Electronic structures in circular, elliptic, and triangular quantum dots

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Electronic structures in circular, elliptic, and triangular shaped quantum dots containing single or a few electrons are calculated by numerically diagonalizing the N-electron Hamiltonian (for N up to 12). In a circular quantum dot, the addition energy shows a clear structure as a function of N due to the shell filling and the spin-polarized half filling. In an elliptic quantum dot, however, the structure is found to be diminished, which is attributed to the splitting of the degenerated single-particle states due to the asymmetric confining potential. The states with $N=3$, 6, and 9 electrons in a triangular quantum dot are found to be slightly stable compared to a circular quantum dot, which is interpreted in terms of a geometrical effect. [S0163-1829(97)03835-6]

I. INTRODUCTION

Recent progress in microfabrication technology has enabled us to investigate quantum mechanics in semiconductor microstructures such as quantum wells, quantum wires, and quantum dots in which the motion of electrons is restricted in two, one, and zero dimension. Although electrons involved in a quantum well and a quantum wire are numerous, we are able to restrict the number of electrons to several in a quantum dot (QD) where electrons are confined three dimensionally by artificially created potential. The N-electron ground state energy in a QD was probed by the transport spectroscopy[1] and by the single-electron capacitance spectroscopy.[2,3] The energy levels in a QD which contains a few electrons ($N \lesssim 10$) are modified by the electron-electron interaction, even in the zero magnetic field.[3]

Recently Tarucha *et al.*[4] reported an experimental result on the tunneling of electrons through a QD, and showed that the addition energy of an electron in a QD with a few electrons reveals an existence of a clear shell structure. They showed that the electron number of $N=2$, 6, and 12 is the ''magic number'' reflecting the shell structure. In addition they observed a maximum of the addition energy for $N=4$, which is explained in terms of the Hund's rule.[4] The theoretical calculations of the chemical potential difference (addition energy) and the capacitive energy in an isolated QD (Refs. 6 and 7) and in a QD coupled to leads[8] were performed by using the self-consistent technique, which show the several structures with respect to the shell filling feature.

In the present work we evaluate the exact eigenstates in vertical QD's,[4,5] which contain many interacting electrons, by diagonalizing the complete N-electron Hamiltonian with the Coulombic interaction. We especially focus on the effects of the symmetry of confining potential on the electronic states, since the observed shell structure is expected to be reduced for systems with stronger asymmetry. In this paper we proceed as follows. A model for QD's is given in Sec. II together with an analytical form of lateral confining potential used in the present work. A calculation method for obtaining many electrons states in QD's is then shown in Sec. III. Numerical results of electron number dependence of addition energy for circular, elliptic, and triangular shaped QD's are presented in Sec. IV. A summary and discussion are given in Sec. V.

II. MODEL

A schematic illustration of the model for a QD formed in a vertical $Al_xGa_{1-x}As/In_{0.05}Ga_{0.95}As/Al_xGa_{1-x}As$ double heterostructure[4,5] is shown in Fig. 1, where the x-y plane and the z direction are taken to be parallel and perpendicular to the heterointerfaces, respectively. The confining potentials in the vertical (z) direction and in the plane parallel to the heterointerfaces (x-y plane) are assumed to be separable, and for confining potential in the z direction ($H(z)$), we assume an infinite square potential well of width W for simplicity. In order to analyze effects of symmetry of the lateral confining potential ($V(x,y)$) on the electronic states, we model $V(x,y)$ by the following equation:

$$V(x,y)=\frac{1}{2}m^*(\omega_x^2x^2+\omega_y^2y^2)\left\{1+\alpha\frac{2}{7}\cos 3\phi\right\}, \qquad (1)$$

where ω_x and ω_y are the confining energies along the x and y directions, respectively, α ($=0$ or 1) is a parameter to specify the shape of the lateral confining potential, and ϕ is the angle with respect to a specific axis in the x-y plane. When $\alpha=0$, the contour line of the lateral confining potential becomes an ellipse (for $\omega_x \neq \omega_y$) or a circle (for

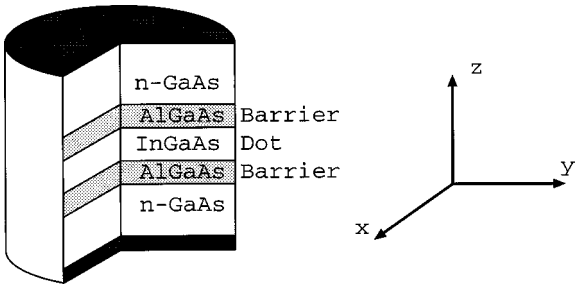

FIG. 1. Schematic illustration of a vertical quantum dot fabricated in semiconductor heterointerfaces. Electrons are confined in the $In_xGa_{1-x}As$ layer. As shown in the figure, the x-y plane and the z direction are taken to be parallel and perpendicular to the heterointerfaces, respectively.

