A THEORY OF CORRELATION EFFECTS IN TWO-ELECTRON QUASI-ONE-DIMENSIONAL NANOCLUSTERS WITH PARABOLIC BOUNDARIES

S.YA. GOROSHCHENKO

M.M. Bogolyubov Institute for Theoretical Physics, Nat. Acad. Sci. of Ukraine
(14b, Metrolohichna Str., Kyiv 03143, Ukraine)

UDC 538.915

We study the energy spectra and electron density distributions in model quasi-one-dimensional nanocluster systems with two electrons interacting via the Coulomb law (long-range interaction) or in a contact manner (short-range interaction) covering various regimes of the electronic correlation (by dealing with clusters of different lengths). It is shown that, in a strong correlation regime, the general structure of energy spectra turns out to be invariant relative to the nature of interaction. In this case, the system with the Coulomb interaction becomes a quasi-classical one in which the electron density is localized at the edge points of a cluster, whereas the system with a contact interaction remains in a quantum state where the density spreads over the whole cluster. The verification of a strongly correlated energy structure by using the methods of dipole and quadrupole spectroscopies is assumed.

1. Introduction

The progress in nanotechnology, which manifested itself in the creation of elliptic quantum dots [1] and quantum rings [2], starts the systematic investigations of quasi-one-dimensional (Q1D) cluster systems in semiconducting heterostructures [3—6]. On the preceding stage of the studies of nanostructures, the main attention has been paid to two-dimensional (2D) quantum dots with the axial symmetry [7—10] and to quantum wires which are one-dimensional (1D) or Q1D infinite systems [11—13] (we mention the problem of Wigner crystallization in such systems [7, 12, 14]). The Q1D cluster systems combine individual features of the mentioned structures and are considered as Q1D quantum wells or quantum wires of a finite length [3] (including the closed ones [5]) with a finite electron occupation close to the occupation in the quantum dots.

The practical possibility to change a geometry and sizes of nanoclusters gives an opportunity to vary the regime of electron correlation in such systems, which must be reflected in the corresponding changes of their electronic structure. The correlation regime is supposed to be weak (strong) if the interaction factor insignificantly (decisively) affects the electron structure of a system against the background of the action of the other factors. The first calculations of the electronic structure of model Q1D clusters with occupations from 2 to 4 electrons ($N_e = 2 \div 4$) were carried out even before the experimental creation of such systems [15, 16]. In [15], the diversity of electronic structures for planar geometrically similar Q1D clusters of various lengths ($L_y = 10L_x$, $L_y = 10^k$ nm, $k = 0 \div 3$) with $N_e = 2$, 2D Coulomb interaction, and absolutely rigid boundaries, is obtained. Only the lowest state of a transversal quantization is taken into the account. It was shown that, in a nanorange of lengths, there exists a possibility to realize all the regimes of electron correlation: from a weak one (short clusters, L_y is of about several nm), when the electronic structure almost cannot be distinguished from that in the systems without interaction, to a strong regime (long clusters, $L_y \gtrsim 100$ nm) with the absolutely different electronic structure which already has features of the Wigner structure for infinite systems (level degeneration, density localization). However, at the large length, the other states of a transversal quantization, beside the ground state, also must affect the electronic structure of the geometrically similar Q1D clusters. In [16], a 1D description of Q1D nanoclusters (also the geometrically similar ones) with $N_e = 2 \div 4$,

in which the cluster transversal size is taken into the account by adding a core to the 1D Coulomb interaction, is used. The smallness of the core value ($\sim 10^{-4}$ as much of the cluster length) makes, however, the interaction to be exclusively 1D Coulomb, which excessively strengthens the correlation regime in short clusters and leads to low-probability effects of the density localization [6].

The chain of transformations of the electronic structure with a change of the correlation regime from the states of a Wigner-type crystal to the states of the Fermi-liquid type was recently presented for 3D spherical Coulomb nanoclusters with $N_e = 2$, $N_e = 3$, and parabolic boundaries (parabolic confinement) [17]. But, in [18], a wide mainly classical view on the electronic structure of 2D elliptic quantum dots with $N_e = 2$ and Coulomb interaction, but with certain limitations from above (below) on the confinement parameters (on the range of correlation regimes), is given. Clusters with small occupation are evidently the most suitable objects for establishing the correspondence between peculiarities of the electronic structure and the correlation regimes. The circle of Q1D cluster systems used in the given context [15, 16, 18] is quite limited and, in the light of modern experimental possibilities, will undergo the development, particularly by attracting Q1D clusters of the "wire" configuration. The investigation of such a cluster model is the subject of the present work.

So, as a model object of investigation, we choose a Q1D cylindric two-electron cluster with the elliptic confinement: it is variable parabolic in the longitudinal direction (the x axis) and constant parabolic in the transversal direction (the yz plane). The energy spectra and electron density distributions in the cases of the Coulomb and contact interactions of carriers in the dependence on the cluster length with the coverage of all the regimes of electron correlation are calculated and compared. A system with the contact interaction is introduced as a model alternative by the interaction nature (short-range — long-range interactions) to the Coulomb system. Numerical estimations in the Coulomb system are made with material parameters which correspond to GaAs: the effective mass of carriers $m^* = 0.067m_e$ and the dielectric coefficient $\epsilon = 12.4$. In the system with the contact interaction, we took the parameters m^* and W, where W is an integral three-dimensional interaction power. As reference parameters, the effective Bohr radius $a^* = \hbar^2\epsilon/e^2m^*$ and the atomic unit of energy (Hartree) $E^* = \hbar^2/m^*a^{*2} = e^2/\epsilon a^*$ are also used. In GaAs $a^* = 9.8$ nm, $E^* = 11.9$ meV.

