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Electronic structure of hexagonal quantum-disc clusters*

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Within the effective-mass approximation, we investigate the electronic structure of hexagonal quantum-disc clusters using the finite element method. With an increasing amount of quantum dots in the cluster, the electronic energy levels quickly expand into mini-bands, each consisting of discrete, unevenly distributed energy levels. The corresponding electronic eigenfunctions are linear combinations of the electron orbits in each quantum dot. The spatial symmetry of the combination is the same as the electronic eigenfunction of a single quantum dot.

Keywords: energy band, linear combination, spatial symmetry
PACC: 7320D, 7125W

1. Introduction

Collections of essentially isolated quantum dots (QDs) have been extensively studied theoretically and experimentally. Great efforts have also been devoted to the interaction of QDs in arrays because of their potential applications, especially those related to QD superlattices (QDSLs).[1,2] But the understanding of coupled QD arrays lags behind their isolated counterpart. We focus our attention on the issue of electronic states in coupled QD arrays.

The coupling of two[3,4] or a large number of QDs[5,6] has been studied experimentally, and the localizing properties of the electron states in these systems have also been examined. In the two-dot coupling system, both covalent bond states and ionic bond states are observed using the microwave spectrum.[3] Recently, the extended states or mini-bands formed in QD arrays have been confirmed by time-resolved photoluminescence (TRPL).[1,5] This means that two-dimensional (2D) QDSLs with artificial electronic structures have been realized. Lan *et al*[1] treated the 2D QDSL as a disordered system containing both extended states and localized states. It is understood that the extended states or mini-bands originate from strong coupling of uniform small QDs; while the localized states come from the large islands that are excluded from the coupling due to their size, which is far larger than the uniform small QDs.

In the literature, most theoretical works on QD arrays use the Hamiltonians of the simple Anderson–Newns or Hubbard-type models.[7,8] The effect of disorder and interaction among QDs are included in the Mott–Hubbard model of finite quantum-disc arrays, and their influence on the persistent current are investigated.[7] In most of the works mentioned above, each QD is regarded as an atom, in accordance with the often well-justified approximation of viewing QDs as artificial atoms. However, it is not self-evident that such treatment will accurately describe real QD array systems.

We study a QD array system by viewing how QD clusters change from QD molecules to QDSLs. This is a new and special approach to understanding the electronic structure of QDSLs. By watching the evolution of electronic structures with different sizes in a QD array system, we are able to study the QDSL formation process by gradually adding QDs. This also provides a special stage for the understanding of the basic principles of quantum mechanics. The finite element method[9,10] is a powerful tool to deal with the eigenvalue problem of the asymmetric system. We use this tool to investigate the formation process of the ar-

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tificial solid.

2. Model of the hexagonal quantum-disc cluster

In the 2D lateral inter-dot coupling system, QDs are organized into a 2D QDSL. This type of 2D QDSL is attractive because it possesses a significant negative differential conductance (NDC).[11] The QDSL sample has been imaged by atomic force microscopy (AFM), and the image shows that the sample has uniform QDs with sizes of around 25nm, exhibiting a close-packed and highly-ordered array. So we adopt a large hexagonal quantum-disc cluster (see Fig.1) to simplify the sample.

With the effective-mass approximation, we choose the single-conduction-band effective-mass envelope functions to describe the confined electrons in the quantum-disc cluster. Such an approach is valid if the characteristic energy corresponding to the envelope function is much smaller than the fundamental bandgap. In small QDs, a single-particle description is a good approximation for few electrons in QDs.[12] The Hamiltonian H of an electron in the quantum-disc cluster is written as

$$H = \frac{p^2}{2m^*} + \sum_{i=1}^{n} V_i(\boldsymbol{r}), \qquad (1)$$

where m^* is the electron effective mass, $\boldsymbol{r}$ is the position vector of the electron, $V_i(\boldsymbol{r})$ is the confining potential of the ith quantum disc, and n is the number of QDs in the cluster. Here the effect of spin is neglected. The electronic structures of the QD cluster are investigated by solving the Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$.

