行政院國家科學委員會專題研究計畫期中（第一年）報告

半導體奈米元件的軌道與電子自旋磁性

Orbital and spin magnetism in semiconductor nano-objects

計畫編號：NSC 97-2112-M-009-012-MY3

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一 摘要 (Abstract)

英文

This report summarizes the major results obtained from the first year program of the ”Orbital and spin magnetism in semiconductor nano-objects” project. Two directions of research have been pursued, as described in detail in the report: problems of a general description of the magneto-optical response form systems of semiconductor nano-objects with unusual orbital magnetism and the first stage of analysis of the magnetic qubit implementation in non-magnetic semiconductor nano-object. In addition we proposed a computational method which allows us to map realistic geometry and material content (known from experiments) of semiconductor nano-objects on smooth three dimensional potentials for electrons and holes confined in the object. Several publications were performed based on this year’s results.

中文

這份報告總結了第一年計畫 "半導體奈米元件的軌道與電子自旋磁性" ， 報告有兩個研究方向 ： 特殊軌道磁性半導體奈米結構的磁光反應通用描述 ，非磁性半導體奈米結構的磁量子位元初階分析，此外我們提出一種精細的三維計算方法去估算半導體奈米結構中的電子與電洞的波函數與對應能量，模型考慮了真實結構形狀與材料成分產生的平滑位能，研究成果已經有數個發表。

二 General description of the magneto-optical response form systems of semiconductor nano-objects with unusual orbital magnetism

We discuss fist a general computational hybrid multi-scale (hierarchical) mmethod which allows us to simulate the coherent manipulation of the quantum mechanical states of electrons and holes confined in semiconductor nano-objects and monitor the manipulation by means of traditional magneto-ellipsometry. In our hybrid discrete-continuum model (Wijers at al., 2006) each embedded nano-object gets represented by a single discrete dipole, characterized by a bare excess polarizability. This polarizability includes the screening by the surrounding continues dielectric medium. To obtain the collective optical response one should solve the system of equations similar to known from the discrete-dipole approximation (Fig. 1). Our general method allows us to simulate the nano-objects of arbitrary shapes. We have shown that parameters of the electron and hole quantum states localized in the nano-objects can be retrieved from the collective magneto-optical response of systems of such nano-objects. As an example of the method implementation we consider impact of the coherent manipulation of electronic states in the double vertical lens-shaped circular quantum dot molecule on the collective magneto-optical response from a layer of those nano-objects (see Fig.2). The manipulation is performed by an external magnetic field applied upon InAs/GaAs quantum dot molecules assembled from the dots with substantially different lateral radii. We treat the semiconductor quantum dot molecules within complete three-dimensional description which allows us to simulate arbitrary directions of the external magnetic field (Fig. 2) in contrast to most of the calculations done before. It brings up much wider opportunities to dynamically manipulate electron and hole states in quantum dot molecules. Recently it was demonstrated that in the asymmetrical quantum dots molecules the non-uniform diamagnetic shifts of the lowest electron energy levels lead to their anticrossing which yields in a positive peak of the differential magnetic susceptibility of the system (O. Voskoboynikov, 2008) . In this work we show unusual consequences of the electronic non-uniform diamagnetic shifts for the magneto-optical transitions (Fig. 3) and corresponding overlap integrals (Fig. 4). The described above effects very clearly result in the ellipsometric angles Ψ and Δ for the light reflected from the layers on the semiconductor quantum dot molecules (Fig. 5). As it was already mentioned changes in magneto-optical response of a layer of quantum dot molecules emerge from the changes in the quantum mechanical configuration of the molecules. The direct accessibility of the quantum information from the QDMs such as individual dipole strengths, transition energies, and overlap integrals by means of the measurement of the ellipsometric parameters is one of the attractive aspects of our approach.

