

## Correlation effects in vertical gated quantum dots

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The influence of the electron-electron correlation on the electronic properties of vertical gated quantum dots with three-dimensional confinement has been studied by the configuration interaction method. We have found that the correlation is essential in the weakly confined electron systems and becomes negligibly small for the strongly confined electrons. We have determined the role of the correlation in the single-electron transport-spectroscopy experiments in the gated quantum dots. The correlation slightly changes the stability diagram, but considerably affects the magnetic-field dependence of the confined-electron energy spectra.

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The single-electron transport in the vertical gated quantum dot<sup>1,2</sup> (QD) has been described<sup>3,4</sup> with the use of the Hartree-Fock (HF) method. Although this method does not take into account the electron-electron correlation, good agreement has been obtained<sup>3,4</sup> with the stability diagram measured<sup>2</sup> without a magnetic field. However, the computational results<sup>5</sup> exhibit systematic deviations from the experimental data obtained in the magnetic field,<sup>1</sup> which can be ascribed to the electron-electron correlation. The configuration interaction (CI) method was applied<sup>6-8</sup> to the correlation in QD-confined electron systems in the framework of the two-dimensional parabolic confinement potential model. The parabolic potential was also used in calculations,<sup>9,10</sup> which account for the electron-electron correlation in the spin local density approximation. Matagne and Leburton<sup>11</sup> used the spin local density approach with the confinement potential derived from the Poisson equation. The results obtained<sup>11</sup> are rather far from the experimental data.<sup>1,2</sup> Based on the existing calculations,<sup>6-11</sup> one can hardly estimate the role of the correlation in the transport-spectroscopy experiments.<sup>1,2</sup> In the present paper, a systematic study of the correlation effects is performed for the vertical QD's by the CI method. We apply the model parabolic potential as well as the realistic confinement potential obtained from the self-consistent solution<sup>4</sup> of the Poisson-Schrödinger problem and discuss the role of the correlation in the single-electron transport via the vertical gated QD's.

We consider the three-dimensional system of  $N$  electrons confined in the QD of the cylindrical symmetry. First, we solve the one-electron eigenproblem using trial wave functions of the form

$$\psi(\mathbf{r}) = \sum_{k_x, k_y=0}^{k_x+k_y \leq k} c_{k_x k_y} x^{k_x} y^{k_y} \exp[-\alpha(x^2+y^2) - \beta z^2], \quad (1)$$

where  $\alpha$  and  $\beta$  are the nonlinear and  $c_{k_x k_y}$  the linear variational parameters. Next, we use one-electron wave functions (1) to build the Slater determinants, which form the basis set for the diagonalization of the  $N$ -electron Hamiltonian by the CI method. The  $N$ -electron eigenstates possess definite  $z$  components of the total angular momentum and the total spin; so they are labeled by the corresponding quantum numbers ( $L, S$ ). Basis (1), complemented by the spin wave func-

tion, allows for a construction of  $\binom{k+1}{N} \binom{k+2}{S}$  Slater determinants with definite  $L$  and  $S$ . For each  $N$ -electron state we use the basis composed of all Slater determinants with the required spin-orbital symmetry. The Gaussians in Eq. (1) lead to the analytical expressions for the Coulomb matrix elements. In the present paper, we consider the systems of two, three, and four electrons with  $L=0, \dots, 6$ .

The conditions of the single-electron tunneling<sup>4</sup> are determined by the chemical potentials, defined as  $\mu_N = E_N - E_{N-1}$ , where  $E_N$  is the ground-state energy of the  $N$ -electron QD. In the vertical QD,<sup>1</sup> the confinement of electrons in the growth ( $z$ ) direction is much stronger than the lateral confinement in the  $x$ - $y$  plane. Therefore, in the  $N$ -electron QD, all the confined electrons occupy the ground state of the quantized motion in the  $z$  direction, which allows us to describe this state by a single  $z$ -dependent Gaussian [cf. Eq. (1)]. This leads to a slight overestimation of the ground-state energy, which is the same for all the occupied states; so it has no influence on the relative values of the chemical potentials of the electrons in the QD.