For semiconductor quantum discs, the size in the z-direction is much smaller than that in the xy plane. In the adiabatic approximation,[13,14] we take advantage of the fact that the electronic wavefunction is strongly confined to the lowest subband in the z-direction,[15] so the wavefunction of the electron is written as $\Psi(x,y,z) = \phi(x,y)\psi_0(z)$, where $\phi(x,y)$ is the wavefunction in the xy plane and $\psi_0(z)$ is the ground-state wavefunction in the z-direction. The laterally coupled QDs are simplified to a 2D system, and the Schrödinger equation in the rectangular coordinates is written as

$$-\frac{\hbar^2}{2m^*}\left\{\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2}\right\} + \sum_{i=1}^{n} V_i(x,y)\phi = E\phi. \qquad (2)$$

By adopting reduced atomic units (a.u.*), which correspond to a length unit of one effective Bohr radius, $a^* = \hbar^2\varepsilon/m^*e^2$, and an energy unit of one effective Rydberg, $R_y^* = m^*e^4/2\hbar^2\varepsilon^2$, Eq.(2) can be rewritten as

$$-\left(\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2}\right) + \sum_{i=1}^{n} V_i(x,y)\phi = E\phi. \qquad (3)$$

Here, we assume that the effective mass of an electron in the QDs is the same as that in the quantum discs.[16] The eigenstates of the system are obtained by solving the Schrödinger equation (3) using the finite element method.[9,10] By adding the number of QDs one by one, the formation process of the mini-band are vividly shown by the calculated results.

3. Numerical calculation: results and discussion

In order to investigate the electronic structure of a QD cluster, we assume that all the radii of the QDs are $1a^*$ and that the confining potentials are square-well potentials with a height of $40R_y^*$. The distance between adjacent QD centres is $2.2a^*$.

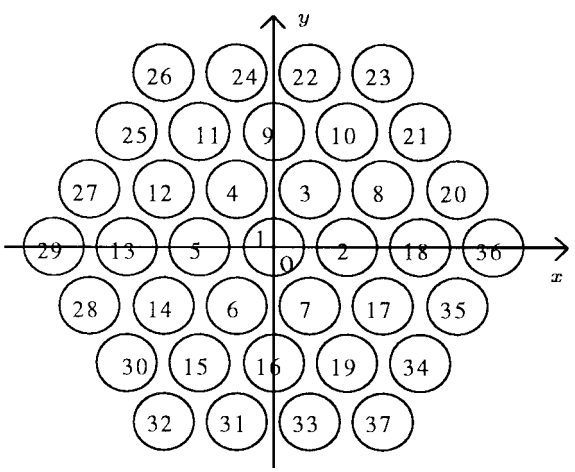


Fig.1. Schematic diagram of a laterally coupled hexagonal quantum-disc cluster.

If the origin of the coordinates is chosen at the centre of a disc (see Fig.1), the centres of the discs are respectively at $\left(\pm 2.2m, \pm 2.2\sqrt{3}l\right)$ or $(\pm 2.2m + 1.1, \pm 2.2\sqrt{3}l + 1.1\sqrt{3})$ for such 2D hexagonally packed quantum discs, where m and l are integers. The confining potential $V_i(x,y)$ in Eq.(3) is written as

$$V_i(x,y) = \begin{cases} 0, & if\ \sqrt{(x-x_i)^2 + (y-y_i)^2} \le 1 \\ 40R^*, & if\ \sqrt{(x-x_i)^2 + (y-y_i)^2} > 1 \end{cases}, \qquad (4)$$

where (x_i, y_i) are the coordinates of the QD centres in Fig.1. Inserting expression (4) into Eq.(3), the eigenstates for the packed QD clusters are obtained by solving this Schrödinger equation (3) numerically using the finite element method.[9]

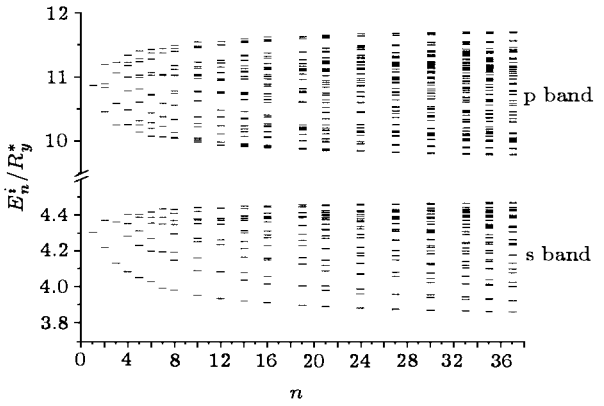


Fig.2. Energy eigenvalues of QD clusters as functions of n (the number of QDs in a QD cluster).

