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Effect of Shape of Quantum Dots on the Energy Levels of Electrons

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ABSTRACT: Quantum dots (QDs) are solid-state nanostructures that can confine electrons or holes in all three spatial dimensions, which leads to discretization of energy levels. It can also be defined as a semiconductor whose excitons are confined in all three spatial dimensions. As a result, they have properties that are between those of bulk semiconductors and discrete molecules. The QD with the confined electrons can be treated as an artificial atom. Semiconductor quantum dots have emerged as strong candidates for quantum computation due to significant progress in ultrafast optoelectronics, nanostructure fabrication and characterization techniques, and possibility of large scale integration. The spin of the electron or hole can be used for the quantum bits due the low de-coherence of the spin degree of freedom which allows sufficient time for carrying out any gating operation on these qubits. So, effect of shape of Quantum Dots have been investigated in this paper.

I. INTRODUCTION

Semiconductor quantum dots have emerged as strong candidates for quantum computation due to significant progress in ultrafast optoelectronics, nanostructure fabrication and characterization techniques, and possibility of large scale integration. The spin of the electron or hole can be used for the quantum bits due the low de-coherence of the spin degree of freedom which allows sufficient time for carrying out any gating operation on these qubits.

Interest in quantum computation was sparked when the algorithms of Shor and Grover demonstrated that the computation problems which require extensive resources and time on a classical computer become feasible on a quantum computer. Investigations into a physically realizable quantum computer have been carried out on ion-trap systems, as well as cavity quantum electrodynamic systems, and in nuclear magnetic resonance systems.

The two qubit operations are required for making a universal gate which would need the preparation of entangled states. Coupled quantum dots or the quantum dot molecules provide a powerful system for producing controllable entanglement between spin qubits. The exchange coupling between the electrons/holes establishes the necessary entanglement between the spin.

In recent papers, one can find many theoretical proposals for the implementation of quantum dots (QDs) in quantum computation. These proposals consist in application of either the orbital or spin states of electrons confined in the QDs. The orbital states of electrons in the coupled QDs were proposed for a possible realization of a quantum controlled-NOT (CNOT) gate. Spin states of coupled QDs are intensively studied as possible candidates for qubits and quantum logic gates due to the long relaxation time. In order to use the qubits as efficient information carriers and to perform a unitary time evolution of them we have to maintain the coherent quantum states for a time that exceeds the quantum gate operation time by many orders of magnitude. This requirement is very difficult to satisfy in solid-state devices and a lot of research is being carried out to overcome this difficulty. The present paper is organized in following sections:

1. Introduction to Quantum Dots
2. Applications of Quantum Dots
3. Introduction to Quantum Computation
4. Fabrication of Quantum Dots
5. Effect of Size of Quantum Dots
6. Method of solving the schrodinger equation.
7. Effect of shape of Quantum Dots.
8. Bibliography and references.

II. INTRODUCTION TO QD'S

Quantum dots (QDs) are *solid-state nanostructures* that can confine electrons or holes in all three spatial dimensions, which leads to discretization of energy levels. It can also be defined as a semiconductor whose excitons are confined in all three spatial dimensions. As a result, they have properties that are between those of bulk semiconductors and discrete molecules. The QD with the confined electrons can be treated as an artificial atom.

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Quantum dots are semiconductor nanocrystals with a length of approximately 2-10 nanometers. These nanocrystals have wavelength smaller than that of an optically-excited electron-hold pair (coherent length).

III. APPLICATIONS OF QUANTUM DOTS

Researches are going on for the implementation of quantum dots in the fields such as:

- single-electron transistor
- Implementations of Qbits for quantum Information processing
- Diode Lasers
- Optical Amplifier
- Biological Sensors
- Optical encoding and multiplexing applications
- *Single Electron Memory*
- *Nano-electronic Integrated Circuit (NIC)*
- *Quantum Cellular Automata*

The new generations of quantum dots have far-reaching potential for the study of intracellular processes at the single-molecule level, high-resolution cellular imaging, long-term in vivo observation of cell trafficking, tumor targeting, and diagnostics.