2. Basic Model Relations

The starting (3D) Hamiltonian of the investigated two-electron cluster system which contains the kinetic energy, potential of confinement, and interaction between electrons can be written in the effective mass approximation as

$$H^{\rm 3D} = \sum_{i=1,2} \left\{ -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial \mathbf{r}_i^2} + \frac{m^*}{2}\left(\omega_x^2 x_i^2 + \omega_\perp^2 (y_i^2 + z_i^2)\right)\right\} + $$

$$+ V_{\rm int}^{\rm 3D}(\mathbf{r}_1 - \mathbf{r}_2), \qquad (1)$$

where $\mathbf{r}_i = (x_i, y_i, z_i)$, ω_x, and $\omega_\perp$ are the frequency parameters of the longitudinal and transversal confinements which are related to the corresponding length parameters $l_x = (\hbar/m^*\omega_x)^{1/2}$ and $l_\perp = (\hbar/m^*\omega_\perp)^{1/2}$. The interaction of electrons $V_{\rm int}^{\rm 3D}(\mathbf{r}_1 - \mathbf{r}_2)$ is given by means of the Coulomb potential

$$V_{\rm Coul}^{\rm 3D}(\mathbf{r}_1 - \mathbf{r}_2) = \frac{e^2}{\epsilon|\mathbf{r}_1 - \mathbf{r}_2|}, \qquad (2)$$

or the contact potential with the power W

$$V_\delta^{\rm 3D}(\mathbf{r}_1 - \mathbf{r}_2) = W\delta(\mathbf{r}_1 - \mathbf{r}_2). \qquad (3)$$

The transversal confinement parameter $l_\perp$ determines the transversal cluster size. Let $l_\perp$ be comparable with the electron layer thickness in GaAs-heterostructures [10] (the tough version of the transversal confinement): $l_\perp/a^* = 0.3$ ($l_\perp \simeq 3$ nm, $\hbar\omega_\perp \simeq 130$ meV). The parameter l_x is supposed to be free, which allows us to change the cluster length. The general distinction of the introduced cluster model from the models considered in [15,16,18] lies in the initial three-dimensionality and the mutual independency of parameters of the longitudinal and transversal confinements.

Applying the coordinate transformation

$$\mathbf{R} = (X, Y, Z) = (\mathbf{r}_1 + \mathbf{r}_2)/2, \quad \mathbf{r} = (x_r, y_r, z_r) = \mathbf{r}_1 - \mathbf{r}_2 \quad (4)$$

to Hamiltonian (1), we separate the center-of-mass motion (with the mass $M^* = 2m^*$) and the relative motion (with the mass $\mu^* = m^*/2$): $H^{\rm 3D} = H_{\rm c.m}^{\rm 3D} + H_{\rm rel}^{\rm 3D}$,

$$H_{\rm c.m}^{\rm 3D} = -\frac{\hbar^2}{2M^*}\frac{\partial^2}{\partial \mathbf{R}^2} + \frac{M^*}{2}\left(\omega_x^2 X^2 + \omega_\perp^2 (Y^2 + Z^2)\right), \quad (5)$$

$$H_{\rm rel}^{\rm 3D} = -\frac{\hbar^2}{2\mu^*}\frac{\partial^2}{\partial \mathbf{r}^2} + \frac{\mu^*}{2}\left(\omega_x^2 x_r^2 + \omega_\perp^2 (y_r^2 + z_r^2)\right) + V_{\rm int}^{\rm 3D}(\mathbf{r}). \quad (6)$$

Let us assume that a model system is quasi-one-dimensional if $l_x > 3l_\perp$ ($\hbar\omega_\perp/\hbar\omega_x > 9$). Intending to proceed to the 1D description, we demand that the energy shift of the ground state in systems without interaction which is conditioned by the interaction (perturbation), $\Delta E^{3D}_{\rm int} = \langle {\rm gr.st.}|V^{3D}_{\rm int}|{\rm gr.st.}\rangle$, be noticeably smaller than $\hbar\omega_\perp$. The energy shifts are given by the expressions

$$\Delta E^{\rm 3D}_{\rm Coul} = E^* \sqrt{\frac{2}{\pi}} \frac{a^*}{\sqrt{l_x^2 - l_\perp^2}} ln \frac{l_x + \sqrt{l_x^2 - l_\perp^2}}{l_\perp}$$

$$(l_x > l_\perp), \tag{7}$$

$$\Delta E^{\rm 3D}_{\delta} = \frac{W}{\sqrt{2\pi} l_x 2\pi l_\perp^2}. \tag{8}$$

