

IRSTI 29.19.17

Ionization equilibrium between electrons and holes in bilayers and adiabatic approximations

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We analyze the ionization equilibrium between the charges in nonlinear bilayers formed by triangular planar atomic lattices. We consider a system consisting of two separated by a dielectric medium and independently gated layers 1 and 2 separated by a dielectric medium with ϵ with equal density of electrons in first layer 1 and holes in second layer 2. Assuming that the upper layer is doped with electrons and in the lower layer is doped with holes, we study of the formation, the dynamics and the thermodynamics of bound states. Beside electron – hole pairing we are including bound states with solitonic excitations. We investigate the ionization of electron – hole pairs and discuss the influence of solitons on bound electron-hole pairs; here we use the adiabatic approximation assuming at any time local equilibrium. So far we concentrated here on several thermodynamics and dynamic effects, as the Coulomb attraction between electrons and holes, the formation of electron – hole atoms and degeneration effect. Further we investigated the ionization equilibrium and the coupling to solitonic excitations.

Key words: ionization processes, electrons, holes, solitons, bose condensation.

PACS numbers: 05.60.-k, 05.45.Yv, 63.20.Ry, 71.38.-k, 73.63.-b.

1 Introduction

Ionization problems are a classical topic of plasma physics [1, 2]. In recent time new problems have appeared in connection with plasmas in low-dimensional nanosystems [3, 4, 5], in particular with plasmas in bilayers [3]. The coupling of electrons injected into one layer to holes injected into a second layer has been studied already long ago [6, 7, 8, 9] including the prediction of observing electron – hole pairs, which are rather stable bosons including possible high – temperature electron – hole superfluidity and other interesting effects [3, 6, 8, 10, 11]. We plan to study here related problems from the point of view of plasma physics including some problems related to the coupling of the charge dynamics to the lattice excitations in nonlinear lattices. An example is the interaction of acoustic lattice soliton excitations in 2d – lattices to imbedded electrons, and the effect of electron surfing [12, 13, 14] including transport [13, 14, 15], and control effects [15, 16]. The lattice excitations may have different origin such as thermal excitations or e.g. mechanical or electrical shocks generated by

contacts of the tip of an electron field microscope with a suitable anharmonic crystal lattice layer. For example in simulations a few hundred atoms on a plane forming triangular [13] or hexagonal lattices [16] interacting with one or a few added, excess electrons were studied.

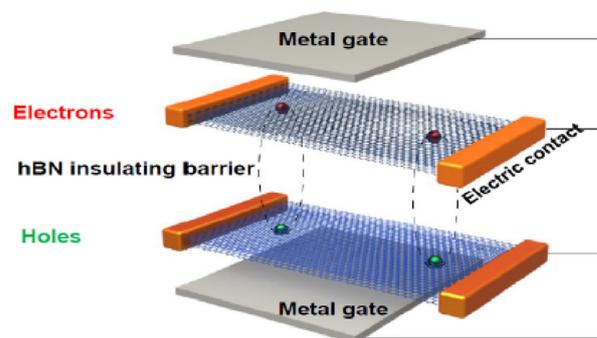


Figure 1 – Schema of a bilayer located between two metal gates and with an insulating layer in between adapted after [3]. The layers have electric contacts and may be doped with electrons in the upper layer and with holes in the lower one. The electrical attracting forces are demonstrated by dashed lines between electrons and holes [3]

Here we want to study similar effects in bilayers, consisting of two lattice layers in small distance. The recent fabrication of two very close, but electrically isolated, conducting bilayer graphene sheets, one doped with electrons and the other with holes with tunable densities, raises exciting new possibilities [17, 18, 19].

We will discuss the following problems:

1) electron and a hole are able to form a stable localized pair already in unperturbed bilayer lattices. The pairs are like a Hydrogen atoms, which are near to classical pairs. Collaps is prevented due to existence of a minimal length given by the distance of the layers.

2) The excitations of solitons in either of the lattices may carry not only individual charges but also pairs.

3) This leads to a variety of possibilities, among them new "vacuum cleaner" effects, a soliton will trap an already localized electron-hole pair and we may control this way the motion of pairs.

