Ground state and structural transitions in mesoscopic electron hole bilayers

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Few-particle clusters of spatially separated electrons and holes in vertically coupled two-dimensional quantum dots are analyzed. As a function of interdot distance d, the inlayer interaction between electrons (and holes) changes from Coulomb repulsion at large d to dipole repulsion of e-h pairs at small d. The change of the structural properties (cluster shell configuration and symmetry) and energy with variation of d is investigated.

1 Introduction

Mesoscopic systems of a small number N of charged particles continue to attract increased interest due to their unusual properties. In particular, they exhibit unique strong coupling phenomena which are of interest for dense plasmas, ions in traps, dusty plasmas and semiconductor quantum dots. Of particular interest is the formation of a mesoscopic Wigner crystal, e.g. [1] with nontrivial melting properties and potential applications to single-electron control devices [2]. An even larger variety of phenomena is observed in *coupled* quantum dots such as mesoscopic electron-electron bilayers, e.g. [3, 4], and coupled dots with spatially separated electrons and holes. The latter system is of particular interest since here the interaction between the particles can be controlled (changing from Coulomb to dipole) by variation of the interlayer separation d and crystallization may interfere with exciton formation [5, 6] and Bose condensation.

In the present paper, we extend our previous investigations of few-particle e-h-bilayers [5, 6] to an analysis of the ground state configurations. We demonstrate that, when the interlayer separation is varied, there may occur one or several (depending on N) structural transitions where the configuration symmetry or the shell structure changes. Similarities with and differences to single-layer systems are explored.

2 Electron-hole bilayers. Model and results

Let us consider a system of two vertically coupled two-dimensional layers (quantum dots, QD) containing electrons and holes, interacting through the Coulomb potential. In the classical case, the ground state of this system is described by the Hamiltonian $H = H_e + H_h + H_{e-h}$, where $H_{e(h)}$ is the Hamiltonian of a single-layer Coulomb cluster whereas H_{e-h} contains the attractive inter-layer particle interactions. In the following we focus on symmetric electron-hole bilayers (SEHB) where electron and hole numbers are equal, $N_e = N_h = N$, electrons and holes have the same mass, $m_e = m_h = m$, and the confinement potentials $H^{\rm conf}_{e(h)}$ of both QDs are identical,

$$H_{e(h)} = H^{\rm corr}_{e(h)} + H^{\rm conf}_{e(h)} = \frac{q^2}{\varepsilon_b}\sum_{i>j}^{N}\frac{1}{r_{ij}} + \frac{1}{2}m\omega_0^2\sum_{i}^{N} r_i^2, \quad H_{e-h} = -\frac{q^2}{\varepsilon_b}\sum_{i}^{N_e}\sum_{j}^{N_h}\frac{1}{\sqrt{r_{ij}^2+d^2}}. \quad (1)$$

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Further, d is the distance between the planar layers, r_{ij} is the in-layer projection of the distance between two particles, q is the particle charge, ε_b the background dielectric constant and ω_0 the harmonic trap frequency. After introducing the length and energy scales, $r_0 = (2q^2/m\varepsilon_b\omega_0^2)^{1/3}$, $E_0 = q^2/\varepsilon_b r_0$, the transformations $\{r \to r/r_0, E \to E/E_0, d \to d/r_0\}$ allow us to rewrite the Hamiltonian in dimensionless form:

$$H = \sum_{i>j}^{N_e} \frac{1}{r_{ij}} + \sum_{i}^{N_e} r^2 + \sum_{i>j}^{N_h} \frac{1}{r_{ij}} + \sum_{i}^{N_h} r^2 + \sum_{i}^{N_e}\sum_{j}^{N_h} \frac{1}{\sqrt{r_{ij}^2 + d^2}}. \quad (2)$$

In the following all energies will be given per electron-hole pair excluding the dimensionless vertical electron-hole coupling energy $1/d$ (exciton binding energy) as it has no influence on the in-layer particle arrangement (this is not true in the quantum case) but only assures exact vertical alignment of e-h pairs.

Computation of the classical ground state configurations. For the numerical analysis we used molecular dynamics simulations (MD) with an adaptive stepsize controlled Runge-Kutta 4th order integrator. For any fixed particle number N and interlayer distance d, the simulations started from a random initial configuration with subsequent cooling to zero temperature.