Figure 2 shows the energy eigenvalues as functions of n. Note that the two energy levels in a QD expand rapidly into two mini-bands consisting of n energy levels and $2n$ energy levels (for convenience, we call these the s band and p band respectively). We can see that the energy levels in each band are not evenly distributed. When n is larger than 19, the widths of the mini-bands reach their limits which are approximately $0.61R_y^*$ (s band) and $1.91R_y^*$ (p band), and the energy gap between the two mini-bands also takes a limit of around $5.3R_y^*$. After this, a further increase of n makes no change in the width of each band, and the increased energy levels all fall into the mini-bands. So the widths of the mini-band and energy gap are independent of the amount of QDs when large enough. Note that the height of the potential and the distance between two adjacent discs do not change with increasing n; in other words, the coupled strength between the two adjacent discs does not vary. So the widths of the mini-band and energy gap are related to the coupling between two adjacent dots and the size of each QD. The widths of the bands will become larger when the dots are closer to each other or the dots are wider in size.[17] For example, if the radii of each QD changes into $1.1a^*$ with the same centre distance $2.2a^*$, the QDs are tangent with each other. The widths of the s and p bands change into $1.7R_y^*$ and $4.3R_y^*$ respectively, and the energy gap decreases to $2.5R_y^*$.

In order to further study the electronic structure of the QD cluster, we have examined the electronic wavefunctions of QD clusters with different sizes. We have found that all the eigenfunctions of the QD clusters are linear combinations of the electronic orbits inside each QD. The spatial symmetry of the electronic eigenfunction in the QD cluster is the same as the electronic eigenfunction of the ex-tangent hexagonal quantum disc (EHQD). Generally, the wavefunction of the ground state possesses the highest spatial symmetry, and the spatial symmetry of the excited wavefunctions decreases with higher energy levels, just as in the EHQD. As an example, Fig.3 shows the contour maps of the two lowest eigenstates inside the cluster with 37 QDs and two lowest eigenstates inside the EHQD.

The electronic wavefunction of the ground state of a QD cluster is shown in Fig.3(a), as compared with the electronic wavefunction of the ground state in the ex-tangent hexagonal disc shown in Fig.3(c). It is noted that the linear combination of the 37 s electronic orbits forms the ground state of the QD cluster, and there are overlaps between two adjacent discs. All the QDs form a bonding state. It is very clear that the spatial symmetry of the combination is the same as that of the wavefunction of the ground state in the EHQD (see Fig.3(c)).

The wavefunction of the first excited state of the QD cluster is shown in Fig.3(b), as compared with the wavefunction of the second eigenfunction inside the EHQD in Fig.3(d). Note that it is also a linear combination of the 37 s electronic orbits, but there is no overlap between the upper and lower halves of the QDs (see Fig.3(b)). The two parts form an antibonding state. Again, the spatial symmetry of the combination is the same as that of the wavefunction of the second eigenfunction in the EHQD (see Fig.3(d)). The combination coefficients are zero for the s electronic orbits located at the nodes of the eigenfunction of the EHQD. The nodes of the wavefunction may affect the electron transport characteristics of the QD cluster.