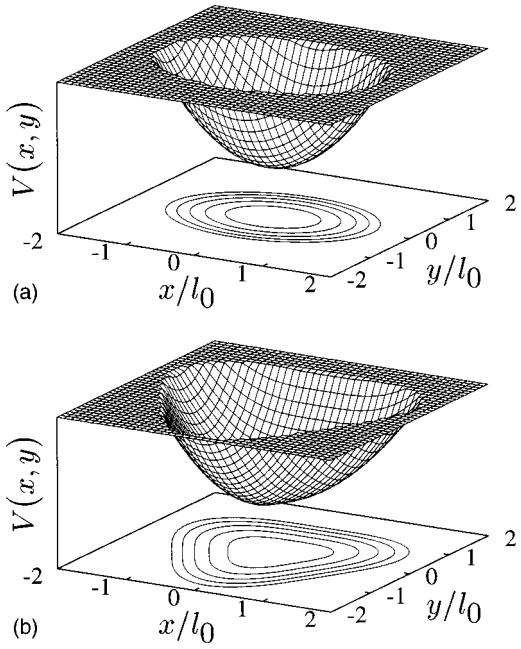

FIG. 2. Three-dimensional view and contour lines of elliptic (a) and triangular (b) shaped confining potentials in quantum dots modeled by Eq. (1).

$\omega_x=\omega_y$). The three-dimensional view and contour lines of an elliptic confining potential is shown in Fig. 2(a) as an example. Figure 2(b) also shows a triangular shaped confining potential and its contour line, which is obtained by setting 1 for the parameter α and putting $\omega_x=\omega_y$.

III. METHOD

For the QD modeled in the previous section, the N-electron Hamiltonian can be written as follows:

$$\mathcal{H}=\sum_{i=1}^{N}\mathcal{H}_0+\sum_{i<j}\frac{e^2}{4\pi\epsilon|\boldsymbol{r}_i-\boldsymbol{r}_j|}, \tag{2}$$

where $\mathcal{H}_0=(\boldsymbol{p}+e\boldsymbol{A})^2/2m^*+V(x,y)+H(z)$ is the single-electron Hamiltonian with $\boldsymbol{A}$ being the vector potential. The second term in Eq. (2) represents the Coulomb interaction energy. In the present paper we will be concerned only with the case without applied magnetic field, and the electronic states of QD's under magnetic field will be dealt with in the separate paper. We therefore put $\boldsymbol{A}=\boldsymbol{0}$ in the present analysis. The material parameters for $In_{0.05}Ga_{0.95}As$ are computed by the linear interpolation of the parameters between InAs and GaAs, which gives the effective mass of electrons of $m^*=0.065m_0$ and the static dielectric constant of $\epsilon=12.9\epsilon_0$.

The N-electron Hamiltonian of Eq. (2) is numerically diagonalized by using Slater determinants for $N=1-12$ electrons system. The method has been employed to obtain the electronic states in QD's with electrons up to $N=4$.[9–16] We constructed the N-particle Slater determinants from a single-particle eigenfunction, or the solutions of single-particle Hamiltonian $\mathcal{H}_0$, as a basis set. In our system the confining potential is separated in the x-y plane and z direction, and thus we can divide the single-particle Hamiltonian into the x-y plane and the z direction. We use the lowest 26 single-particle eigenstates associated with the quantum confinement in the x-y plane parallel to the heterointerfaces. Since the confinement along the z direction is strong in a real QD (Refs. 4,5) compared to the confinement in the x-y plane, many eigenstates fall in the lowest subband formed by the z direction confinement. It is therefore a good approximation in the calculation to take into account the lowest subband associated with the quantized z motion, as shown below. Consider an example of the confining energies $\omega_x=\omega_y=3$ meV and the well width $W=12$ nm, which are the typical value in the calculation, the energy separation between the lowest 26 single-electron states in the x-y plane is 12 meV, whereas the energy separation between the ground and the first exited states along the z directions is 121 meV. Therefore the first exited single-particle state along z direction can be safely ignored.