Both these relations are monotonously decreasing functions of l_x. For Q1D clusters with a chosen value $l_\perp$ and at $l_x > 3l_\perp$, we get the estimation $\hbar\omega_\perp/\Delta E^{\rm 3D}_{\rm Coul} > 6.7$ in the Coulomb case. But, in the case of the contact interaction, we consider the inequality $\hbar\omega_\perp \gg \Delta E^{\rm 3D}_{\delta}$ as a limitation from above on the initially indeterminate parameter W: $W \ll \sqrt{(2\pi)^3} l_x \hbar^2/m^*$. If the conditions $\hbar\omega_\perp \gg \hbar\omega_x$, $\Delta E^{\rm 3D}_{\rm int}$, are fulfiled, the transition to the 1D description is carried out by averaging the interaction in (6) with the non-perturbed wave function of the ground state of the relative motion in the transversal direction,

$$\psi_{\perp {\rm gr}}(y_r, z_r) = \frac{1}{\sqrt{2\pi} l_\perp} \exp\left(-\frac{y_r^2 + z_r^2}{4l_\perp^2}\right), \tag{9}$$

and leads to the 1D Hamiltonian $H^{\rm 1D} = H^{\rm 1D}_{\rm c.m} + H^{\rm 1D}_{\rm rel}$. Using the units $\hbar\omega_x$ for energies and l_x for lengths here and further (in this case, a unit of mass is m^*, and a frequency unit is ω_x), we present its constituents as

$$H^{\rm 1D}_{\rm c.m} = -\frac{1}{4}\frac{\partial^2}{\partial X^2} + X^2 \qquad \left(E^{\rm 1D}_{\rm c.m} \equiv E_N = N + \frac{1}{2}\right), \tag{10}$$

$$H^{\rm 1D}_{\rm rel} = -\frac{\partial^2}{\partial x_r^2} + \frac{x_r^2}{4} + V^{\rm 1D}_{\rm int}(x_r). \tag{11}$$

The energy reference point in the 1D description is the ground state energy of the transversal motion of a non-disturbed system. In a Coulomb system, the effective interaction $V^{\rm 1D}_{\rm int}(x_r)$ in (11) takes the form

$$V^{\rm 1D}_{\rm Coul}(x_r) = \frac{l_x}{a^*}\left\{\frac{l_x}{\sqrt{2} l_\perp}\sqrt{\pi} \times \right.$$

$$\left. \times \exp\left(x_r^2 \frac{l_x^2}{2l_\perp^2}\right) {\rm erfc}\left(|x_r| \frac{l_x}{\sqrt{2} l_\perp}\right)\right\} \tag{12}$$

(${\rm erfc}(z) = 1 - {\rm erf}(z)$ is the probability integral) with the following behavior at the zero (finiteness) and at large distances:

$$V^{\rm 1D}_{\rm Coul}(x_r = 0) = \frac{(l_x/a^*)^2}{l_\perp/a^*}\sqrt{\frac{\pi}{2}},$$

$$V^{\rm 1D}_{\rm Coul}(|x_r| \to \infty) = \frac{l_x/a^*}{|x_r|}. \tag{13}$$

In the system with the contact interaction,

$$V^{\rm 1D}_{\delta}(x_r) = \frac{l_x}{a_\delta}\delta(x_r), \tag{14}$$

where

$$a_\delta = \frac{\hbar^2/m^*}{W/2\pi l_\perp^2} \tag{15}$$

is the length parameter interchangeable through inverse proportionality with the effective 1D power $W/2\pi l_\perp^2$ of the contact potential. To a certain degree, this parameter plays the role of the Bohr radius for a Q1D system with δ-interaction. (In particular, in such a system, but with an attractive interaction, the parameter a_δ characterizes the spatial scale of bound states.) Through the above-mentioned limitation on the parameter W from above, we get the corresponding limitation on the admissible values of a_δ from below in the framework of the 1D description: $a_\delta \gg (l_\perp^2/l_x)/\sqrt{2\pi}$. For Q1D clusters with $l_x > 3l_\perp$ and $l_\perp \simeq 3$ nm, it is sufficient to assume that the inequality $a_\delta \gtrsim 4$ nm ($a_\delta \gtrsim 0.4a^*$) is fulfilled. As will be shown below, the electron correlation regime in the corresponding systems is determined by the coefficients l_x/a^* and l_x/a_δ which appear in the effective interactions (12) and (14).

3. Energy Spectra

The energies and electron density distributions in Q1D cluster systems were found by means of the numerical solution of the problem on eigenvalues and eigenfunctions with Hamiltonian (11) and the effective interactions (12) and (14). In Fig. 1, the energy spectrum $E_{Nn} = E_N + E_n$ of a cluster (in units of $\hbar\omega_x = \hbar^2/m^* l_x^2$) with the Coulomb interaction is shown versus the parameter l_x/a^* which characterizes the Q1D cluster length. The energies $E_N = N + 1/2$ correspond to the center-of-mass motion, and the energies E_n to the relative motion (N, n = 0, 1, 2, ...). The energies of levels in the system without interaction, where $E_{Nn} = N + n + 1$ (Fig. 1,*a*, dashed curves) are also

shown. In clusters with parabolic boundaries, only the relative motion undergoes the influence of the pairwise interaction. The region of values $l_x > 3l_\perp$ which corresponds to Q1D clusters is located to the right of a vertical dashed line. Formally, the solutions of the Q1D model were found also for $l_x < 3l_\perp$ (to the left of a vertical dashed line), where the cluster cannot be supposed quasi-one-dimensional and is three-dimensional in the general case. In the given region, the solutions approximately reproduce only the individual fragments of the energy spectrum of a 3D cluster, namely those fragments, from which the Q1D spectrum of the system originates as the cluster length increases to values $l_x \approx 3l_\perp$ (in this case, the rest of the total 3D spectrum will be located much higher than the depicted levels). Fig. 1,*a* illustrates that the weak electron correlation regime is realized exactly in a 3D cluster, when the energies of systems with and without interaction differ insignificantly.

