

# DUBNA-NANO2012



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Section

**QUANTUM DOTS**

**BINDING ENERGIES OF  $D^0$ ,  $D^-$  CENTERS AND RESULTANT DIPOLE  
MOMENT OF  $D^-$  CENTER IN SEMICONDUCTOR QUANTUM DOT WITH  
GAUSSIAN CONFINEMENT**

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The stability of  $D^0$  and  $D^-$  centers in a three-dimensional quantum dot is investigated by a variational method with a very simple wave function containing a Jastrow-like factor. The ground state binding energies are calculated as a function of the quantum dot radius, and the confinement strength and compared with the results available in the literature. It is observed that the energies of  $D^0$  and  $D^-$  systems decrease as the dot size increases. The binding energies of  $D^0$  and  $D^-$  complexes however increase as the dot size decreases in the beginning and then reach a maximum value and finally decrease with further decrease in the dot size. Our results are found to be in good agreement with those obtained from the exact matrix diagonalization method. The resultant dipole moment of a  $D^-$  complex is also calculated for different potential strengths as a function of quantum dot size.

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## ENTANGLEMENT OF ELECTRON ORBITAL MOTION IN OPEN TWO-ELECTRON QUANTUM DOTS

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Recently we developed an analytical approach to study quantum properties of electrons in an exactly solvable model of an isolated two-electron QD in a magnetic field [1]. In this model, electrons were assumed to move in a two-dimensional parabolic confining potential under the perpendicular magnetic field. The interaction between electrons was approximated by the effective harmonic potential of the Johnson–Payne type. We performed a detailed study of the degree of the orbital entanglement of the QD ground state and its first excited states for various values of a QD shape, the strength of the interaction and the magnetic field [2].

In the present report, we investigate effects of decoherence in an open QD coupled with its environment. We analyse the degradation of electron entanglement depending on the temperature of environment and the QD parameters.

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## ELECTRON TUNNELING IN DOUBLE QUANTUM RINGS AND DOTS

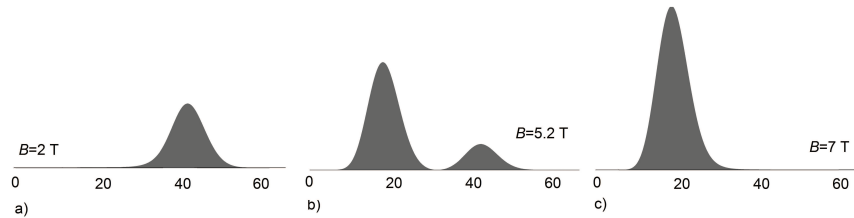
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We are investigating electron wave function localization in double quantum rings (DQR) [1] and dots (DQD). The electron tunneling under a perpendicular magnetic field is considered for weakly coupled double quantum ring, a possible situation occurs when the single electron energy levels associated with different rings may cross. Degeneracy is avoided by anti-crossing of corresponding levels of DCQR. We show that in this DCQR the electron spatial transition between the rings occurs due to the electron level anti-crossing [2]. The anti-crossing of the levels with different radial quantum numbers and equal orbital quantum numbers provides conditions for the electron tunneling between rings. Results of numerical simulation for the electron transition are presented for the DCQR with the geometry parameters corresponding to experimentally fabricated DCQR in [1] (see Fig. 1). We also studied the spatial transition of both electrons and holes in double lateral quantum dots and rings when placed in an electric field that lies along the x-axis.



**Figure 1.** Profiles of the normalized square wave function of electron in DQR for different magnetic field  $B$ . Electron is located a) in outer ring, b) in whole volume of DQR and c) in inner ring. The radial coordinate is given in nm. The quantum numbers of the states are (1-1), outer and (1,-1), inner for a) and c), respectively.