三 Magnetic qubit implementation in non-magnetic semiconductor nano-object

The coupling and entangling control in quantum dot molecules can be performed by variation of the distance between dots (static tuning) or external fields (dynamic tuning). In this work we theoretically study coherent manipulation of electronic states in an asymmetrical quantum dot molecule performed by changing external magnetic field. A magnetic qubit manifests itself by turning the magnetic susceptibility of the quantum dot molecule into the paramagnetic domain. This result is particularly interesting because the system is built from diamagnetic semiconductor materials. We consider a system of two vertical lens-shaped circular InAs/GaAs quantum dots (Fig. 2). The calculations are done for the full three-dimensional model of InAs/GaAs QDM with the hard-wall confinement potential. This allows us to simulate the magnetic dependence of the electron energy states in a system of very asymmetrical shape: the quantum dots have substantially different diameters (19 and 50 nm) and different heights in contrast to most of the known simulations. In our approach we use realistic semiconductor material parameters (for instance the band offset of the InAs/GaAs strained heterostructure, corrected to the strain conditions band parameters, etc.). For our system (with a relatively large inter-dot distance) we can consider two iso-spin states, in which the electron occupies the lower or upper dot. When the two states are energetically close and the temperature is low we can omit other upper states in the quantum dot molecule and the system can be approximated by a two-level model (qubit). The non-uniform diamagnetic shift of the lowest energy levels in different dots leads to their anti-crossing and the relocation electronic wave ground state functions from lower dot to upper dot. This can be presented as an operation with a magnetic iso-spin qubit (Fig. 6). A few single-qubit quantum gates can be performed. The magnetic susceptibility of the system is reflecting the iso-spin configuration and can be used to observe the coherent manipulation of the qubit (Fig. 7). It follows from this theoretical study that experimental investigation of the magnetic properties of asymmetrical quantum dot molecules will yield interesting results for further development of the quantum informatics.

四 Realistic geometry and material content mapping on smooth three dimensional potentials in semiconductor nano-objects

A number of methods for simulation of the egienstates and wave functions of electrons in semiconductor nano-objects have been proposed and developed. Most of them require very large scale computation including complex chemical, mechanical, and structural modeling. But, if we want to study physical properties of the nano-objects it is very important to go far beyond the solutions of the basic egienvalue problems. Therefore, there is a need on a method which efficiently generates physical properties of the nano-objects on the base of cumulative experimental knowledge of their geometrical, structural, and material composition.

In this work we propose a computational method which allows us to map realistic geometry, strain and material composition of semiconductor nano-objects (known from experiments) on smooth three dimensional potential's and parameter's profiles for electrons confined in the objects. The method allows us very efficiently and economically to simulate and study physical properties of semiconductor nano-objects within a wide range of the parameter's change (Fig. 8). To demonstrate the method efficiency in this paper we consider the application of the mapping procedure to the simulation of the magnetization of a single electron asymmetrical InAs/GaAs nano-ring (Fig. 9). The resulting mapped confinement potential for electrons in the nano-ring is shown in Fig. 10. It carefully reproduces all known three-dimensional experimental geometry and composition data. A three-dimensional mapped effective Hamiltonian for electronic band was derived and used in simulation of the magnetic response of InAs/GaAs nano-rings. Our method us efficiently and economically to simulate and study physical properties of semiconductor nano-objects and adjust important parameters of them.

Publications:

1. Thu Le Minh and O. Voskoboynikov, “Magneto-optics of layers of double quantum dot molecules”, submitted to Physical Review B (2009).
2. O. Voskoboynikov, "Hybrid Model for Simulation of Magneto-Optical Response of Layers of Semiconductor Nano-Objects", accepted like an invited paper to the International Journal for Multiscale Computational Engineering, to be published in 2009.
3. C. M. J. Wijers and O. Voskobyonikov, "Magnetic qubit in a non-magnetic semiconductor quantum dot molecule", invited and submitted to the Journal of Computational and Theoretical Nanoscience, planed to be published in 2009.
4. Thu Le Minh and O. Voskoboynikov, " Magneto-Optics of Layers of Semiconductor Double Quantum Dot Molecules Like a Source of Quantum Mechanical Information ", accepted for oral presentation in the Int. Conf. on Computational Methods for Coupled Problems in Science and Engineering, Italy, June , 2009.
5. 2. Thu Le Minh and O. Voskoboynikov," Magneto-optics of two-dimensional arrays of embedded semiconductor quantum dot molecules ", accepted to the 18th International Conference on Electronic Properties of Two-Dimensional Systems, Japan, Kobe, July , 2009.
6. Thu Le Minh and O. Voskoboynikov, " Unusual diamagnetism in semiconductor nano-objects ", accepted to the 14th International conference on Narrow Gap Semiconductors and Systems, Japan, Sendai, July, 2009.
7. L. M. Thu, W. T. Chiu, Shao-Fu Xue, and O. Voskoboynikov, "Binding energy of magneto-biexcitons in semiconductor nano-rings", accepted to the 14th International conference on Narrow Gap Semiconductors and Systems, Japan, Sendai, July, 2009.
8. O. Voskoboynikov, “Theory of diamagnetism in an asymmetrical vertical quantum dot molecule”, Physical Review B, vol. 78, no.11, pp. 113310-1-4, Sep. (2008).
9. Thu Le Minh and O. Voskoboynikov, "Magneto-optics of layers of triple quantum dot molecules", Physica Status Solidi B 246, No. 4, 771– 774 (2009).
10. Thu Le Minh and O. Voskobyonikov, “Optical Response of Layers of Embedded Semiconductor Nano-Objects: From Quantum Mechanics to Ellipsometry and Back”, The IEEE Nanotechnology Materials and Device Conference, Kyoto, Japan, Oct. (2008).