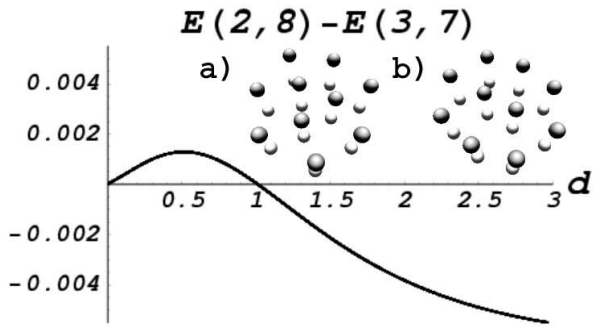

Fig. 1 Energy difference between the two energetically lowest shell configurations for $N = 10$ e-h pairs. At small d, the ground state has the shell configuration $(3,7)$ which changes around $d/r_0 = 1$ to the configuration $(2,8)$. The inset shows the ground state configurations at $d = 1.00$ (a) and $d = 1.02$ (b).

For small (mesoscopic) clusters which are the subject of this paper the method rapidly converges. In the case of several energetically close states, each of the configurations was analyzed separately over the whole range of $d-$values. The results were verified by independent Monte Carlo simulations. For the limiting cases of $d \to \infty$ and $d \to 0$, we found exact agreement with the known single-layer energy results for Coulomb [9] and dipole clusters [10], respectively[1].

The interesting property of the present system is that, by varying the interlayer distance d, the *in-layer* interaction changes from *Coulomb* repulsion, for $d/a \gg 1$, to *dipole* repulsion, for $d/a \ll 1$, where a is the mean inter-particle distance in each layer. In the intermediate range around $d = a$, in-layer and intralayer correlations are of the same order and the system exhibits *three-dimensional behavior*. From an analysis of the ground state configurations for many different particle numbers, in the whole range of d, we found that for certain e-h pair numbers N the ground state configuration changes with d, i.e. we observe structural transitions. We found the following three different scenarios:
I) the ground state configuration does not depend on d, II) the two limits of independent layers ($d/a \gg 1$) and strongly coupled layers ($d/a \ll 1$) have different configurations, characterized by different particle numbers on the shells, III) in both limits, the same configuration exists, but in a transition region between both limits, another groundstate configuration is observed.

Figs. 1 and 2 illustrate the cases II) and III) on the examples $N = 10$ and $N = 12$, respectively. For $N = 10$, only one transition takes place, close to $d = 1$ (see table). At this point, the $(2,8)$ ground state known from a single-layer Coulomb cluster changes to the $(3,7)$ configuration found in a single-layer cluster with dipole-dipole interaction [10]. In the limit of $d \to 0$, the energies of both configurations vanish, but the ratio of the two energies remains larger than one, $E(2,8)/E(3,7) \to 1.004$, i.e. the configuration (3,7) remains stable. However, the behavior for $N = 12$, is different, see Fig. 2. Here, we observe case III), i.e. at small d, the large-distance configuration $(3,9)$ reappears, while at intermediate d-values the $(4,8)$ configuration is more stable.

The physical explanation for the observed behavior is the following: the large d configuration is obviously that of a single layer Coulomb cluster. On the other hand, with reduction of d, the correlation energy becomes purely dipole-like and vanishes with d as $E_{\rm corr}(d) \sim d^{4/5}$ [6]. Thus the total potential energy is dominated by the confinement energy and the ground state configuration by minimization of $E_{\rm conf}$. At finite d the confinement favors large particle numbers in the central region (inner shell), as seen in both figures. Furthermore, the asymptotic

[1] Some care has to be taken in the comparison of the zero $d-$limit: this limit of the bilayer system yields N dipoles with twice the mass of that of the single layer system. In the dipole limit, the ground state total energy depends on d and m as $E \sim d^{4/5}m^{3/5}$. This means that the ratio of the bilayer energy to the single layer energy is proportional to $2^{3/5}$.

configuration for $d \to 0$ shows a tendency towards close packed (hard sphere like) hexagonal configurations, cf. inset a) of Fig.2. These asymptotic configurations are the same as in a single layer containing N dipoles (see Sec. 3), and may ($N = 12$) or may not coincide ($N = 10$) with the configuration of an N-particle Coulomb system.

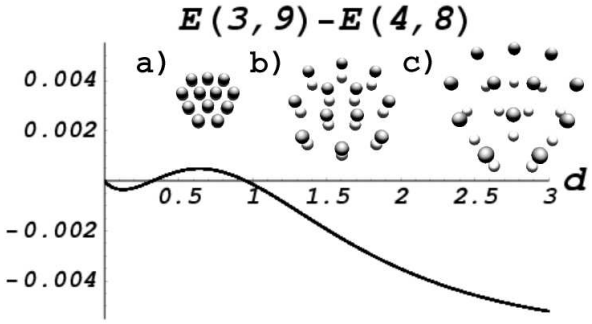

Fig. 2 Energy difference between the two lowest energy configurations for $N = 12$ e-h pairs. At small and large d, the ground state is given by the configuration (3,9), whereas at intermediate d the configuration (4,8) is energetically more advantageous. Also shown (insets) are the ground state configurations at a) d=0.12, b) d=0.65, c) d=1.50.