In the Q1D region, the spectral picture of a system with interaction as a whole shifts noticeably upward relative to the levels of a system without interaction, especially for the extended clusters at large l_x. In addition, a reorganization of the whole spectral structure takes place. Here, the regimes of intermediate and strong electron correlations occur. The reorganization of the spectral structure with a change of the correlation regime is shown in Fig. 1,*b*, where the fine structure of the energy spectrum is shown, and the level indexation is given. In this figure, the energies are reckoned from the interaction-conditioned shifts of the level with $n = 1$ in the relative motion: $\Delta E_{n=1} = E_{n=1} - 1.5$. On the linear scale in the vertical direction, the intervals between the levels E_{Nn} neighboring by the center-of-mass index N are equidistant, and the levels $E_{N,n=1}$ are depicted as the horizontal lines $N + 2$. Fig. 1,*b* demonstrates the peculiarities of the energy structure for all regimes of electron correlation and clarifies the limits of a realization of individual regimes. In the weak correlation regime (a 3D cluster, and small l_x), the levels related to the longitudinal motion are in fact degenerated with the multiplicity $N+n+1$, as in the case of the absence of interaction, what indicates the domination of the factor of the longitudinal confinement over the interaction factor. With increase in the cluster length, this degeneration is removed, so that the levels $E_{N,2k}$ and $E_{N,2k+1}$ even and odd by internal motion begin to approach one another. The approaching finishes by the asymptotic degeneration of each pair of levels at $l_x/a^* \gtrsim 5$. As a result, a new steady structure of twice degenerated levels is created that indicates the attainment of the strong correlation regime, where the factors of interaction and confinement act in balance.

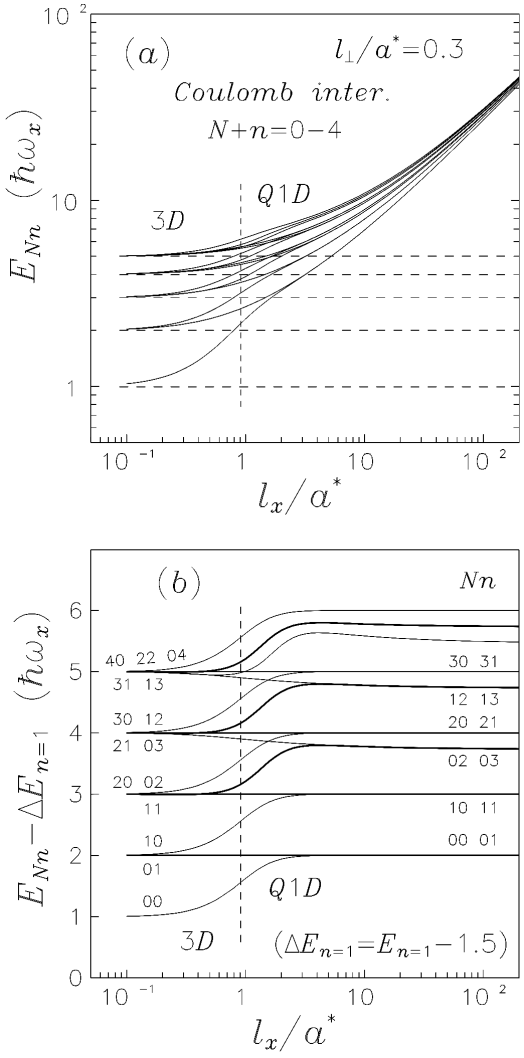

Fig. 1. *a* — energy spectrum E_{Nn} of a model two-electron Q1D cluster system with the Coulomb interaction (see the text) as a function of the cluster length. The lowest levels E_{Nn} with $0 \le N + n \le 4$ are presented. The mutual position of the spectra in systems with interaction (solid curves) and without interaction (dashed horizontal curves). *b* — the transformation of a spectral cluster structure with the variation of both its length and the electron correlation regime changing from a weak (small l_x/a^*) to strong one (large l_x/a^*)

For $0.2 \lesssim l_x/a^* \lesssim 5$, the regime of intermediate electron correlation takes place both in 3D and Q1D clusters. In this regime, the energy structure is not strictly determined or regular and strongly depends on l_x. If a somewhat smaller value of the parameter $l_\perp$

($l_\perp < 0.3a^*$) is taken in calculations, then, according to (12), the influence of the interaction factor will increase, and the transition to the strong correlation regime will happen at smaller values of l_x. On the contrary, for $l_\perp > 0.3a^*$, the transition occurs at larger l_x. Thus, at the chosen value of $l_\perp \approx 3$ nm, the regimes of intermediate and strong electron correlations will exist in a Q1D cluster, and the regimes of weak and intermediate correlations are characteristic of a 3D cluster.