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## SPECTRAL AND OPTICAL CHARACTERISTICS OF SPHEROIDAL QUANTUM DOTS

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In effective mass approximation for electronic (hole) states of spheroidal quantum dots (SQDs) with and without external fields are constructed in the framework of Kantorovich and adiabatic methods [1]. Absorption coefficients for ensemble of SQDs are calculated by using of the eigenvalues and eigenfunctions. Comparison analysis of absorption coefficients for oblate and prolate SQDs reveals different behavior vs aspect ratio of minor to major semiaxis (see Figure 1). Possibility of verification of considered models is discussed.

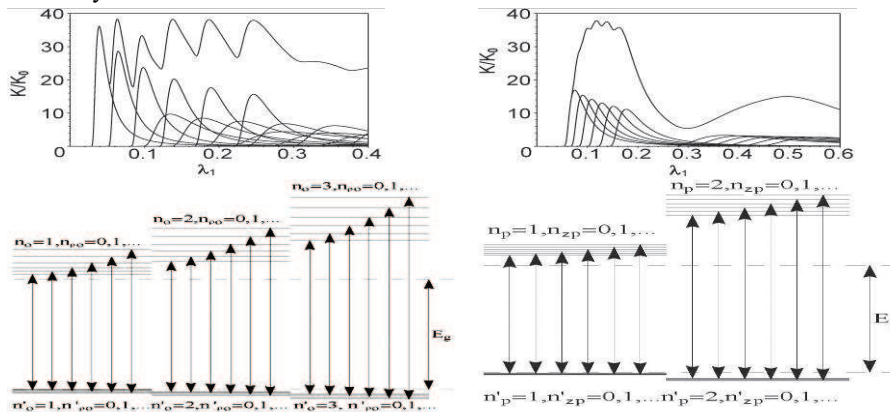


Figure 1. Absorption coefficient  $K/K_0$  consists of sum of the partial contributions vs the energy  $\lambda_1 = (\hbar\omega - E_g)/E_g$  of the optic interband transitions (ITs) for the Lifshits-Slezov distribution (upper) and plots of ITs (lower) for ensemble of oblate (left) and prolate (right) GaAs SQDs with  $c = 0.5$ ,  $a = 2.5$  and  $\bar{a} = 0.5$

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## SEMICONDUCTOR AND GRAPHENE QUANTUM DOTS

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We describe progress in theory and experiments on semiconductor and graphene quantum dots with potential applications in nanoelectronics, nanospintronics, nanophotonics and quantum information processing. The lateral quantum dots defined using metallic gates in GaAs/GaAlAs field effect transistor are one of the most advanced artificial quantum systems in solid state. We will describe a stability diagram and spin blockade in triple quantum dot molecule with controlled electron numbers in each dot[1], discuss potential use of such a molecule in entanglement and Berry's phase generation[2], chirality based qubits[3] and as building block of a FET with a macroscopic quantum groundstate[4]. We next turn to hybrid systems of self-assembled semiconductor CdTe quantum dots containing single magnetic impurities. Such impurities can be thought of as an atomic limit of quantum memory directly integrated into a semiconductor host. We show that the optical detection and manipulation of impurity spins is governed by the quantum interference between the electron, hole and impurity spin[5,6]. Finally, we discuss one atom thick semiconductor quantum dots made of graphene[7-10] or MoS<sub>2</sub>[11]. We show that their electronic, optical and magnetic properties can be engineered by the size, shape, type of edge and number of layers[7-10]. We focus on their optical and magnetic properties, and their control with external gate, electric field and photons. Possibility of realizing a fully integrated carbon-only quantum circuit will be discussed.

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## MAGICS FOR MAGNETIZED FERMI DROPLETS OF NM&FM SIZES

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Shell effects arise whenever the Fermi particles are confined to a finite spatial volume due to quantization phenomena. Such features are usually displayed as oscillations of various observables around its smooth behavior as a function of a size of, e.g., nano-crystals, atomic clusters and nuclei, and/or quantum dots referred for, hereafter, as the Fermi droplets (FDs).