Let us consider now the forces and other physical effects in doped bilayers:

We consider a system consisting of two separated by a dielectric medium and independently gated layers 1 and 2 separated by a dielectric medium with ε with equal density of electrons in first layer 1 and holes in second layer 2. Let us first discuss the physical effects to be expected. At large distances, the two layers are uncoupled and the state is expected to be similar to what we observed and described on one – layer systems [13, 14, 15, 16]. In the case that the two layers come closer together, the Coulombic forces between electrons and holes come into play and at small distances e-h pairing can occur due to Coulomb interaction. At lower densities we may neglect the Coulombic forces between the electrons in one layer and the holes in the other one. The forces are repulsive and try to keep the charges far from each other, therefore a close meeting of two equally charged particles is rather seldom.

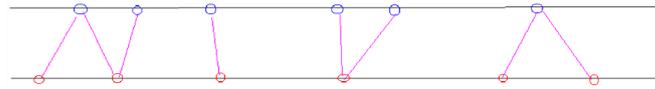


Figure 2 – State of a bilayer: The upper layer is doped with electrons and the lower one with holes. The attracting Coulomb forces between electrons and holes lead to pairing effects. Thermal effects tend to destroy the pairing at mediate and higher temperatures

We assume the following interaction between an electron in upper layer 1 and a hole in lower layer 2. For the electron – hole interaction we assume the true Coulomb potential

$$V_{eh}(x_i^1, y_i^2, x_j^2, y_j^2, d) = -\frac{e^2}{\varepsilon[(x_i^1 - x_j^2)^2 + (y_i^1 - y_j^2)^2 + d^2]^{1/2}}. \quad (1)$$

where $\varepsilon \simeq 3$ is an effective dielectric constant, $d \simeq 1nm$ is the distance between the layers and $x_i^1, y_i^2, x_j^2, y_j^2$ are the respective coordinates in the upper layer 1 doped with electrons and the lower layer doped with holes 2. We mention that this potential has been used in earlier work [20] Note that Efimkin et al. [9] and Conti et al. [11] use different formulae in Fourier representation for the description of the forces, e.g. we find in [11] the "ansatz"

$$V_{eh}(k, k') = -2\pi \frac{e^2 \exp(-d|k-k'|)}{\varepsilon|k-k'|}. \quad (2)$$

At low temperatures and small distances between the layers, bound states will be formed, due to the attracting Coulomb forces between electrons and holes. In particular we expect pairing effects which lead to a kind of excitons which are bosons [6]. Thermal effects will create ionization effects which destroy the pairing at mediate and higher temperatures.

In our simulations we used for modeling the electron dynamics the tight-binding approximation (TBA) (which is entirely different from the tools used by Conti et al. [11]) and for the lattice particles we use her as in earlier work a classical Hamiltonian albeit with the Morse interactions. As a result of this mixed anharmonic classical-quantum TBA dynamics we could show that the charges "like" to follow the trajectories of soliton-like excitations. In the 1d case we have predicted several interesting phenomena, in particular the "vacuum-cleaner" effect, i.e., the electron probability density is gathered by solitons which along their trajectory act as long range correlators.

2 Interactions and solitonic excitations in bilayers

We assume that effects connected with polarization and polaron effects are small. The atoms repel each other exponentially and attract each other with weak dispersion forces. The characteristic length determining equilibrium distance between the particles in the lattice is σ which is used as the length unit. Using the relative distance $r^s = |r_n^s - r_j^s|$ for two atoms in layer with number s we introduce the Morse potential: we set

$$V(r^s) = D\{\exp[-2b(r^s - \sigma)] - 2\exp[-b(r^s - \sigma)]\}. \quad (3)$$

By imposing the cutoff of the potential at 1.5σ , we exclude unphysical cumulative interaction effects arising from the influence of lattice units outside the first neighborhood of each atom [13]. The lattice solitons along crystallographic axes in 2 coupled two-dimensional anharmonic crystal lattices are rather independent.

For the electrons and holes we will use essentially the model described above. Just as an illustration we may show Figs. obtained earlier for one layer systems. In Figure 4 we show an unperturbed triangular lattice.

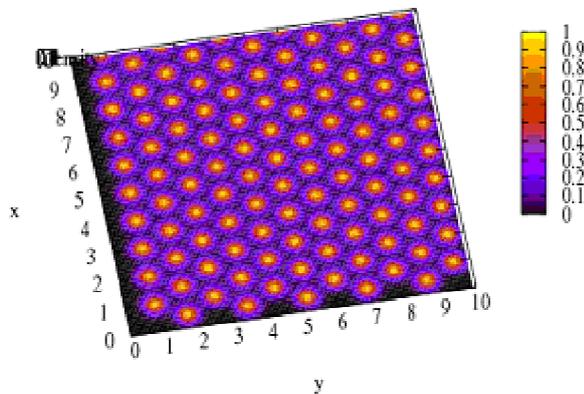


Figure 3 – Triangular Morse lattice. The lattice sites in one layer are represented by small Gaussian clouds

Solitons may be created for example by kicks at the border of the lattice. The soliton which is moving along a crystallographic axis can be excited by a strong pulse of velocity v_0 imposed at $t = 0$. The high-energetic soliton excited this way is quite long lasting in its motion along the chosen crystallographic axis. Transverse excitations and thermal collisions do not play a significant role in the interval of observation.