Let us clarify a structure of the spectrum E_{Nn} in the strong correlation regime. In the asymptotics in l_x, the total potential of interaction and confinement of the relative motion in (11), $V_{Cc}(x_r) = V_{\rm Coul}(x_r) + V_{\rm conf}(x_r)$, becomes a two-well one with a wide Coulomb barrier (quasi-classical two-well potential [19]). At all x_r, except for a small region near $x_r = 0$, the effective interaction (12) can be approximated by a 1D Coulomb potential according to (13). The total potential is as follows:

$$V_{Cc}(x_r) = \frac{l_x/a^*}{|x_r|} + \frac{x_r^2}{4}. \qquad (16)$$

Near the bottoms of wells, whose location we denote as $\pm x_{r0}$, this potential is well approximated by a parabolic function

$$V_{Cc}(|x_r| \simeq x_{r0}) \approx \frac{3}{4}x_{r0}^2 + \frac{3}{4}(|x_r| - x_{r0})^2;$$

$$x_{r0} = \left(2\frac{l_x}{a^*}\right)^{1/3}. \qquad (17)$$

The x_{r0} (presented here in units of l_x) will be further identified as the corrected cluster length at large values of l_x. The first term in (17) sets the scale of a shift $E_{\rm shift} = (3/4)x_{r0}^2$ of the whole spectrum in the strong correlation regime (in comparison with the scale equal to 1 for a system without interaction or $\hbar\omega_x$ in dimensional units, as seen from Fig. 1,*a*). The second parabolic term contains the frequency $\sqrt{3}$ (or $\sqrt{3}\omega_x$ in dimensional units) which characterizes the excitation scale for the relative motion, i.e. the frequency interval between two neighboring pairs of asymptotically degenerated levels $E_{N,2k}$, $E_{N,2k+1}$ and $E_{N,2k+2}$, $E_{N,2k+3}$. From the classical point of view, the frequency $\sqrt{3}$ is related to oscillations of the interparticle distance $x_r = x_1 - x_2$ around x_{r0}, i.e. it is a frequency of "respiratory" oscillations in the strong correlation regime. It can be analytically proved that the same frequency of "respiratory" oscillations is intrinsic to symmetric cluster systems with a parabolic confinement of any dimension and with any amount of electrons which interact by the Coulomb law of the corresponding dimension, in particular to two-dimensional clusters [20]. Thus, the quasiclassical energy of a cluster in the strong correlation regime has a form $E_{Nn} = (N + 1/2) + E_{\rm shift} + \sqrt{3}([n/2] + 1/2)$ with the dominant contribution from the shift $E_{\rm shift}$ which, in turn, consists of two thirds of the interaction contribution and of one thirds of the confinement contribution.

Let us present some estimations of the parameters in Fig. 1 for GaAs-based clusters. Values $l_x/a^* = 0.1 \div 100$ correspond to $l_x \simeq 1 \div 1000$ nm, i.e. the whole nanorange of lengths l_x is covered. In the strong correlation regime, the corrected cluster length x_{r0} equals 1000 nm even at $l_x \simeq 265$ nm ($x_{r0} \sim l_x^{4/3}$ in dimensional units). At $l_x/a^* = 1$, the reference scale is $\hbar\omega_x = E^* \simeq 12$ meV. The increase of l_x by one order lowers this scale by two orders. This yields that a spectral structure in the strong correlation regime at $l_x/a^* = 10$ ($\hbar\omega_x \simeq 0.12$ meV $\simeq 1.5$ K) can be resolved at sufficiently low temperatures. It is known that, in clusters with the parabolic confinement and the pairwise interaction, only spectral branches related to excitations in the center-of-mass subsystem [21] are verified by dipole spectroscopy. It can be assumed that the optical methods are valid also for the identification of characteristic resonance excitations of the internal subsystem in the strong correlation regime, but the spectroscopy must be quadrupole, because, under the pairwise degeneration of levels, the closest levels will differ by the index of internal motion n at least by $\Delta n = 2$.

In Fig. 2, the energy spectrum of a cluster with the contact interaction versus the parameter l_x/a_δ which characterizes the cluster length and the relative power of the effective 1D $\delta-$interaction (14) is shown. With regard for the limitation from below on a_δ, we set, for definitness, $a_\delta = a^*$. In this case, the separating line between the 3D and Q1D regions of the spectrum will take the same place as in Fig. 1, which is convenient for the comparison of both spectral pictures. Here, the regimes of weak and intermediate electron correlations are also realized in the region $l_x \sim l_\perp$ (3D cluster) as in Coulomb clusters. But, at $l_x > 3l_\perp$ (Q1D cluster), the regimes of intermediate and strong correlation are observed. However, the change of regimes happens slower than in Coulomb clusters. With increase in l_x, the even and odd levels of relative motion will approach to one another pairwise up to the asymptotic degeneration in the strong correlation regime which is reached at $l_x \simeq$ 1000 nm, which is much larger than the corresponding values in Coulomb clusters. In contrast to the Coulomb case, the shift of the whole energy structure doesn't occur here. This is explained by the fact that the contact

potential does not influence the odd levels of relative motion, because it acts at a point of the location of the central nodes of the corresponding wave functions. However, each even level undergoes the action of the contact potential and shifts to the closest odd level as the cluster length increases (the strengthening of the correlation regime). Thus, the whole collection of odd levels of relative motion remains beyond the scope of the influence of the contact interaction, "attracting" the collection of even levels in sufficiently extended clusters to itself. This leads to the formation of a general structure of asymptotically degenerated pairs of the levels (as in Coulomb clusters) resulting, in essence, to the appearance of the strong regime of electron correlation. The energies in this regime are given by expressions $E_{Nn}=E_N+E_n$, $E_N=N+1/2$, $E_n=2[n/2]+3/2$ and are equally distributed between the kinetic and potential energies. The asymptotic contribution of the interaction to the energies E_n in the case of even values $n=2k$, $<2k|V_\delta^{1D}|2k>=(l_x/a_\delta)\psi_{2k}^2(0)\sim(l_x/a_\delta)^{-1}\to 0$, is negligibly small. The given estimate is conditioned by the behavior of a pairwise wave function of the internal motion at zero: $\psi_{2k}^2(0)\approx\sqrt{8/\pi}[(2k+1)!!/(2k)!!]/(l_x/a_\delta)^2$ at $l_x/a_\delta\gg 1$. In this case, the total potential of the internal motion can be imagined as two semioscillatory confinement potentials $x_r^2/4$ sewed along the vertical at the point $x_r=0$.