IV. INTRODUCTION TO QUANTUM COMPUTATION

Most of the driving force behind developing the first computers stemmed from an application

- Babbage - accurate logarithmic calculations
- Turing – assist in code breaking
- Zuse – computational devices for engineers

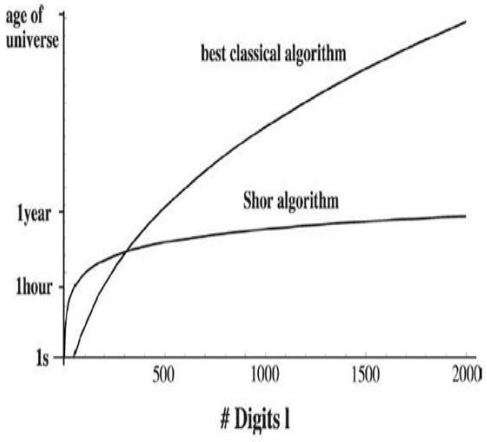
After Deutsch's publication, it would take 9 years before a strong application for a quantum computer would arise

a. Until 1994, only a few contrived mathematical problems would be investigated
b. In 1994, Peter Shor circulated a preprint of a paper in which he set out a method for using quantum computers to crack an important problem in Number Theory

We can list the important developments in this field as follows:

- 1982 - Feynman proposed the idea of creating machines based on the laws of quantum mechanics instead of the laws of classical physics.
- 1985 - David Deutsch developed the quantum turing machine, showing that quantum circuits are universal.
- 1994 - Peter Shor came up with a quantum algorithm to factor very large numbers in polynomial time.
- 1997 - Lov Grover develops a quantum search algorithm with O(√N) complexity

Shor's algorithm which is based on Quantum Computing can be compared by following figure:



Time required for classical factorization algorithm vs. quantum algorithm.

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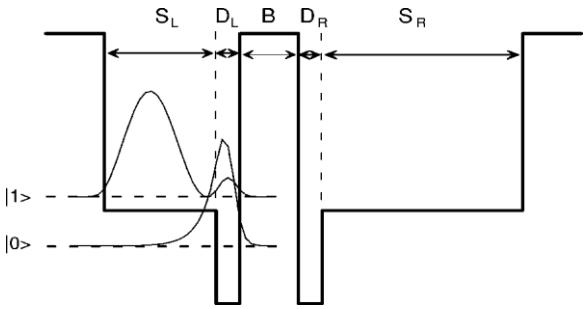
Factorization is required for the famous RSA algorithm for data security.

In recent papers, one can find many theoretical proposals for the implementation of quantum dots (QD) in quantum computation These proposals consist in application of either the orbital or spin states of electrons confined in the QDs. The orbital states of electrons in the coupled QDs were proposed for a possible realization of a quantum controlled-NOT (CNOT) gate. Spin states of coupled QDs are intensively studied as possible candidates for qubits and quantum logic gates due to the long relaxation time of Zeeman-split states in an external magnetic field. Performing a direct measurement, Hanson *et al.* demonstrated that the relaxation time of the spin states of the QD-confined electrons is sufficiently long to use these states as qubits in quantum computation. Hayashi *et al. reported* the coherent manipulation of spin qubits in laterally coupled QDs. The large number of theoretical papers on quantum computation with QDs, is in contrast with the small number of experimental studies. The discrepancy between the numbers of theoretical and experimental papers mainly results from the decoherence problem. In order to use the qubits as efficient information carriers and to perform a unitary time evolution of them we have to maintain the coherent quantum states for a time that exceeds by many orders of magnitude the quantum gate operation time. This requirement is very difficult to satisfy in solid-state devices.

Quantum logic operations:

We consider two electrons confined in two coupled asymmetric QDs. The barrier separating the QDs is taken to be sufficiently wide so that the tunneling of electrons between the individual QDs is neglected. Such a nanostructure can be formed, e.g., in a quantum wire, which is fabricated from different materials. We assume that the nanostructure possesses cylindrical symmetry and lateral confinement of the electrons, i.e., the confinement in the *x-y* plane, perpen dicular to the growth szd axis, is much stronger than the vertical szd confinement. The lateral confinement is approximated by a harmonic-oscillator potential and the vertical confinement has the form of asymmetric potential wells separated by the barrier



As a result we find CNOT Gate which act on computational basis states as follows:

$$U_{\mathrm{CNOT}}|00\rangle = |00\rangle,$$

$$U_{\mathrm{CNOT}}|01\rangle = |01\rangle,$$

$$U_{\mathrm{CNOT}}|10\rangle = |11\rangle,$$

$$U_{\mathrm{CNOT}}|11\rangle = |10\rangle.$$

Simillerly to get all gate functions a gate which operates on three qubits is called a ***Controlled Controlled NOT (CCN) Gate.*** Iff the bits on both of the control lines is 1,then the target bit is inverted.