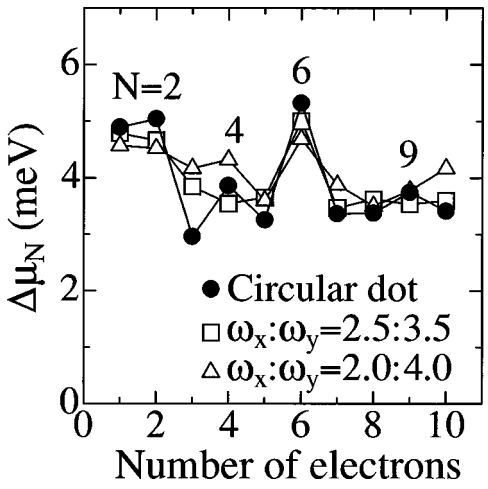

FIG. 3. Chemical potential differences (addition energy) in elliptic quantum dots as a function of the number of electrons. Solid circles are results for a circular quantum dot with confining energy $\omega_x=\omega_y=3.0$ meV. The open squares are for the QD with confining energies of $\omega_x=2.5$ meV and $\omega_y=3.5$ meV, and the open triangles for a QD with $\omega_x=2.0$ meV and $\omega_y=4.0$ meV.

IV. RESULT AND DISCUSSION

In this section we will present calculated results for several QD's with different lateral confining potentials. Figure 3 shows the chemical potential difference $\Delta\mu(N)\equiv\mu(N+1)-\mu(N)$ in two different elliptic QD's with the average confining energy of $(\omega_x+\omega_y)/2=3$ meV as a function of electron number $N=1\sim11$. The chemical potential is defined by $\mu(N)\equiv E(N)-E(N-1)$ with $E(N)$ being the ground state energy for N electrons. The open squares are for the QD with confining energies of $\omega_x=2.5$ meV and $\omega_y=3.5$ meV, and the open triangles are for a QD with $\omega_x=2.0$ meV and $\omega_y=4.0$ meV. The results for a circular QD with confining energy of $\omega_x=\omega_y=3.0$ meV are also plotted in Fig. 3 by solid circles for comparison. The chemical potential difference $\Delta\mu(N)$ in a QD corresponds to an energy required to add one more electron into the QD which initially contains N electrons. From this definition, the chemical potential difference $\Delta\mu(N)$ is referred to as ''addition energy'' of a QD with N electrons. It is evident from

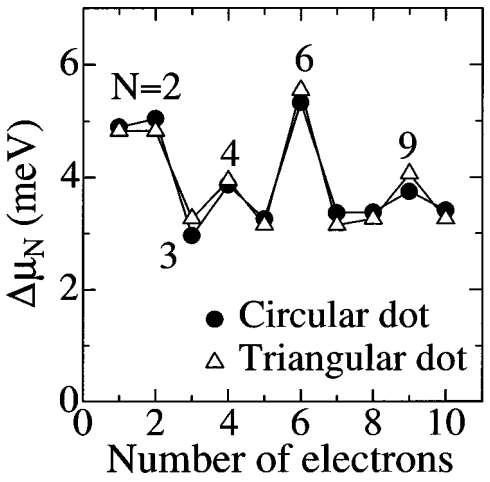

FIG. 4. Chemical potential differences (addition energy) in a circular quantum dot (solid circles) and a triangular quantum dot (open triangles) as a function of the number of electrons. The confining energies ω_x and ω_y in both circular and triangular quantum dots are 3 meV.