The asymptotic degeneration in the strong correlation regime, strictly speaking, is higher than the twofold one. Since the frequencies of the closest excitations in the relative motion exactly two times higher than the similar frequencies in the center-of-mass subsystem, the degeneration multiplicities $g(E_{Nn})=2,2,4,4,6,6,...$ of the asymptotic level structure will increase with the level energies ($E_{Nn}=2,3,4,5,6,7,...$). At any small expansion of the δ-interaction, the mentioned frequency balance will be broken. As a consequence, the enhanced degeneration will be taken off.

Independently of the interaction nature, the degeneration multiplicity of levels in the strong correlation regime doubles, if we account the total spins of the states with energies E_{Nn}: $S=0$ for even n, and $S=1$ for odd n.

In the framework of the 1D description, the reproduction of various electron correlation regimes is also related to the manner of accounting the effective interaction. In the general case, the effective 1D interaction can keep the main physical features of the 3D interaction, from which it is originated. For example, the power of the effective 1D Coulomb interaction must

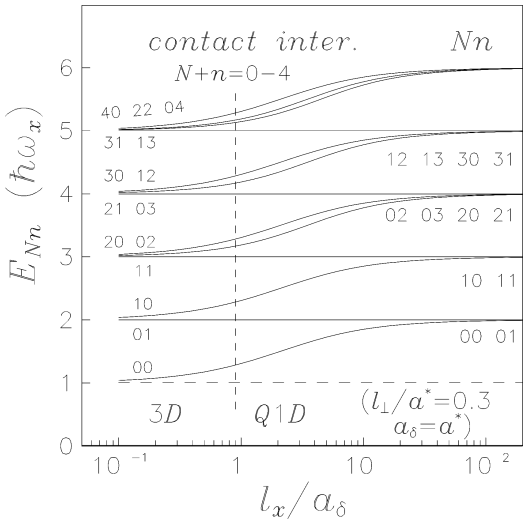

Fig. 2. Energy spectrum E_{Nn} ($0\le N+n\le 4$) of a model two-electron Q1D cluster system in the case of the contact δ-interaction of carriers depending on the cluster length. The interaction intensity W and the transversal size of a cluster $l_\perp$ are accounted by the parameter a_δ according to Eq. (15). The horizontal dashed curve is the ground state energy in a system without interaction. The vertical dashed curve which separates the regions of 3D and Q1D spectra corresponds to $l_x=3l_\perp$ (the case where $a_\delta=a^*$)

be finite in any finite interval, as it is natural to the 3D Coulomb interaction (and also to the model 2D one) in any finite region of the 3D (2D) space, in spite of the presence of a singular point. Therefore, the effective 1D interaction cannot have nonintegrable singularities in finite intervals, in particular, cannot be simulated by exclusively the 1D Coulomb one. This allows one to avoid the problems of twofold degeneration of levels and the separation of the ground state at the 1D description of Q1D systems [22,23] (otherwise, all possible correlation regimes, except the strong one, will remain beyond the consideration). The effective 1D interactions (12) and (14) are physically acceptable by the mentioned feature, i.e. they satisfy the requirement of integrability in any finite intervals and therefore foresee the realization of different regimes of electron correlation.

4. Electron Density

We restrict ourselves by consideration of the electron density distributions in clusters which are in the lowest energy center-of-mass state ($N=0$) and in any state of