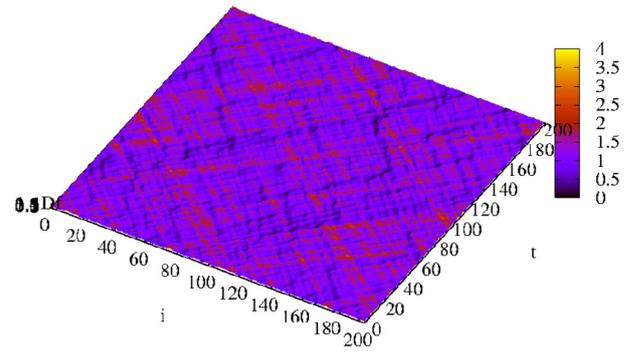


Figure 4 – Solitonlike excitation along a one-dimensional crystallographic axis represented as a stripes showing position over time. We show only the lattice sites in one layer, by small Gaussian clouds

Solitonic excitations may also be created by thermal collisions [13, 14]. Since solitons are local compressions of the lattice these clusters of atoms generate a potential hole in which charges density might be concentrated. Any displacement of the atoms changes the polarization energy. The charge density will try to follow up these changes. This is the basic effect leading to the effect of soliton formation [13, 14]. For the following discussion we have to notice that any soliton created in the lattice by mechanical or thermal effects, acts as an attractor for the charge density.

Solitons and electrons may form solitons, no doubt may be that the same may happen with holes leading to solitonic holes – solholes. So far we do not know much about the masses. Small masses are of large interest for BEC-effects

The soliton as it travels disturbs the lattice. This is connected with the emission of phonons, this process occurs in the phonon band. Only after a finite time which is about 5 time units in our example the lattice returns to the ordered crystalline state. In the intermediate time the lattice is in a non-crystalline state and unable to allow solitons to cross the path. Any second soliton which will cross the trace of an soliton in the delay time will get stuck. We have shown how this effect may be used for control.

The potential for the electron – hole interaction may be represented as

$$V_{eh}(x_i^1, y_i^2, x_j^2, y_j^2, d) = -\frac{e^2}{\epsilon d \sqrt{1 + \frac{\rho^2}{d^2}}}, \quad (4)$$

$$\rho^2 = x^2 + y^2; \quad x = (x_i^1 - x_j^2); \quad y = (y_i^1 - y_j^2) \quad (5)$$

Here is ρ the horizontal distance.

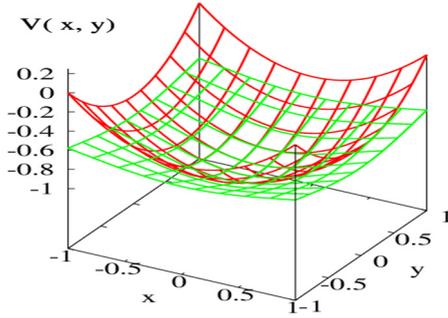


Figure 5 – The potential of the effective horizontal force between electron and hole, including also the parabolic approximation which is valid only for small $\hbar\omega$

3 Modeling charge pairing and bound states

For the quantum – mechanical treatment of electron – hole pairs, a parabolic approximation of the quite difficult interaction potential is useful. For small distances ρ follows in quadratic approximation

$$V_{eh}(\rho, d) = -\frac{e^2}{\varepsilon d \sqrt{1+(\rho^2/d^2)}} \simeq \frac{e^2}{\varepsilon d} \left[-1 + \frac{\rho^2}{2d^2} \right] + \dots$$