Before considering the real QD,<sup>1,2</sup> we study the correlation effects in the idealized QD described by the model confinement potential, which is assumed to be a rectangular potential well in the  $z$  direction and a lateral potential  $U_{conf} = m_e \omega^2 (x^2 + y^2)/2$ , where  $m_e$  is the electron effective band mass and  $\hbar \omega$  is the confinement energy. We take the parameters of the nanostructure, which correspond to the cylindrical QD of Tarucha *et al.*<sup>1</sup>; e.g., the quantum well has width 12 nm in the  $z$  direction and depth 220 meV. The values of all the other parameters are the same as in Ref. 4. In the gated QD,<sup>1,2</sup> the lateral confinement energy  $\hbar \omega$  is not constant<sup>4</sup> but decreases from  $\sim 6.7$  to  $\sim 5.4$  meV when  $N$  increases from 1 to 4. Therefore, in the present calculations with the model confinement potential, we take on  $\hbar \omega = 6$  meV. Moreover, we neglect the spin Zeeman effect.

In order to check the convergence of the present CI results, we have performed test calculations whose results are listed in Table I for  $N=3$ . In the further calculations, we adopt basis (1) with  $k=5$ . Based on the results of Table I, we estimate the precision for the energy levels considered to be about 0.1 meV. Therefore, throughout the present paper, we will call these CI results "exact." Table I also shows that the accuracy of the HF method<sup>12</sup> is different for the different

TABLE I. Results of test calculations for the three-electron system confined in the lateral parabolic potential with  $\hbar\omega=6$  meV and vertical double-barrier potential at  $B=0$ .  $k$  determines the number of elements in one-electron basis (1). In the subsequent columns, we quote the energy (in meV) of the three lowest-energy states with quantum numbers  $(L,S)$ , given in the first row, calculated by the CI method with the numbers of Slater determinants given in parentheses. The results obtained by the HF method are listed in the last row. One-electron ground-state energy  $E_1 = -188.04$  meV. The top of the potential barrier is taken as the reference energy ( $E=0$ ).

$k$	(1,1/2)	(2,1/2)	(3,3/2)
2	-536.82 (15)	-533.33 (11)	-529.56 (2)
3	-538.20 (56)	-534.91 (49)	-530.66 (10)
4	-538.34 (161)	-535.19 (145)	-531.63 (38)
5	-538.40 (377)	-535.27 (354)	-531.66 (96)
6	-538.42 (785)	-535.29 (744)	-531.71 (218)
HF	-536.84	-532.89	-531.42

states. The difference between the exact and HF energy, i.e., the correlation energy, is considerably smaller for the spin-polarized state (3,3/2) than for the spin-unpolarized states (1,1/2) and (2,1/2). At zero magnetic field, the ground states of the systems with  $N=2, 3$ , and 4 electrons are labeled by (0,0), (1,1/2), and (0,1), respectively. For these states, using basis (1) with  $k=5$ , we have constructed 70, 377, and 2174 Slater determinants, respectively, and obtained the following total ground-state energies:  $-367.94$  ( $-366.84$ ),  $-538.42$  ( $-536.84$ ), and  $-704.06$  ( $-702.31$ ) [in meV], where the HF estimate is given in the parentheses. These results show that the absolute errors of the HF total energy estimates increase with  $N$ . However, these errors partly cancel out when calculating the chemical potentials. The related differences of the chemical potentials calculated by the HF and CI methods are the following:  $\Delta\mu_2 = 1.10$  meV,  $\Delta\mu_3 = 0.48$  meV, and  $\Delta\mu_4 = 0.17$  meV.

The magnetic-field evolution of the three-electron energy levels is displayed in Fig. 1, which shows that the correlation energy is nearly constant for each state considered, i.e., independent of the magnetic field. We note that the HF method can fail in predicting the ground state of the system. For the three-electron system the ground state changes with the magnetic field as follows: this is state (1,1/2) for  $B < 4.6$  T, state (2,1/2) for  $4.6 \text{ T} \leq B \leq 5.7$  T, and state (3,3/2) for  $B > 5.7$  T. However, according to the HF approach, state (1,1/2) would possess the lowest energy for  $B < 3.8$  T, while for the higher magnetic field state (3,3/2) would become the ground state. As a result, the HF method underestimates the magnetic field, which induces the spin polarization, and does not predict state (2,1/2) to be the ground state.