Magnetic field brings new dimension to shell oscillations. In this contribution we analyze similarities and difference in magnetization of atomic clusters and nuclei, i.e., nm and fm size droplets. As is shown recently [1,2] shell effects dominate magnetic phenomena for fermionic aggregates of sufficiently small size. We incorporate the harmonic oscillator spectrum to analyze FD magnetism. As is demonstrated the oscillations of thermodynamic potentials (i.e., the binding energy at zero temperature) as a function of field strength represent perhaps the most interesting universal feature of magnetic reactivity. The Zeeman splitting in varying magnetic fields originates such a behavior.

The change in the level structure caused by magnetic field results in rather different field dependence of relative binding energy for magic and anti-magic systems at vanishing field. At increasing strength  $H$  in the range of relatively "small" fields the binding of magics is weakened, while the anti-magic aggregates become more bound. Such a behavior is related to magic--anti-magic switching [2] in fermionic shell structure at varying magnetic field.

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## ON THE SYMMETRY OF THE ELECTRONIC DENSITY IN THE THREE-ELECTRON PARABOLIC QUANTUM DOT

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An effective analysis of the electronic structure of quantum dots requires the knowledge of the basis properties of their wave functions. Namely, one should be able to make such a choice of the arguments of the wave function so that its variation with respect to some (“fast”) variables will be much larger than the variation with respect to the other (“slow”) variables.

In the few-body Coulomb problem it is usually believed that the hyperradius is the slow variable. It will be shown that in the case of circular parabolic three-electron quantum dots the slow variable is one of the hyperangles from the set of Gronwall-Dalitz-Fabri coordinates [1, 2, 3].

The consideration is based on the direct numerical diagonalization of the Hamiltonian using the basis of Fock-Darwin states [4]. Then, the technique of Dalitz plots [2] has been used to visualize the electronic density in the three-electron circular parabolic quantum dot.

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## CORRELATION EFFECTS IN VERTICAL TWO-ELECTRON QUANTUM DOTS IN A MAGNETIC FIELD

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Can a mesoscopic system with a few particles moving in one-body potential exhibit a quantum phase transition (i.e. a phase transition driven by quantum fluctuations) due to two-body interaction? The related question is, if such a transition occurs, what are the concomitant structural changes? Two-electron quantum dots (QDs) being mesoscopic systems have drawn a great deal of experimental and theoretical attention in recent years. In particular, this interest is due to the fact that QDs may provide answers on the above questions.

Using a three-dimensional (3D) parabolic approximation for a confining potential, two-electron QDs in magnetic field are studied for various strengths of the electron-electron interaction. We found that in 3D QDs, the Wigner molecule formed in the ground state can be localized only in the lateral plane even for very strong magnetic fields, in contrast to excited states which electron density distributions may take orientation along the direction of the applied magnetic field.

To get a deep insight into this phenomenon we analyse the entanglement for the ground and for a few excited states. We found that these states become more entangled when the electron-electron interaction becomes stronger. As a general trend, we also observe that the entanglement of the eigenstates tends to increase with the states's energy. There are, however, entanglement level-crossings where the entanglement of a state becomes larger than the entanglement of other states with higher energy. In particular, at a specific magnetic field value the dot attains a spherical symmetry [1]. The transition from the axial to the spherical symmetry manifests itself as a drastic change of the entanglement of the lowest state with zero angular momentum projection. The entanglement of this state, being first a decreasing function of the magnetic field, starts to increase after the transition point with the increase of the magnetic field. This behaviour can be associated with a topological transition from the lateral to the vertical localization of the two-electron probability density for this state in the QD. **References**

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## MATHEMATICAL MODELING OF INTRINSIC JOSEPHSON JUNCTIONS WITH CAPACITIVE AND INDUCTIVE COUPLINGS

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Intrinsic Josephson junctions (IJJ) in high temperature superconductors attract much interest due to the perspective of generation of coherent radiation in terahertz region and different applications in superconductive electronics. Up to now, several papers on numerical study of sine-Gordon equations describing vortex dynamics and electromagnetic wave radiation in IJJ with inductive coupling are published (see Ref.[1]). Current voltage characteristics (CVC) of IJJ with capacitive coupling were also intensively investigated (see for example Refs.[2, 3]). However, CVC of IJJ with both types of couplings were not investigated before and parametric resonance in this system [4] has never been examined.