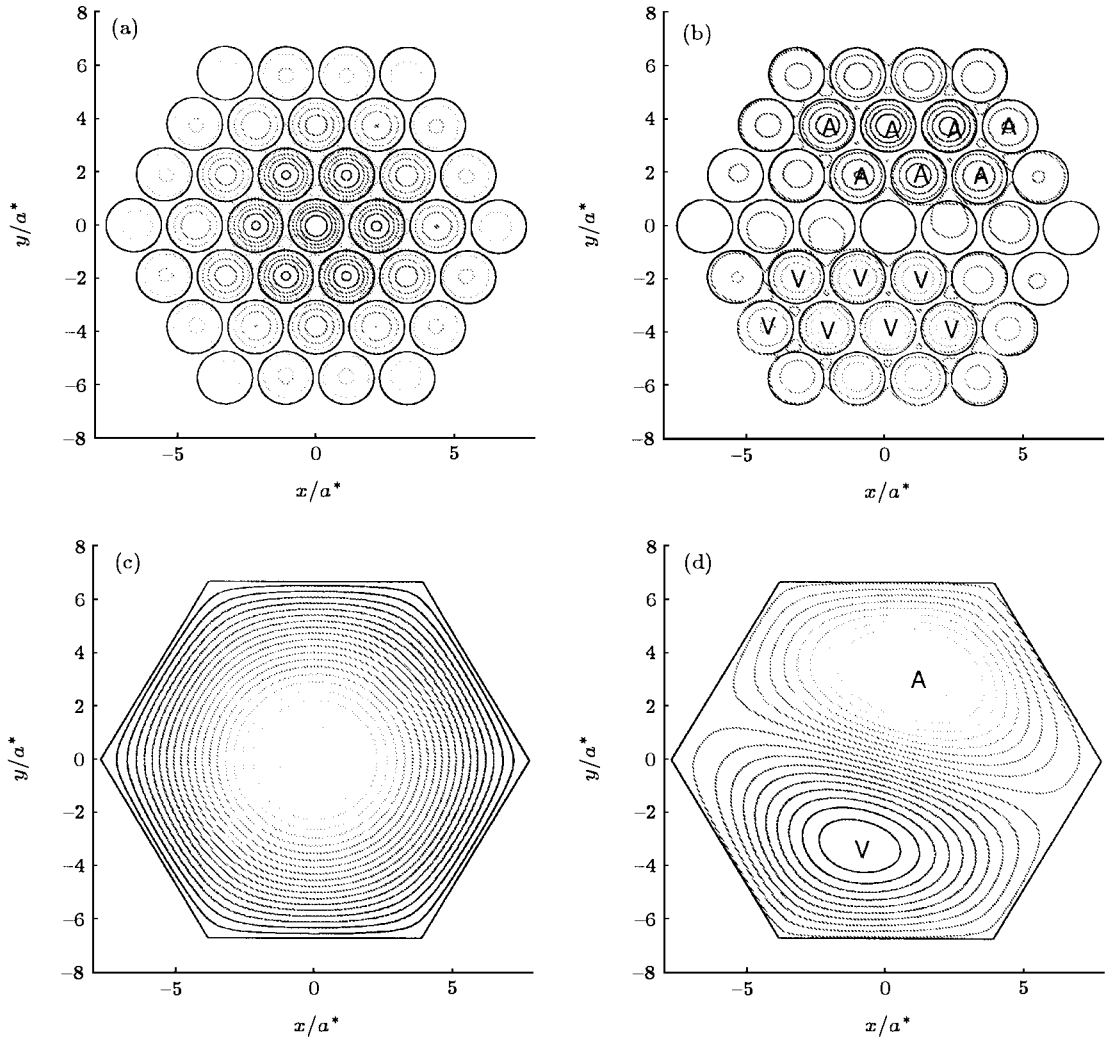


Fig.3. (a) and (b) show the contour maps of the first and second eigenfunctions of the cluster with 37 QDs, which are linear combinations of the orbit s in each disc. (c) and (d) show the contour maps of the first and second eigenfunctions inside the EHQD. 'A' denotes a peak while 'V' denotes a valley.

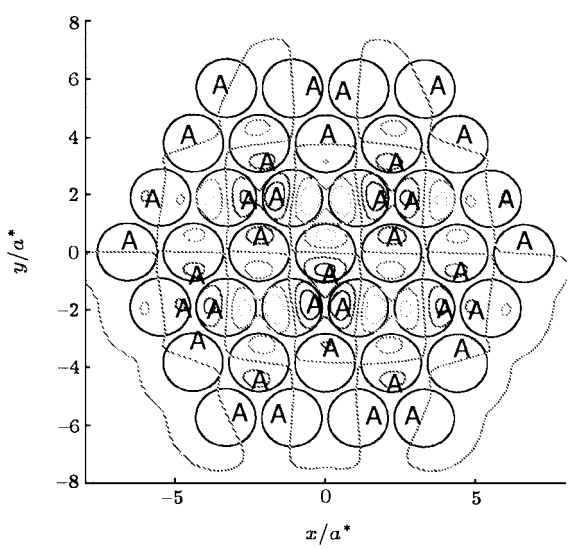


Fig.4. The contour map of the eigenfunction of the lowest level in the p band. It is a linear combination of orbit p in each disc. 'A' denotes the peak.

The wavefunctions of the other 35 energy levels in the s band are also the linear combinations of the 37 s electronic orbits, and also show the above features.

Similarly, the wavefunction of the lowest energy level in the p band is the linear combination of the 37 p electronic orbits (see Fig.4). There are also overlaps between all adjacent dots for this wavefunction, so the combination forms a bonding state. All the nodes of the wavefunctions are located inside the QDs.

4. Conclusion

In conclusion, we have studied the electronic structure of the hexagonal QD cluster using the finite element method. We found that by increasing the amount of the QDs in the cluster, the electronic energy levels quickly evolve into mini-bands, each con-

sisting of discrete, unevenly distributed energy levels. The widths of each energy band and gap are determined by the coupling between QDs and the size of each dot. The corresponding electronic eigenfunctions are linear combinations of the electron orbits in each QD. The spatial symmetry of the combination is the same as the electronic eigenfunction inside the EHQD. In this paper we have given a complete picture of how a QD crystal is formed, providing a blueprint for wavefunction engineering.

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