The parabolic approximation corresponds to a two-dimensional oscillator with frequency

$$m\omega^2 = \frac{e^2}{\varepsilon d^3} \quad (7)$$

The classical value of the ground state energy of an electron – hole pair, which is a lower bound reads $e^2/\varepsilon d$, and the quantum-mechanical bound states in

this potential are in first approximation the known oscillator states

$$E_{n_x, n_y} = -\frac{e^2}{\varepsilon d} + \hbar\omega \left[\frac{1}{2} + n_x + n_y \right] \quad (8)$$

with the ground state

$$E_{0,0} = -\frac{e^2}{\varepsilon d} + \frac{1}{2} \hbar\omega \quad (9)$$

The condition for the existence of discrete bound states is

$$\hbar\omega < 2 \frac{e^2}{\varepsilon d} \quad (10)$$

or expressed in other parameters

$$\frac{\varepsilon}{d} > 4 \frac{e^2}{\hbar^2}. \quad (11)$$

As we see, the condition for the existence of discrete bound states, which we need, is that the distance between the layers is sufficiently small. In order to give an example we assume $\varepsilon \sim 3$ and $d \sim 1$ nm, then we arrive at Bohr radii of about a few nm and ground state energies with an order of magnitude around 0.1 eV or maybe more generally binding energies in the range $10^{-2} - 10^{-1}$ eV. A rule of thumb known from plasma physics is that interesting ionization phenomena are to be expected at temperatures in the region of $T \sim 0.1 |E_0/k_B|$ and this estimate leads in our case to temperatures around 100 K (or maybe more generally in the range 10 K – 200 K). To be more precise, we need the exact data of the sample. Here we consider only the order of magnitude.

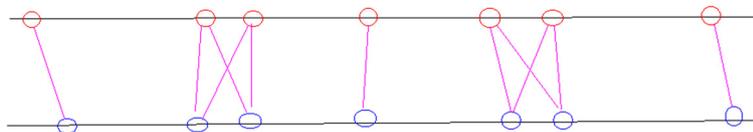


Figure 6 – Model of a bilayer at low temperatures with examples of pairing ("atoms", "molecules").

The electrons in the upper layer and the holes in the lower layer are mostly paired and behave like excitons or H – atoms which are bosons.

Further we showed also two less stable molecules (double pairs) consisting of two electrons and two holes which appear to be similar to H_2 -molecules and are also bosons

The potential of the horizontal forces between electrons and holes is represented in Figure 5 including the parabolic approximation.

What we can say about the possibility to form a kind of molecules e-h-e-h. A classical estimate of the energy of two pairs in a line in distance x is

$$E_0^{(2)}(x) = -2\frac{e^2}{\varepsilon d} + \left[2\frac{e^2}{\varepsilon x} - 2\frac{e^2}{2\varepsilon[x^2+d^2]^{1/2}}\right] \quad (12)$$

As far as we can see, the additional term is for any x – value positive, i.e. the formation of double pairs as shown in Figure 6 is of no energetic advantage. The only possibility to get negative additional contributions is to introduce between the two layers materials with still lower dielectric constant or a vacuum. We will therefore ignore here the formation of molecules, since quantum effects can only

increase the ground state energy. We mention also the early finding of Lozovik and Yudson [6] that excitons in $2d$ repel each other what ensures the stability of an exciton gas against coalescence into biexcitons, droplets etc.. Lozovik and Yudson pointed out that this property, which is characteristic for the $2d$ case, makes transitions to a superfluid state possible. New in comparison to earlier studies is that we include the excitation of the quasiparticles solitons, being nonlinear compressions in the lattice (see Figure 7)

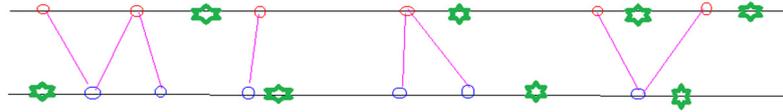


Figure 7 – Bilayer with electrons and holes including the excitation of solitons (here symbolized by green stars). These quasi-particles which are typical excitations in nonlinear lattices attract charges and may form bound states with them, being in upper layer the "solelectrons" and in lower layer the "solholes"

4 Adiabatic Schrödinger equation in the presence of solitons

Let us assume that a soliton is passing an electron – hole pair and takes it with it. We may image that the $e - h$ – pair is surfing on the top of the solitonic excitation. This is a process of high complexity which may however be simplified and reduced in adiabatic approximation to a tractable model. The idea of adiabatic approximation for solelectron systems has been developed in [12]. Let us assume that the soliton generates just a moving potential in which the electron and the hole are moving. Following the model developed earlier [15]. This model is based on a continuous description which consists of two equations, one for the effective Schrödinger equation for the wave function ϕ of the charges and the other one for the deformation density of the lattice. The effective Schrödinger equation for the charges $\rho(x, t)$ reads in the one – dimensional case [15]

$$i\hbar\phi_t(x, t) + \frac{\hbar^2}{2m}[\phi_{xx}] + g\rho(x, t)\phi(x, t) = 0, \quad (13)$$