In this paper we developed a method for simulation of CVC of IJJ with two types of couplings between junctions: capacitive and inductive. A system of coupled sine-Gordon equations is solved by different methods. We show the distribution of the magnetic field and voltage as a functions of coordinate and time at different values of bias current. Results of detailed investigation of the effect of model parameters on CVC are presented. The influence of inductive coupling on parametric resonance in coupled Josephson junctions is discussed.

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## EFFECT OF CORRELATION AND RASHBA INTERACTION ON THE ENERGY LEVELS OF PARABOLICALLY CONFINED QUANTUM DOT

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We present a theoretical study of the ground state energy of a parabolically confined quantum dot in the presence of the Rashba spin-orbit interaction (SOI) and electron-electron interaction in an external magnetic field. With a simple and physically reasonable model potential for electron - electron interaction term, we have solved the problem exactly. Our results indicate that the presence of SOI reduces the total energy of the system quadratically. With increasing number of electrons in the system, the reduction in energy due to SOI becomes stronger. The effect of SOI becomes more significant at larger magnetic fields. Electron – electron interaction increases the total energy of the system. It increases quadratically with the number of electrons in the system. Also electron – electron interaction energy increases linearly with an increase in external magnetic field. Our results are found to be in excellent agreement with exact numerical solutions reported in the literature.

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## PERSISTENT CURRENTS IN VERTICALLY COUPLED QUANTUM DOTS

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The system of Kohn-Sham equations for vertically coupled quantum dots in strong magnetic field  $B$  with the number of spin-polarized electrons  $N$  from 2 to 100 was solved numerically. Many-body effects are taken approximately into account by the use of local intra-layer exchange energy. The dots are identical and two-dimensional. Calculations for different values of the tunneling gap and the distance  $d$  between the quantum dots were carried out.

It is shown that the dependence of the angular moment of electrons from magnetic field represents a series of a plateau. In the strong coupling regime the period of oscillations of persistent current  $I$  is well described by the formula

$$\Delta B = 2B_1 / (N+1), \quad (1)$$

where  $B_1$  corresponds to the middle of the first plateau.

For large values of  $d$  quantum dots become independent and the period of oscillations of persistent current is described by the formula (1) for each quantum dot. At intermediate values of  $d$  dependence of  $I(B)$  inside of each period becomes nonmonotonic. This is due to the fact that the transitions of electrons between symmetric state and antisymmetric state are possible as the magnetic field changes.

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## **X-RAY STUDIES OF ZNO NANOPARTICLES BY WILLIAMSON-HALL AND SIZE-STRAIN PLOT METHODS**

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ZnO nanoparticles (ZnO-NPs) were prepared by a sole-gel combustion method from a zinc acetate precursor and acetic acid. The ZnO-NPs were synthesized at calcination temperatures of 650 C° and 750 C° for 1 h. The synthesized ZnO-NPs were characterized by X-ray diffraction analysis (XRD) and TEM. The XRD results revealed that the sample product was crystalline with a hexagonal wurtzite phase. High magnification transmission electron microscopy (TEM) showed single-crystal ZnO-NPs with nearly spherical shapes. The crystalline development in the ZnO-NPs was investigated by X-ray peak broadening. The Williamson-Hall (W-H) analysis and size-strain plot method were used to study the individual contributions of crystallite sizes and lattice strain on the peak broadening of the ZnO-NPs. The physical parameters such as strain, stress and energy density values were calculated more precisely for all the reflection peaks of XRD corresponding to the wurtzite hexagonal phase of ZnO lying in the range of 20°-100° from the modified form of the W-H plot assuming a uniform deformation model (UDM), uniform stress deformation model (USDm), uniform deformation energy density model (UDEDm) and by the size-strain plot method (SSP). The results obtained showed that the mean particle size of the ZnO NPs estimated from the TEM, W-H analysis and the SSP method were highly intercorrelated.