The chemical potentials calculated by the CI and HF methods are displayed in Figs. 2(a)–2(c) for different confinement strengths. In the case of weak confinement [Fig. 2(a)], the HF results become unreliable both quantitatively and qualitatively. In particular, the HF method predicts the incorrect symmetry of the ground state. For example, the low-spin state (2,0), which is the ground state of the four-

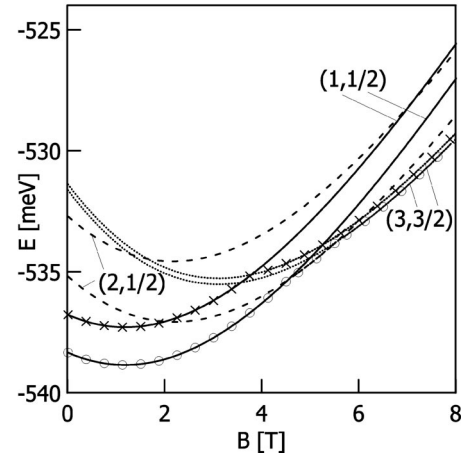


FIG. 1. Energy  $E$  of the three-electron system in the vertical QD with the parabolic lateral confinement ( $\hbar\omega=6$  meV) as a function of magnetic field  $B$ . Solid lines correspond to state (1,1/2), dashed lines to state (2,1/2), and dotted lines to state (3,3/2). For each pair of the curves the lower (upper) one shows the CI (HF) results. The ground-state energy determined by the CI (HF) method is marked by circles (crosses).

electron system in a wide range of the magnetic field, is erroneously predicted to be the excited state in the HF method. QD's with the weak confinement were fabricated by Ashoori *et al.*<sup>13</sup> However, the experimental spectra for these dots are affected by random local fluctuations of the confinement potential. Therefore, the parabolic model potential seems to be oversimplified for these QD's.

Figure 2(b) shows the results for the intermediate confinement. With one exception, the increasing magnetic field leads to the increase of the total spin in the ground-state transformations. Since the HF method works better for the spin-polarized states, the critical values of the magnetic field for these transformations are underestimated. In the four-electron system, the transition  $(0,1) \rightarrow (2,0)$  at  $B=0.5$  T is the only one in which the total spin decreases and the corresponding critical magnetic field is overestimated by the HF method, which prefers the spin polarization. We note that the intermediate confinement corresponds to the QD of Tarucha *et al.*<sup>1</sup> In this case, the HF results are in qualitative agreement with the exact results. The only exception is the omission of the (2,1/2) ground state in the three-electron system [Fig. 2(b)]. However, the cusp corresponding to the (1,1/2)  $\rightarrow$  (2,1/2) transition is rather smooth. Therefore, this transition is hardly visible in the experimental data.<sup>1</sup>

The results for the strong confinement are displayed in Fig. 2(c), which shows that the agreement between the HF and CI results is better than in the case of the intermediate confinement. In the strongly confined electron systems, the multiconfiguration basis reduces to one dominating configuration; i.e., the correlation is small. The results of Fig. 2(c) indicate that the HF method can be used as a computational tool of sufficiently high precision for the QD's with the strong confinement potential, e.g., for the self-assembled quantum dots, in which  $\hbar\omega > 10$  meV.<sup>14</sup>