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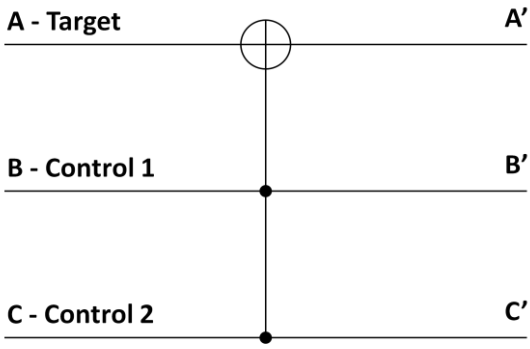

A	B	C	A'	B'	C'
0	0	0	0	0	0
0	0	1	0	0	1
0	1	0	0	1	0
0	1	1	1	1	1
1	0	0	1	0	0
1	0	1	1	0	1
1	1	0	1	1	0
1	1	1	0	1	1

V. FABRICATION METHOD OF QUANTUM DOTS

There are three primary methods of making a Quantum Dots with the goal to engineer potential energy barriers to confine electrons in 3 dimensions

- Lithography,
- Colloidal Synthesis, &
- Epitaxy.

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VI. EFFECT OF SIZE OF QUANTUM DOTS

5 nm dots: red - 1.5 nm dots: violet(QDs prepared by colloidal synthesis)

By changing size, shape, and composition, quantum dots can change their absorptive and emissive properties dramatically.

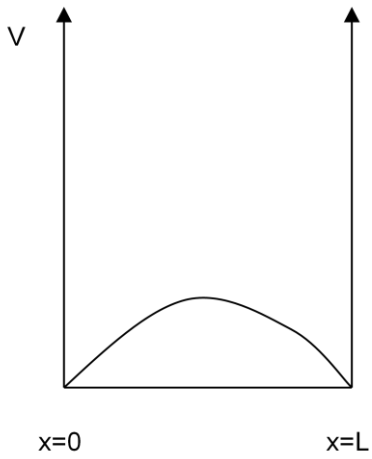
VII. METHOD OF SOLVING THE SCHRODINGER EQUATION

Quantum confinement produces discrete states Energy levels from solutions to Schrodinger Equation:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(r)\Psi = E\Psi$$

For 1D infinite potential well

$$\Psi(x) \sim \sin(\tfrac{n\pi x}{L}),\ \mathrm{n} = \mathrm{integer}$$



I am using direct relaxation method for calculating Eigen values and Eigen function using fourier method proposed by R. Kosloff:

Description of the method:

In quantum mechanics the state of the system is represented by wave function ψ, while the time evolution is governed by the schrodinger equation

$$i\frac{d\psi}{dt} = \hat{H}\psi$$

It consists of three steps, of which step one is setting up a grid and constructing on it an initial wavefunction. Grids in Cartesian as well as skewed, cylindrical or spherical coordinates can be used. Step two is the calculation of the Hamiltonian operation: φ equals to $\hat{H}\psi$

where $H = P^2/2m + V$

Because the potential energy operator V is local in coordinate space, its operation is a simple multiplication of the wavefunction at grid point i by V in grid point i.

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A similar procedure is possible for the kinetic energy operator if the wavefunction is represented in momentum space. The transformation to momentum space is done by a fast Fourier transform or by a fast Hankel transform for radial problems. The third step is to propagate the wavefunction in imaginary time. The solution of the time-dependent Schrodinger then becomes:

$$\psi(\tau) = e^{-\hat{H}\tau}\psi(0)$$

Where $\tau = it$. Expanding the initial wavefunction in eigenfunctions ψ_n, of the Hamiltonian:

$$\psi(\tau) = e^{-H\tau}\sum_n c_n \psi_n(0) = \sum_n c_n e^{-E_n\tau}\psi_n(0).$$

Examining this equation we find that each eigenfunction relaxes to zero at a rate which is proportional to its eigenvalue. This means that the ground state which relaxes most slowly, persists. As a consequence, after a time τ the component of the eigenfunction n is reduced relative to the ground state by the ratio:

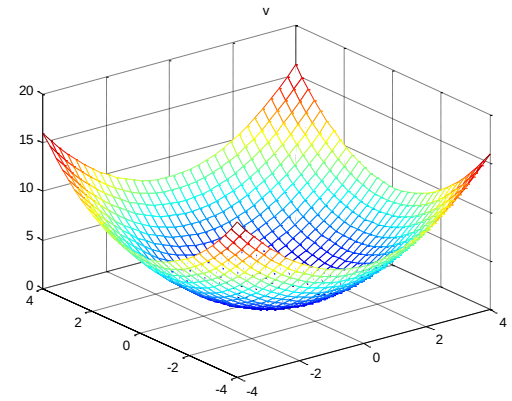
Obtaining excited states:

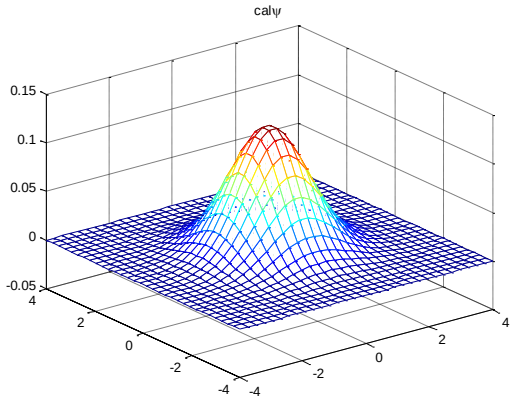
The first excited state is obtained by removing the ground state from the Hilbert space. This makes the first excited state the ground state of the new space.

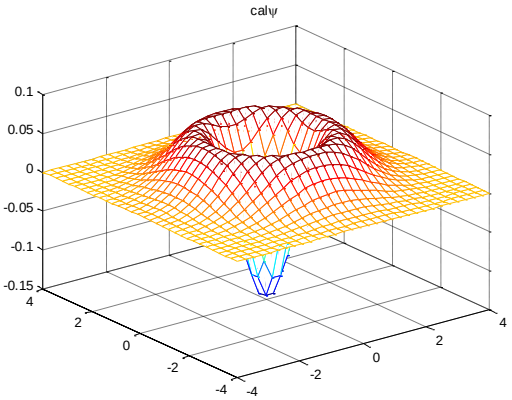
If $P_0 = |\psi_0><\psi_0|$ is the projector operator of the ground state, then the ground state of the operator:

$$\hat{H}_1 = (I - \hat{P}_0)\hat{H}(I - \hat{P}_0)$$

is the first excited state. This procedure is repeated, to obtain the next excited state by removing the first excited state. Continuing this procedure the ground state of the operator is the nth excited state can be calculated.







These figures I have taken from the matlab program I have developed. Figure 1 is showing the potential well, 2 is showing ground state wavefunction, and 3 is showing the first excited state.

I have taken many shape of the confinement potential, which is basically representing the shape of Quantum Dots.

Quantum Dots fabricated by modern semiconductor nanotechnology possess various shapes. Semiconductor nanocrystals with nearly spherical boundries emedded in insulating materials are examples of spherical QD's. Excess electrons confined in nanometer-sized QD's can form bound atomiclike states. The confinement potential, which

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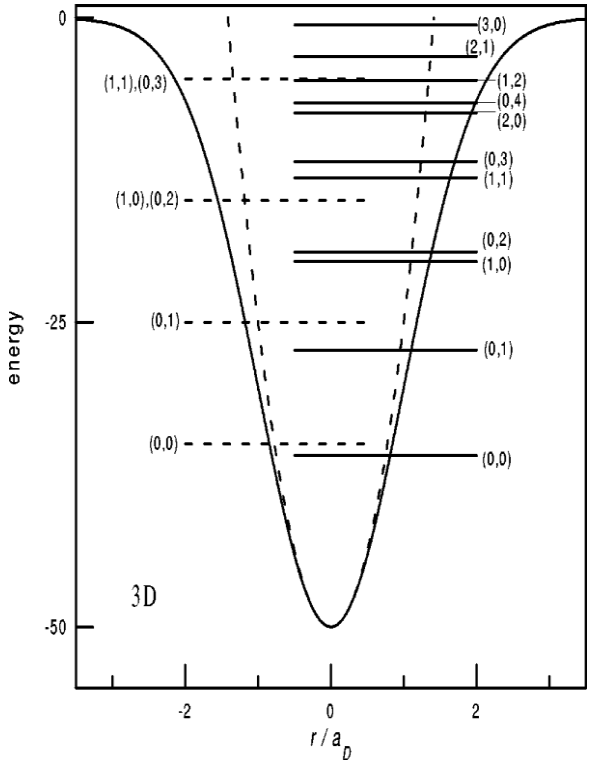
results from a conduction- band discontinuity at the QD boundary and external voltages applied to the nanostructure, is usually approximated by a three dimensional potential well.