The nonlinearities in the electron-lattice coupling appear in quite symmetrical way in the coupling constant

$$g = \chi + \alpha V_0$$

The term $(-g\rho)$ plays the role of an external potential in the Schrödinger equation. The compression density ρ is to be found from the Boussinesq equation [15]

$$\rho_{tt} - k_0\rho_{xx} + \gamma_0(\rho^2)_{xx} - \frac{1}{12}\rho_{xxxx} + g(\phi)_{xx} = 0 \quad (14)$$

In our case we have two dimensions x, y and two charges interacting by by a potential V . Further the Boussinesq equation is to be replaced by the Kadomzev – Petviashvili equation or generalizations as given in [21]. A generalization is the following modified Boussinesq equation for solelectrons which differs from the original one only by shifted coefficients

$$\frac{\partial^2 \rho(x, y, t)}{\partial t^2} - v_0^2 \frac{\partial^2}{\partial x^2} - \frac{a^2}{12} \frac{\partial^4}{\partial x^4} \rho(x, y, t) \quad (15)$$

$$= \frac{v_0}{2} \frac{\partial^2}{\partial y^2} \rho(x, y, t) - (v_0^2 \gamma_0 \frac{\partial^2}{\partial x^2} \rho^2(x, y, t) - g \frac{\partial^2}{\partial x^2} \int dx' dy' \rho^2(x', y', t)) \quad (16)$$

We generalize also the Schrodinger equation for this case and assume

$$i\hbar\phi_t(x^1, x^2, y^1, y^2) + \frac{\hbar^2}{2m}\Delta\phi(x^1, x^2, y^1, y^2) - [V_{eh}(x, y) - g\rho(x, y)]\phi(x^1, x^2, y^1, y^2) = 0, \quad (17)$$

The adiabatic approximation is based on the following assumptions:

(i) The center of the exciton (e – h – pair) and the center of the soliton are located at the same place.

(ii) the exciton follows the moving soliton without delay.

similar as known from standard quantum mechanics we may go now to traveling center of mass coordinated and relative coordinates x, y and get finally the Schrodinger equation

$$i\hbar\phi_t(x, y, t) + \frac{\hbar^2}{2m}[\phi_{xx} + \phi_{yy}] + [g\rho(x, y, t) - V(x, y)]\phi(x, y, t) = 0, \quad (18)$$

The wave function amplitude $\phi(x, y, t)$ may be considered as the limit of the amplitude of the coefficients $c_n(t)$ in the discrete description [15]. Note that the validity of the continuous approximation is restricted to small nonlinearities (small α, χ, γ_0). In spite of these known limitations we will use here the continuous theory for analytical estimates, as far as other analytical estimates are not available. Solutions of special interest to us are the so – called lump solitons, they are like moving hills. A special solution for the envelope of a lump-type soliton reads [21]:

$$\rho(x, y, t) = \rho_0 \frac{[v_s y^2 + 3/v_s - (x - v_s t)^2]}{[v_s y^2 + 3/v_s + (x - v_s t)^2]^2} \quad (19)$$

Note that this special solution depends only on one parameter, the soliton velocity v_s . The compression density $\rho(x, v, t)$ is always positive around the center of the moving lump but has also negative parts at larger distance from the maximum. This is related to the property that the integral is zero

$$\int dx dy \rho(x, y, t) = 0; \rho_0 = \frac{v_s}{3}. \quad (20)$$

In figure 7 we represented the envelope of a lump soliton at two subsequent time instants. Such lump solutions we have found also numerically for Morse lattices [15, 21]

In parabolic approximation the density of a lump soliton may be represented as:

$$\rho(x, y, t) = \rho_0 - \frac{1}{2}r_x x^2 - \frac{1}{2}r_y y^2 \quad (21)$$

This way we get for the total effective potential acting on a n electron – hole pair moving in the field of a soliton:

$$V_{eh}^{eff} = V_{eh}(x, y) - g\rho(x, y)\phi(x^1, x^2, y^1, y^2) \simeq \simeq V_{eh}(x, y) + \frac{1}{2}gr_x x^2 + \frac{1}{2}gr_y y^2 \quad (22)$$

for $t = 1, 5, 9$; $v_s = 1.5$;

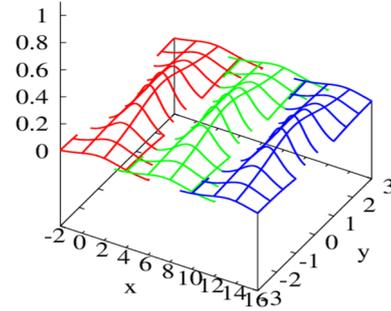


Figure 8 – Solution of the KP equation showing a traveling lump soliton at three successive time instants

5 Ionization equilibrium in bilayer plasmas and BEC condition

In our bilayer system, due to the existing attractive and repulsive forces, we may find different species and quasi-species as e.g.: electron, holes, solitons, solectrons, solholes, excitons, biexcitons, quasimolecules, etc.