While the two asymptotic configurations are fixed by the respective single-layer Coulomb and dipole ground states, the configurations at intermediate d are a peculiar property of the two-layer system, cf. the case of $N = 12$, Fig. 2. Here, the configuration $(4, 8)$ arises from a competition of in-layer and inter-layer correlations and shows the strongest deviations from the hexagonal two-dimensional ground state: the two layers behave like a piece of a 3D system with a mixture of 4-fold and 5-fold coordination, see inset b) of Fig. 2. Similar behavior is observed also for other particle numbers which possess two energetically close shell configurations [12]. The critical data of the transitions are summarized in the table. We mention that in all cases we observed a continuous change of the ground state energy with d, but jumps of dE/dd resembling first-order structural transitions.

Ground state of mesoscopic quantum clusters. Now the question arises if these ground states and structural transitions are a property of the classical limit. To answer this question, we considered mesoscopic *quantum* e-h-clusters.

Then the ground state Hamiltonian (1) contains in addition the quantum kinetic energy term: $H_{e(h)} \to H_{e(h)} - \hbar^2/2m \sum_{i=1}^{N} \nabla_i^2$, which leads to quantum fluctuations and finite spatial extension of the electron (hole) wave functions. This gives rise to a nonzero overlap of individual electrons (holes) in each layer which, in principle, might affect the ground state configurations. To investigate this question, we performed path integral Monte Carlo simulations, for details see [1]. Our first preliminary results are shown in Fig. 3 for $N = 10$. We observe the same configurations at large and small d as in the classical case, and also a transition $(2, 8) \to (3, 7)$ around $d = a$ (in this figure, the vertical axis is scaled with $r_s \equiv a/a_B$). The precise value for d_{cr} depends on the density and will be given in Ref. [12].

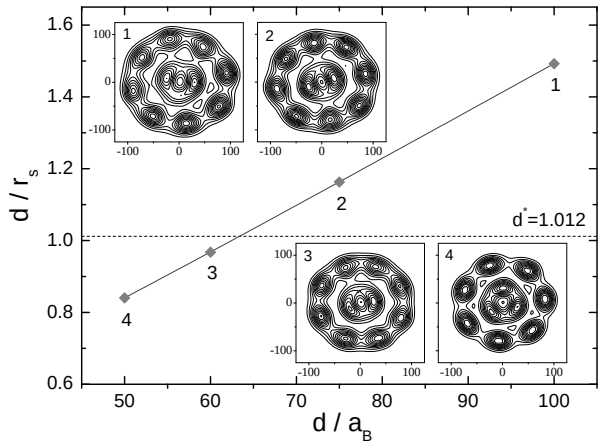

Fig. 3 Ground state configuration of the quantum e-h cluster with $N = 10$ for 4 different layer separations. The horizontal line indicates the critical distance for the structural transition $(2, 8) \to (3.9)$.

N	d_{cr}	shell configuration change	E
10	1.012	$(2, 8) \to (3, 7)$	3.9167
12	0.953	$(3, 9) \to (4, 8)$	4.3463
	0.325	$(4, 8) \to (3, 9)$	2.1293

Table 1 Critical distances d_{cr} where the structural transitions occur and total energy at the transition point. The arrows indicate the configuration change when d is reduced to d_{cr}.

3 Comparison to single a layer with varying interaction potential

As we have seen above, in the two limiting cases of large and small d, the bilayer system behaves like a single layer with Coulomb or dipole repulsion, respectively. It is, therefore, interesting to ask if the same behavior would occur in a single layer in which the interaction law is changed accordingly. A similar analysis has been performed for dusty plasmas where the interaction potential is a Debye/Yukawa potential [9, 11]. By changing the screening length, this system also becomes dipole or Coulomb like, respectively. Here we study a different type of interaction – a power law, $1/r^\alpha$, – and analyze the ground state as function of the exponent. This, naturally, includes the Coulomb and dipole cases, $\alpha = 1$ and $\alpha = 3$, respectively but also other exponents which occur in other systems, including colloidal plasmas or selforganized atom layers on surfaces ($\alpha = 2$) or quadrupoles ($\alpha = 5$), for details, see [12]. We, therefore, will extend the analysis to both small and large α. Then, the dimensionless ground state Hamiltonian is $H = \sum_{i>j}^{N} r_{ij}^{-\alpha} + \sum_i^N r^2$.