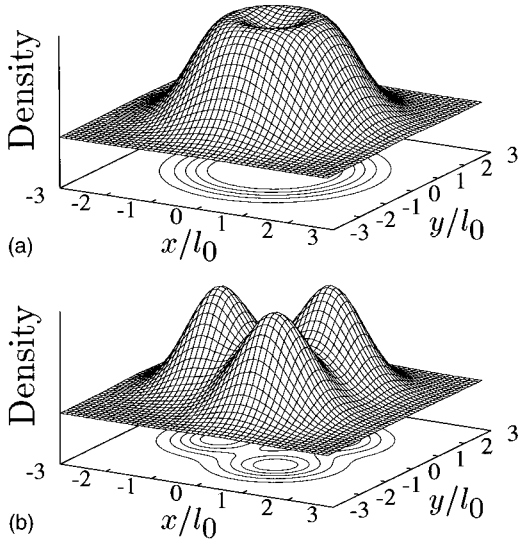

FIG. 5. Density distribution of electrons in QD's containing three electrons with a circular (a) and a triangular (b) shaped confining potential in plane parallel to the heterointerface. l_0 is 20 nm.

this definition that an eigenstate with large addition energy is energetically stable.

We find in Fig. 3 that the addition energy has peaks at $N=2$ and 6 in the circular QD (solid circles). In a circular QD, a complete shell filling structure takes place for 2,6,12,$\cdots$ electrons, resulting in maxima of the addition energy $\Delta\mu(N)$. In addition we find a weak structure at $N=4$ and 9. Such a feature is not expected from the calculations based on a simple single-particle picture. From the present results obtained by the exact diagonalization method, it is found that spin triplet states with total spin $S=1$ ($S_z=-1$, 0, and 1) give rise to the ground state in a circular QD with four electrons. In spin triplet states, two electrons with spin antiparallel occupy the first orbit, and another two electrons with spin parallel occupy the second orbit in the QD. The electrons in the second orbit will stay apart from each other due to the Pauli's exclusion principle, resulting in diminishing Coulomb interaction energy between the electrons in the second orbit and forming a relatively stable state. The weak structure of the addition energy at $N=4$ and 9 may, therefore, be interpreted in terms of the spin polarized half filling shell structure.[4,8] In elliptic QD's (open squares and open triangles in Fig. 3), on the other hand, $\Delta\mu(N)$ no longer has clear structures except the peak at $N=6$. This is because the asymmetry of these systems results in the splitting of the degenerated single-particle eigenstates and in the mixing of many eigenstates with various angular momenta.

Figure 4 shows the results of a triangular QD, where the result of the circular QD are again plotted by solid circles for comparison. In Fig. 4 the addition energies of the circular (solid circles) and the triangular (open triangles) QD's are found to exhibit almost the same characteristics. The addition energy $\Delta\mu(N)$ of the triangular QD containing electrons $N=3$, 6, and 9, however, is found to be slightly larger than that of a circular QD. This feature may be explained as follows. The density of electrons in QD's containing three electrons is shown in Fig. 5(a) for the circular QD and Fig. 5(b) for the triangular QD. As seen in Fig. 5(a) electrons in the circularly shaped lateral potential form a rotationally symmetric distribution, and the electron density becomes small in the center of the QD due to the electron-electron interaction. On the other hand, in the triangular QD each electron moves toward each corner of the triangle and forms a more stable state as shown in Fig. 4(b), giving rise to a slightly larger addition energy. For the same reason electronic states for $N=6$ and 9 in the triangular QD become slightly stable compared to the case of the circular QD.

V. CONCLUSION

We calculated N electron eigenstates in QD's with vertical confinement of heterointerfaces and with lateral confinement of circular, elliptic, and triangular potentials. The eigenstates are obtained by diagonalizing N-particle Hamiltonian utilizing Slater determinants composed from the single-particle eigenstates. Due to the rotational symmetry in a circular QD, electrons form the complete shell filling structures for $N=2$ and 6, and the spin-polarized half filling structures for $N=4$ and 9. These structures give rise to relatively large addition energies, which are observed in the single-electron tunneling spectroscopy reported by Tarucha *et al.*[4] From the present analysis we find that the Hund's rule is valid in two-dimensional artificial atoms. In elliptic QD's addition energy no longer exhibits clear structure in the plot of addition energy vs the number of electrons N, except for $N=6$. This feature is explained in terms of the asymmetry of these systems which leads to the splitting of the degenerated single-particle eigenstates and the mixing of many eigenstates with various angular momenta. In a triangular QD, on the other hand, slightly stable states due to the localization of the electrons at the corners are realized for electron number $N=3$, 6, and 9, which may be interpreted in terms of a geometrical effect.

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