At low densities the concentrations between different species are in chemical equilibrium. In the thermodynamic equilibrium we may describe the relations between the "elementary" particles / quasiparticles, the electrons, holes and solitons by mass action laws. Let us first describe the most important chemical equilibrium between electrons and holes. We will give a short derivation of the so-called Saha equation formalism for a binary Coulomb system with n_h positive charges (holes) and n_e negative charges (electrons) per cubic centimeter. The density of free e-h-atoms is denoted by n_0 . The total density of charges is $n = n_e + n_h$. In the following we will use the plasma notations, i.e. we call the negative charges "electrons" and the positive charges simply "holes". We assume in the spirit of the ideas of Planck and Nernst a chemical

equilibrium between electrons, holes and atoms [2, 23].

$$e^- + h^+ \rightarrow a_0; \quad \mu_e + \mu_h = \mu_0 \quad (23)$$

Here the $\mu_k = \partial F / \partial N_k$ (F – free energy) are the chemical potentials for the corresponding species, for the e-h-atoms we assume for non-degenerated "atoms" in ground state which is most probably assumed:

$$\mu_0 = k_B T \ln n_0 + k_B T \ln \lambda_0^3 - E_{0,0} \quad (24)$$

and for the charges including an ideal Boltzmann contribution and an excess part stemming from degeneration effects and the charge-charge interactions:

$$\begin{aligned} \mu_e &= \mu_e^{id} + \mu_e^{ex} + k_B T \ln n_e; \\ \mu_h &= \mu_h^{id} + \mu_h^{ex} + k_B T \ln n_h. \end{aligned} \quad (25)$$

The ideal Boltzmann terms contain the chemical constants which were first expressed by Planck's constant in the pioneering work of Sackur and Tetrode:

$$\begin{aligned} \mu_e^{id} &= +k_B T \ln \Lambda_e^3; \quad \mu_h^{id} = +k_B T \ln \Lambda_h^3; \\ \Lambda_k &= h / \sqrt{2\pi m_k k_B T}. \end{aligned} \quad (26)$$

From the condition of chemical equilibrium for the chemical potentials follows neglecting nonideality and nondegeneracy the so-called Saha formula:

$$\frac{n_a}{n_e n_h} = K(T) = \Lambda^3 \exp \left[\frac{-E_{0,0}}{k_B T} \right]; \quad \Lambda = \frac{\Lambda_e \Lambda_h}{\Lambda_a}. \quad (27)$$

The length Λ_e, Λ_h is the de Broglie- wave length of electrons/holes having thermal momentum, n_e, n_h are the densities of free electrons and free holes. Free electrons are formed in chemical equilibrium with bound electrons and Planck's theory is applicable. The theory depends crucially on the ground state energy $E_{0,0}$. In the general case, the excited states have to be taken into account through the Planck-Brillouin-Larkin partition function and degeneracy and charge interaction through standard approximations [2, 23]. Assuming as previously $d \sim 1$ nm and $\varepsilon \sim 2 - 10$, we arrive at bound state energies with an order of magnitude around 0.1 eV and find that the densities of the valley are located at

$n \simeq 10^{12} \text{ cm}^{-3}$ corresponding to weak doping and $n \simeq 10^{18} \text{ cm}^{-3}$ corresponding to strong doping. We show the estimates for different temperatures in the region between $0.3 \cdot 200$ K and $0.8 \cdot 200$ K. In the region of low densities we observe temperature ionization and in the region of high densities we observe density ionization which is mainly due to the lack of space for exciton formation. Taking into account that an exciton, which is in principle like an hydrogen atom needs a space of at least a_B^* to form bound state wave functions. Remember that the Bohr radius in a dielectric medium (m^* – effective relative mass of e-h pairs)

$$a_B^* = \varepsilon \frac{\hbar^2}{m^* e^2} \quad (28)$$

(m^* – effective relative mass of e-h pairs). This may lead to typical Bohr radii around $10^{-6} - 10^{-7}$ cm and therefore to maximal densities for the existence of excitons around $10^{18} - 10^{20} \text{ cm}^{-3}$. It follows, that certain limit densities, which are typically around a doping of $10^{18} - 10^{20} \text{ cm}^{-3}$ electrons and holes in the layers cannot be exceeded.