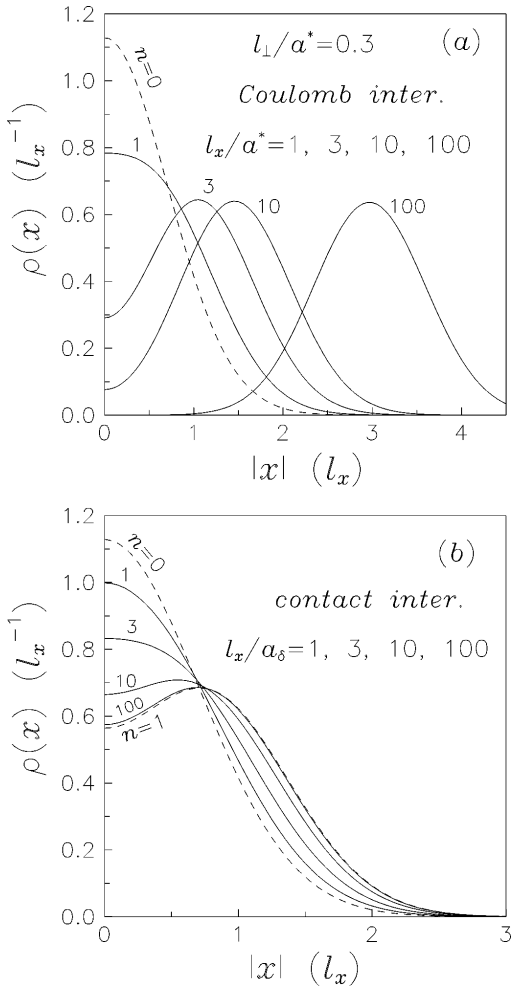

Fig. 3. Electronic density distribution $\rho(x)$ in the ground state ($N = n = 0$) in Q1D clusters of various length in the case of the (a) Coulomb and (b) contact interaction of the carriers (solid curves). At $l_x/a^* = 100$ the distributions in $n=0$ and $n=1$ states in a Coulomb cluster are graphically indistinguishable. The dashed curves correspond to the density distributions in systems without interaction with arbitrary values of l_x and (a) $N = n = 0$, (b) $N=0$, $n=0$; 1

relative motion n. The corresponding density is given by the expression (in units of l_x^{-1})

$$\rho(x; N = 0, n) = \sqrt{\frac{8}{\pi}} \exp(-2x^2) \times$$

$$\times \int dy \psi_n^2(y) \exp(-y^2/2) \mathrm{ch}(2xy), \qquad (18)$$

where $\psi_n(y)$ is the wave function of the relative motion. In the absence of interaction,

$$\rho(x; N = 0, n) = \frac{2}{\sqrt{\pi}} \exp(-x^2)(-1)^n L_n^{-1/2-n}(x^2), \quad (19)$$

where $L_n^\alpha(s)$ is the Laguerre polynomial.

The density distributions in Q1D Coulomb clusters of various lengths are presented in Fig. 3,a. In the applied reference scheme, each distribution in a system with interaction (the solid line with a specific value of the parameter l_x/a^*) can be directly compared with a distribution with the corresponding value l_x for a system without interaction (the dashed line, whose form is not related to l_x according to (19)). The idea of the mutual form of two distributions with different parameters $(l_x/a^*)_i \equiv p_i$ on the same scale can be obtained by means of the simultaneous stretching along the horizontal and the squeezing along the vertical by p_2/p_1 times of the distribution with $p_2 > p_1$ relative to the distribution with p_1.

In the intermediate correlation regime ($l_x/a^* = 1; 3$), the density distributions in the ground state differ sufficiently from similar ones for systems without interaction and cover the whole cluster with a smaller or larger dip at the cluster center depending on its length. In the strong correlation regime, in the presence of a wide barrier in the relative motion, the wave functions of the relative motion can be written in the quasi-classical form $\psi_n(x_r) = \{\varphi_{[n/2]}(x_r) + (-1)^n \varphi_{[n/2]}(-x_r)\}/\sqrt{2}$ [19], where $\varphi_k(\pm x_r)$ are the functions of states in each of two wells of the quasi-classical potential (16) which are approximated with the accuracy of $O(1/x_{r0})$ by the oscillator functions for the individual potential wells (17). The oscillator functions take into the account the length parameter related to the frequency $\sqrt{3}$ and the reduced mass 1/2. In the given approximation, the density distribution along the cluster axis x in the states with $n = 0$ and 1 looks as

$$\rho(x; N = 0; n = 0, 1) \simeq \sqrt{\frac{s}{\pi}} \left\{ \exp\left(-\left(x - \frac{x_{r0}}{2} \right)^2 s \right) + \right.$$

$$\left. + \exp\left(-\left(x + \frac{x_{r0}}{2} \right)^2 s \right) \right\}, \qquad (20)$$

$s = 2\sqrt{3}/(1+\sqrt{3}) \approx 1.27$. The distribution (20), being asymptotic in l_x, consists of two identical components centered on the cluster axis at the points $\pm x_{r0}/2$. The width of each component is proportional by the order of magnitude to 1 (or l_x in the dimensional units). At $x_{r0} \gg 1$, the intersection of components is practically absent. This means that, in the strong correlation regime, the electron density is localized at the distances $x_{r0}/2$ from the cluster center, and the parameter x_{r0} determines, as mentioned above, the effective cluster length.

In clusters with the $\delta-$interaction, all the electron density distributions in the ground state ($n = 0$) are located, according to the energy structure, between two distributions which correspond to the states without interaction with $n = 0$ and $n = 1$, by approaching the latter as the cluster length increases (Fig. 3,*b*). In the strong correlation regime, the asymptotic representation of density distributions will be given by formula (19), which does not account the interaction, with the replacement $n \to 2[n/2]+1$ on the right-hand side. The given distributions, whose density is spread within the whole cluster in the limits of its potential boundaries, are exclusively quantum also in the large-length clusters, in contrast to the quasi-classical localized distributions in the Coulomb clusters. This fact demonstrates the basic difference of the electron structures of nanoclusters with the Coulomb and contact interactions.