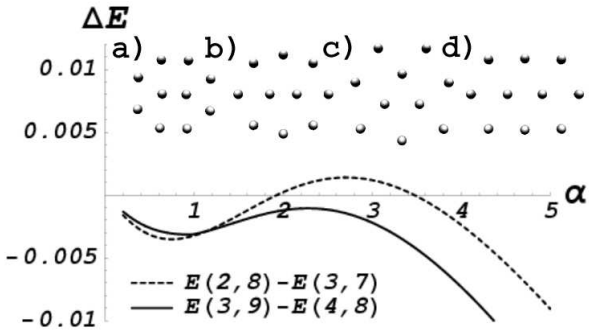

Fig. 4 Energy difference between the two lowest states for $N = 10$ and $N = 12$ electrons in a single layer as a function of the interaction exponent. Insets show the ground state configurations for $N = 10$ and $\alpha = 0.65$ (a), $\alpha = 1.0$ (b), $\alpha = 3.0$ (c) and $\alpha = 7.0$ (d).

In Fig. 4 we present the energy difference of the lowest configurations for the same two particle numbers as in Figs. 1 and 2 above. In the two cases, the same trend is found: the curves start, at small α, at zero energy difference, favoring the configuration with fewer particles on the inner shell due to the dominance of the repulsive correlation energy (as in the Coulomb case, $\alpha = 1$). In the limit of large α where the interaction is becoming weak and extremely short range, the confinement energy dominates the symmetry, favoring a close-packed hexagonal lattice. Thus the ground state is again the configuration with fewer particles in the central region and a parallel alignment of layers, see inset d) of Fig. 4. Comparing this picture with Fig. 1, we see that in the two-layer case of $N = 10$, the dipole interaction is slightly too long-range to reestablish the close-packed configuration $(2, 8)$ (the critical exponent is $\alpha \approx 3.4$).

Let us now consider the range of intermediate α. When α is increased beyond 1, the relative stability of the configuration with more particles on the inner shell increases, due to a weakening of the contribution of the correlation energy to the total energy, relative to the confinement energy, as discussed above. Whereas for $N = 10$ a transition to the shell configuration $(3, 7)$ is observed, for $N = 12$, the energy difference does not change sign. Interestingly, for $N = 10$, as a precursor of the transition a symmetry change of the $(2, 8)$ configuration is observed for $\alpha = 0.94$, cf. insets a) and b) in Fig. 4. (Similar symmetry changes occur for other particle numbers, e.g. in the metastable state $(4, 8)$ for $N = 12$).

Comparing these results to the bilayer case we conclude that the configurations in the Coulomb and dipole cases are the same. Different ground state configurations are, however, observed in the range of intermediate d and α, respectively. For example, for $N = 12$, the single layer system does not show a structural transition in contrast to the bilayer system, cf. Figs. 2 and 4. This indicates that the interaction in the bilayer system at intermediate d is qualitatively different as a result of strong interlayer correlations.

In summary, we analyzed the ground state configurations of classical mesoscopic symmetric electron hole bilayer crystals and presented data for the structural transitions. Quantum Monte Carlo simulations confirmed the same qualitative behavior in quantum e-h bilayers.

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References

[1] A. Filinov, M. Bonitz and Yu.E. Lozovik, Phys. Rev. Lett. **86**, 3851 (2001); phys. stat. sol. (b) **221**, 231 (2000)
[2] M. Bonitz, V. Golubnychij, A.V. Filinov, Yu.E. Lozovik, Microelectronic Engineering **63**, 141 (2002)
[3] A.V. Filinov, M. Bonitz, and Yu.E. Lozovik, Contrib. Plasma Phys. **41**, 357 (2001)
[4] B. Partoens, V.A. Schweigert, and F.M. Peeters, Phys. Rev. Lett. **79**, 3990 (1997)
[5] A. Filinov, M. Bonitz, and Yu.E. Lozovik, J. Phys. A: Math. Gen. **36**, 5899 (2003)
[6] A.V. Filinov, P. Ludwig, V. Golubnychyi, M. Bonitz, and Yu.E. Lozovik, phys. stat. sol. (c) **238**, No. 3 (2003)
[7] E. Anisimovas and F.M. Peeters, Phys. Rev. B **66**, 075311 (2002)
[8] G. Goldoni and F.M. Peeters, Phys. Rev. B **53**, 4591 (1996); I.V. Schweigert, V.A. Schweigert, and F.M. Peeters, Phys. Rev. Lett. **82**, 5293 (1999)
[9] M. Kong, B. Partoens, and F.M. Peeters, Phys. Rev. E **65**, 046602; New J. Phys. **5**, 23.1 (2003)
[10] A.I. Belousov and Yu.E. Lozovik, arXiv:cond-mat/9806108
[11] G.E. Astrakharchik, A.I. Belousov and Yu.E. Lozovik, arXiv:cond-mat/9905193
[12] P. Ludwig, A. Filinov, M. Bonitz, Yu.E.Lozovik, to be published