The interesting result is, that bosonic effects connected with excitons are to be expected only in a valley of intermediate densities and the bosonic region is rather narrow at higher temperatures.

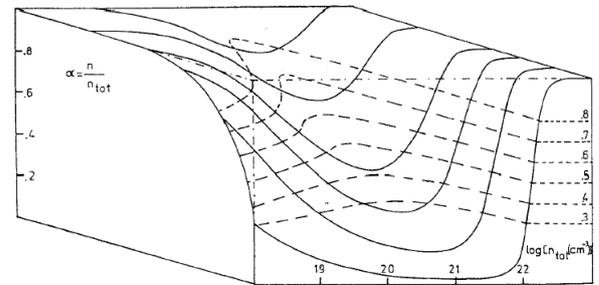


Figure 9 – Ionization equilibrium in bilayers in the region around 160 K (curve above) and 60 K (curve below) showing the region of electron-hole pairing. The electrons in the upper layer and the holes in the lower layer are within the valley mostly paired and behave like excitons. The valley of densities where the excitons are formed is shown which is located usually between $n \simeq 10^{12} \text{ cm}^{-3}$ and $n \simeq 10^{18} \text{ cm}^{-3}$ is shown in our example for a temperature region between 60 K and 160 K.

In principle we may expect also the formation of pairing of sollectrons and solholes leading to molecule – like structures (biexcitons), however this is energetically not of any advantage [6]. For the region of lower temperatures where the particles may

be degenerated, the situation is more complicated and may be in some respect similar to electron – hole systems in semiconductors [6, 8, 22, 23] and in plasmas [2]

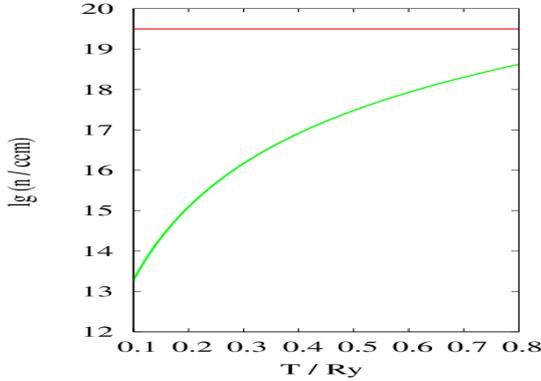


Figure 10 – The region of electron – hole pairs in the density – temperature plane. Formation of pairs (excitons) is expected inside the area formed by the green line, denoting temperatures where temperature ionization begins and the red line giving the high densities where the excitons are destroyed due to lack of space for forming bound state wave functions. The temperature is measured in units of the e-h- ground state energy $T \sim k_B T / E_{0,0}$.

Including Coulomb interactions and all degeneracy effects, the generalization of the Saha equation reads [2]

$$\frac{n_a}{n_e n_h} = \Lambda^3 \sigma_0(T) \exp[-\beta [\mu_e^{ex} + \mu_h^{ex} - \mu_0^{ex}]]. \quad (29)$$

where $\sigma_0(T)$ denotes the excitonic partition function to be calculated using the exciton bound state energies

$$\sigma_0 = \sum_{n_x, n_y} \exp[\beta E_{n_x, n_y}]. \quad (30)$$

The excess chemical potentials describe the Coulomb interaction and degeneracy effects. The most important open question is in this connection, whether the densities of excitons provided by the chemical equilibrium are high enough to allow degeneration and BEC effects. The problem has been studied among others by Mahler and Kilimann for the exciton formation in semiconductors (see e.g. [22, 23]). As well known, in the region of BEC holds for the Bose gas

$$\mu_0^{gas} = 0 \quad (31)$$

In combination with the condition of ionization equilibrium

$$\mu_e + \mu_h = \mu_0 \text{ and } \mu_0 \simeq \mu_0^{gas} + E_{0,0} \quad (32)$$

We find as a first estimate for the existence of BEC effects similar as for semiconductors [22, 23] the condition

$$\mu_e + \mu_h \simeq E_{0,0} = 0 \quad (33)$$

6 Adiabatic approximations for solitonic excitations

So far we studied mostly systems in thermodynamic equilibrium assuming a continuous background. In some earlier works we studied the interaction of acoustic lattice soliton excitations in 2d – lattices to imbedded electrons, and found a form of electron *surfing* [12, 13, 14] including transport effects [15]. In particular we discussed applications to control effects [16]. Briefly speaking, the charges may be transported by lattice excitations. Since the dynamics of electrons and holes is much faster than the lattice dynamics, adiabatic approximations may be quite useful assuming that the charges follow instantaneously the mesoscopic changes in the lattice, as soliton excitations, breathers etc.