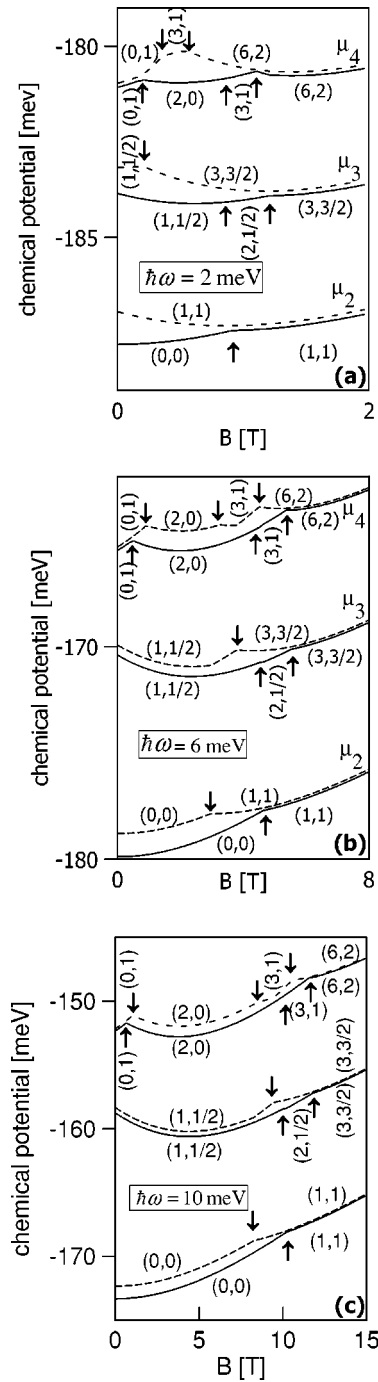


FIG. 2. Chemical potentials  $\mu_N$  of  $N=2, 3, 4$  electrons confined in the vertical QD with the confinement energy (a)  $\hbar\omega=2$  meV, (b)  $\hbar\omega=6$  meV, and (c)  $\hbar\omega=10$  meV, as functions of magnetic field  $B$ . The results obtained by the CI (HF) method are displayed by solid (dashed) lines. Quantum numbers  $(L,S)$  correspond to the ground state. The magnetic-field-induced ground-state transformations calculated by the CI (HF) method are shown by the arrows up (down).

The exact chemical potentials exhibit the same qualitative magnetic-field dependence for the confinement potentials studied [cf. Figs. 2(a)–2(c)]. In all the cases studied in this paper, the magnetic-field induces the ground-state transformations in the same order independently of the strength of

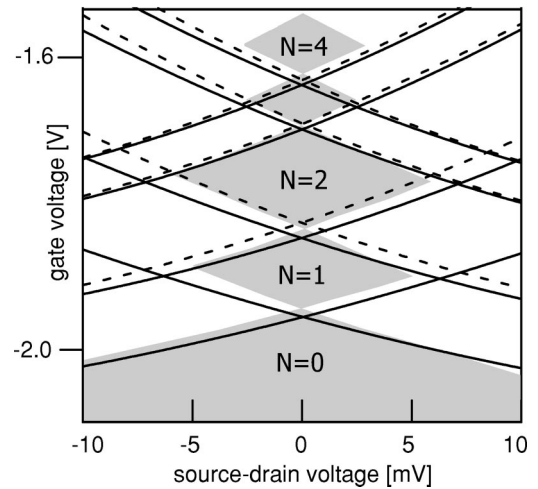


FIG. 3. Stability diagram with Coulomb diamonds. The experimental data (Ref. 2) are depicted by the shaded areas. Solid (dashed) curves show the boundaries of the Coulomb diamonds calculated by the CI (HF) method.

the confinement. In the high-magnetic field regime, states  $(1,1)$ ,  $(3,3/2)$ , and  $(6,2)$  of the two-, three-, and four-electron systems, respectively, correspond to a maximum density droplet (MDD).<sup>15</sup> We note that—for these states—the HF method yields very accurate results. At the higher magnetic fields than those considered in the present paper, the MDD becomes unstable against a formation of a Wigner molecule.<sup>16–19</sup> Based on the high accuracy of the HF method for the high-field spin-polarized states, we expect that the unrestricted HF method with a properly chosen basis<sup>19</sup> will yield reliable results for the Wigner molecules. For the MDD, the unrestricted and restricted HF methods yield the same results. In this state, the electron charge density obtained by both the HF methods reproduces the symmetry of the confinement potential. However, only the unrestricted HF method accounts for the breakdown of the MDD and the formation of the Wigner molecule.<sup>17–19</sup> In this way, the unrestricted HF method can provide at least some collective effects in the confined electron system. Therefore, the results of the restricted HF approach are more suitable as the reference data in the discussion of the correlation effects.<sup>20</sup>