5. Conclusions

The main result of the carried investigation is the demonstration of the fact that the strong correlation regime in Q1D electron nanoclusters with parabolic boundaries can be realized in a system with the long-range (Coulomb) interaction, as well as in a system with the short-range (contact) interaction. The sign of this regime is the specific and fixed (with the cluster length changing in the proper range) general spatial and spin structure of energy spectra which is invariant relative to the interaction nature. The types of interaction in this structure are distinguished by the single parameter, the excitation energy in subsystems with internal motion: $\sqrt{3}\hbar\omega_x$ and $2\hbar\omega_x$ (see Section 2). However, for commensurable values of the parameters a^* and a_δ related to the interactions of different nature, the strong correlation regime in the case of a short-range interaction is reached at much larger cluster lengths. Moreover, absolutely different are those physical mechanisms that are responsible for the formation of an electron structure in the strong correlation regime. This circumstance is revealed in a radical distinction of electron density distributions: the localization on the cluster edges in the Coulomb nanoclusters, i.e. we observe the Wigner quasi-classical structure, and the full occupation of the "cluster space" in systems with the contact interaction which have a spin-nonpolarized structure of the quantum-liquid type (Section 3). Thus, the strong electron correlation regime in Q1D nanoclusters is unambiguously verified only by the features of the energy structure.

The work is performed with the support of the Russian-Ukrainian project on nanophysics and nanoelectronics and the program of NASU, N 0102U002329.

1. *Austing D.G., Sasaki S., Tarucha S., et al.* // Phys. Rev. B.— 1999. — **60**, N 16. — P. 11514—11523.
2. *Lorke A., Luyken R.J., Govorov A.O., Kotthaus J.P.* // Phys. Rev. Lett. — 2000. — **84**, N 10. — P. 2223—2226.
3. *Reimann S.M., Koskinen M, Manninen M.* // Phys. Rev. B. — 1999. — **59**, N 3. — P. 1613—161.
4. *Hirose K., Wingreen N.S.* // Ibid. — N 7. — P. 4604—4607.
5. *Koskinen M., Manninen M., Mottelson B., Reimann S.M.* // Ibid. — 2001. — **63**, N 20. — P. 205323(5).
6. *Reimann S.M., Manninen M.* // Rev. Mod. Phys. —2002. — **74**. — P. 1283—1342.
7. *Bedanov V.M., Peeters F.M.* // Phys. Rev. B. — 1994. — **49**, N 4. — P. 2667—2676.
8. *Jacak L., Hawrylak P., Wojs A.* Quantum Dots. — Berlin: Springer, 1998.
9. *Chakraborty T.* Quantum Dots. — Amsterdam: Elsevier, 1999.
10. *Alhassid Y.* // Rev. Mod. Phys. —2000. — **72**, N 4. — P. 895—968.
11. *Li O.P., Das Sarma S.* // Phys. Rev. B. — 1991. — **43**, N 14. — P. 11768—11786.
12. *Schulz H.J.* // Phys. Rev. Lett. — 1993. — **71**, N 12. — P. 1864—1867.
13. *Calmels L., Gold A.* // Phys. Rev. B. —1995. — **52**, N 15. — P. 10841—10857.
14. *Piacente G., Schweigert I.V., Betouras J.J., Peeters F.M.* // Phys. Rev. B. — 2004. — **69**, N 4. — P. 045324(17).
15. *Bryant G.W.* // Phys. Rev. Lett. — 1987. — **59**, N 10. — P. 1140—1143.
16. *Häusler W., Kramer B.* // Phys. Rev. B. — 1993. — **47**, N 24. — P. 16353—16357.
17. *Sundquist P.A., Volkov S.Yu., Lozovik Yu.E., Willander M.* // Ibid. — 2002. — **66**, N 7. — P. 075335(10).
18. *Drouvelis P.S., Schmelcher P., Diakonos F.K.* // Ibid. — 2004. — **69**, N 3. — P. 035333(15).
19. *Landau L.D., Lifshits E.M.* Quantum Mechanics. — Moscow: Nauka, 1974 (in Russian).
20. *Schweigert V.A., Peeters F.M.* // Phys. Rev. B. —1995. — **51**, N 12. — P. 7700—7713.
21. *Maksym P.A., Chakraborty T.* // Phys. Rev. Lett. — 1990. — **65**, N 1. — P. 108—111.
22. *Bryant G.W., Glick A.J.* // Phys. Rev. B. — 1982. — **26**, N 10. — P. 5855—5866.
23. *Bryant G.W.* // Ibid. — 1984. — **29**, N 12.— P. 6632—6639; — 1985. — **31**, N 12. — P. 7812—7818.

Received 18.04.05
Translated from Ukrainian by R.A. Naryshkin

ТЕОРІЯ КОРЕЛЯЦІЙНИХ ЕФЕКТІВ
У ДВОХЕЛЕКТРОННИХ КВАЗІОДНОВИМІРНИХ
НАНОКЛАСТЕРАХ З ПАРАБОЛІЧНИМИ МЕЖАМИ

С.Я. Горощенко

Р е з ю м е

Досліджено енергетичні спектри та розподіли електронної густини в модельних квазіодновимірних нанокластерних системах із двох електронів, що взаємодіють за законом Кулона (далекодія) або контактним чином (близькодія), за різних режимів електронної кореляції (у кластерах різної протяжності). Показано, що в режимі сильної кореляції загальна структура енергетичних спектрів виявляється інваріантною щодо характеру взаємодії, при цьому система з кулонівською взаємодією стає квазікласичною з електронною густиною, локалізованою на кінцях кластера, а система з контактною взаємодією залишається квантовою, в якій густина розподілена по всій довжині кластера. Передбачається, що верифікація енергетичної структури в режимі сильної кореляції може бути виконана із застосуванням методів дипольної та квадрупольної спектроскопії.