The adiabatic approximations which we developed in our work since 2009 [12] is a very simple tool to estimate the effects of thermal motion including the compression effects on polaron- and soliton – formation. The idea is quite simple. In the first approximation which is correct for fast electron dynamics in comparison to lattice dynamics, the local charge occupation of a lattice point n is given by a Boltzmann, Fermi- or Bose distribution based on the adiabatic quantum states. At small densities we may use the Boltzmann distribution

$$p_n = \text{const} \exp[-\beta \epsilon_n] \quad (34)$$

Here the ϵ_n are the local eigenvalues of the Hamilton matrix, which in adiabatic approximations are assumed to be a function of all coordinates of sites in the lattice. Following Gershgorin's theorem, as shown in [12] what matters are only the elements in some circle (the Gershgorin circle). In our case we need the positions inside some physical distance, say 1.5σ from given lattice point n . In a reasonable approximation the local eigenvalue is given by the mean

compression near to the lattice site n . Still easier is the description in the continuous approximation described above, at least restricting the studies to the parabolic approximation. In the continuous approximation the distribution in space is given by the adiabatic wave functions

$$n_0(x, z, t) = \text{const} \sum_n \exp[-\beta \varepsilon_n] |\psi_n(x, y)|^2 \quad (35)$$

However the levels and the wave functions are fully known only in the parabolic approximation, which however gives at least a qualitative picture. What we need at the end are only the local compressions which have to be calculated appropriately. An preliminary example calculated earlier for a one layer system is shown in figure 11. More precise calculations of the running compressions and the corresponding charge densities in two – layer systems are still to be done.

We studied here bilayers, consisting of two lattice layers in small distance. The coupling of electrons injected into one layer to holes injected into a second layer leads to the formation of electron-hole pairs which are bosons. Since the dynamics of electrons and holes is much faster than the lattice dynamics, we used adiabatic approximations. The idea is to assume that the charges follow instantaneously the mesoscopic changes in the lattice, as soliton excitations, breathers etc. The tool of adiabatic approximations has been developed in several of our works [12]. It is the appropriate and sufficiently simple tool to estimate the effects of thermal motion including the compression effects on polaron- and solectron – formation. This first approximation is correct if the electron dynamics is fast in comparison to lattice dynamics. Then the local charge occupation of a lattice point is given approximately by a Boltzmann, Fermi- or Bose distribution based on the adiabatic quantum states.

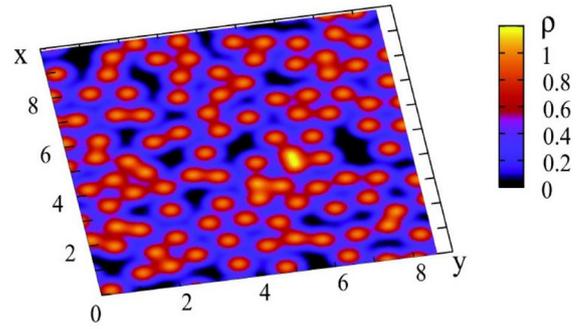


Figure 11 – Adiabatic approximation for the charge distribution in a heated system at $T = 0.2D$ taken from a preliminary calculation given in [12], with several locally percolating regions of high charge density.

7 Conclusions

So far we concentrated here on several thermodynamics and dynamic effects, as the Coulomb attraction between electrons and holes, the formation of electron – hole atoms and degeneration effect. Further we investigated the ionization equilibrium and the coupling to solitonic excitations.

Still to be studied are details on the control of the dynamics of pairs extending [16], transport phenomena extending [15], formation of bosonic electron – hole atoms at higher densities and, possible BE-condensation of e-h-atoms at very low temperatures/high densities [11, 3].

Acknowledgement

The authors profited from contributions to SCCS-2017 in Kiel [3] and from further advice provided by M. Bonitz (Kiel), G. Röpke (Rostock) and V. Filinov (Moscow).

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