Now, we consider the effect of correlation on the single-electron transport in the real QD.<sup>1,2</sup> For this purpose, we have introduced the CI method into the self-consistent procedure, elaborated in our previous work,<sup>4</sup> in order to solve the Poisson-Schrödinger problem for the vertical gated QD.<sup>1,2</sup> We are still using the HF method<sup>21</sup> to determine the confined charge density in the self-consistency loop<sup>4</sup> for the electrostatics of the nanodevice, since the charges outside the QD perceive the averaged confined electron charge only. The CI method is applied to the evaluation of the energy of the  $N$ -electron system confined in the QD, which allows us to increase the accuracy of the energy calculations. The results are displayed in Fig. 3, which shows the stability diagram with the Coulomb diamonds measured by Kouwenhoven *et al.*<sup>2</sup> and their borders calculated by the CI and HF methods. We note that the both the methods lead to similar results.

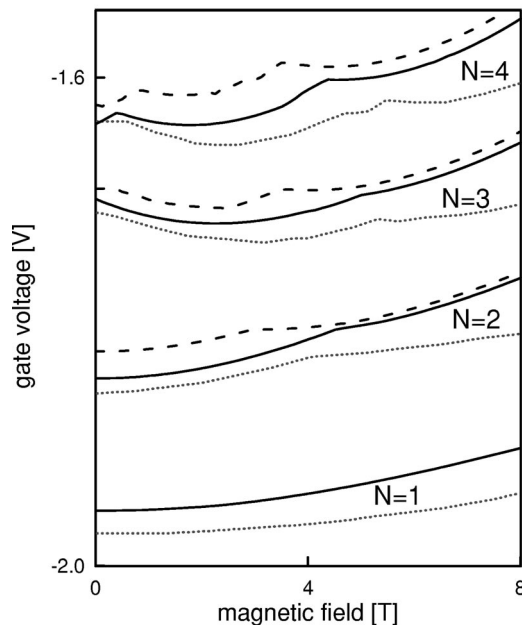


FIG. 4. Gate voltage corresponding to the current peaks as a function of the magnetic field. Dotted, solid, and dashed lines correspond to the experimental (Ref. 2), CI, and HF results, respectively.

The significant differences that occur for the upper boundaries of the first diamond and the lower boundaries of the second diamond are due to the fact that the largest difference between the HF and CI chemical potentials appears for  $N=2$ . It is just chemical potential  $\mu_2$  that determines these boundaries.<sup>4</sup>

The magnetic-field dependence of the gate voltage, at which the single-electron tunneling occurs, is plotted in Fig. 4. The cusps on the curves (Fig. 4) correspond to the magnetic-field-induced ground-state transformations in the

$N$ -electron QD. We see that the CI results are considerably closer to the experimental data than the HF results and the HF method underestimates the critical magnetic fields for the ground-state transformations. This means that the electron-electron correlation plays an important role in the single-electron transport in the external magnetic field. For  $N=1$  there is no correlation; therefore, the discrepancy between the measured and calculated plots (cf. Fig. 4,  $N=1$ ) illustrates the precision of the present modeling of the vertical QD. The difference in the slopes of these plots, which is visible in Fig. 4, indicates that the confinement potential in the real nanostructure is slightly stronger than that used in our modeling.

The conditions of the single-electron transport via the gated QD (Refs. 1 and 2) are determined by the QD chemical potential,<sup>4</sup> which is calculated as the ground-state energy difference. If the ground-state energies are determined with a comparable accuracy, the errors cancel out and the chemical potential can be evaluated with a sufficient precision. This explains why the HF approach<sup>4</sup> leads to a good agreement with experiment<sup>2</sup> for the Coulomb diamonds (cf. Fig. 3). The critical magnetic fields for the ground-state transformations are directly determined by the ground-state energy. The HF method works with the different accuracy for the different states (cf. Fig. 1). Therefore, the magnetic field, which induces the ground-state transformations, i.e., changes the order of the energy levels associated with the states of the different spin-orbital symmetry, can be inaccurately estimated by the HF method.

In summary, we have shown that the correlation considerably changes the energy of the weakly confined electron systems. In the single-electron transport through the vertical gated QD's, the correlation slightly modifies the boundaries of the Coulomb diamonds in the stability diagram, but considerably affects the QD energy spectra in the external magnetic field.

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<sup>21</sup>The HF results for the real QD taken from Refs. 4 and 5 have been obtained by the unrestricted HF method.