One-electron energy levels for the Gaussian (solid lines) and harmonic-oscillator (dashed lines) 3D potential.
The energy levels are labelled by quantum numbers (n,l).
The shapes of both the potential energies are also shown as functions of distance r from the QD center.

REFERENCES

1. J. H. Davies, “The Physics Of Low-Dimensional Semiconductors, An Introduction” Cambridge University Press.
2. S. Datta, “Electronic Transport In Mesoscopic Systems” Cambridge University Press.
3. J. Adamowski, S. Bednarek, B. Szafran “Handbook of Semiconductor Nanostructures and Nanodevices” ISBN: 1-58883-074-8.
4. Quantum Computing by Joseph Stelmach
5. Quantum Dots By Timothy Paik Marcus Dahlstrom Michael Nip
6. Overview of Spin-based Quantum Dot Quantum Computation by Xuedong Hu*and S. Das Sarma phys. stat. sol. (2003)
7. Controlled exchange interaction for quantum logic operations with spin qubits in coupled quantum dots S. Moskal, S. Bednarek,* and J. Adamowski PHYSICAL REVIEW A 76, 032302 2007
8. Synthesis and Analysis of Quantum Dots by Karen S. Quaal[1], Justin LaRocque, Shazmeen Mamdani, Luke Nally, Jennifer Z. Gillies and Daniel Landry' Siena College, Loudonville, NY, (2) Evident Technologies
9. B.Szafran, E. Barczyk, F.M. Peeters, S. Bednarek, "Exciton spectra in vertical stacks of triple and quadruple quantum dots in an electric field" Phys. Rev. B 77, 115441 (2008).
10. [S. Bednarek, B. Szafran " Energy dissipation of electron solitons in a quantum well" Phys. Rev. B 73, 155318 (2006).
11. [Szafran, T. Chwiej, F. M. Peeters, S. Bednarek,J. Adamowski, and B. Partoens " Exciton and negative trion dissociation by an external electric field in vertically coupled quantum dots " Phys. Rev. B 71, 205316 (2005).
12. S. Kapoor, J. Kumar, and P. K. Sen “Optical coherent transient effects in magnetoactive GaAs/AlGaAs quantum well structure” Journal Of Applied Physics 95, (2004).
13. J. Kumar, S. Kapoor, S. K. Gupta, and P. K. Sen, “Theoretical investigation of the effect of asymmetry on optical anisotropy and electronic structure of Stranski-Krastanov quantum dots” Phys. Rev. B 74, 115326 (2006).
14. S K Gupta, S Kapoor, J Kumar and P K Sen, “Strain-induced effects on optical properties of magnetized Stranski–Krastanov quantum dots”, Nanotechnology 18, 325402 (2007).

| ISSN: 2582-7219 | www.ijmrset.com |

| Volume 3, Issue 10, October 2020 |

15. X. Hu and S. D. Sharma, “Overview of Spin-based Quantum Dot Quantum Computation” phys. stat. sol. (2003).
16. J. Adamowski, S. Bednarek, and B. Szafran " Quantum Computing with Quantum Dots " Schedae Informaticae 14, 95-111 (2005).
17. S. Bednarek, B. Szafran, "Spin rotations induced by an electron running in closed trajectories in gated semiconductor nanodevices" Phys. Rev. Lett. 101,216805 (2008).
18. T. Chwiej, S. Bednarek, B. Szafran, J. Adamowski, F.M. Peeters "Broken one-particle symmetry in few-electron coupled quantum dots" Phys. Rev. B 73, 075422 (2006).
19. S.Moskal, S.Bednarek, J.Adamowski, "Controlled exchange interaction for quantum logic operations with spin qubits in coupled quantum dots" Phys. Rev. A 76, 032302 (2007).
20. S.Bednarek ,B.Szafran, K. Lis, J.Adamowski "Modeling of electronic properties of electrostatic quantum dots" Phys. Rev. B 68 155333 (2003).
21. S.Bednarek ,B.Szafran, T.Chwiej, J.Adamowski "Effective interaction for charge carriers confined in quasi-one-dimensional nanostructures" Phys. Rev. B 68 45328 (2003).
22. S. Moskal, S. Bednarek, and J. Adamowski " Time-evolution simulation of a controlled-NOT gate with two coupled asymmetric quantum dots " Phys. Rev. A 71 062327 (2005).