Figures:

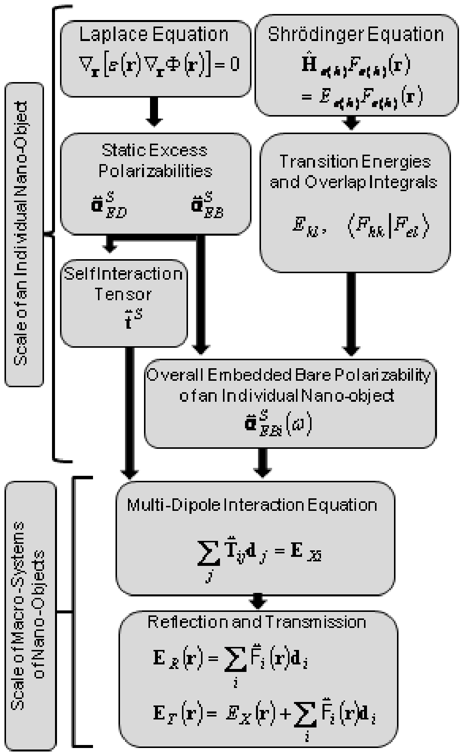

Fig. 1. Flow diagram of the model implementation.

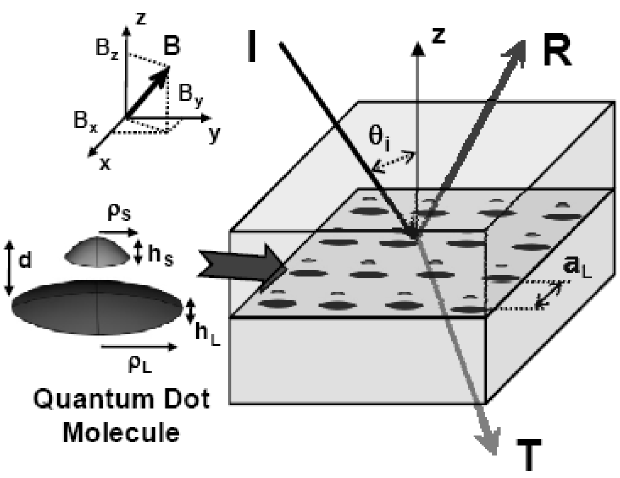

Fig. 2. Schematic of the magneto-optics of a layer of embedded semiconductor quantum dot molecules.

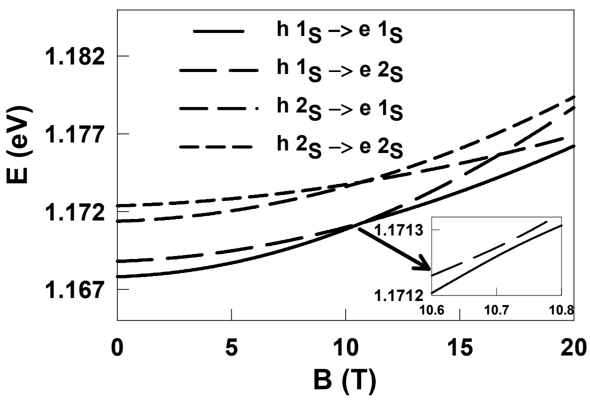

Fig. 3. Lowest transition energies in the double dot molecule as functions of magnetic field B||z. Inset: the anticrossing region.

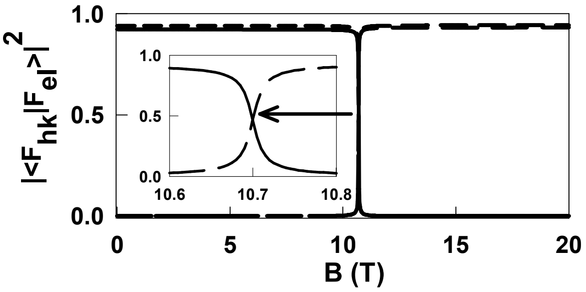

Fig. 4. Overlap integrals for the lowest transition energies in the double dot molecule as functions of magnetic field B||z. Inset: the anticrossing region.

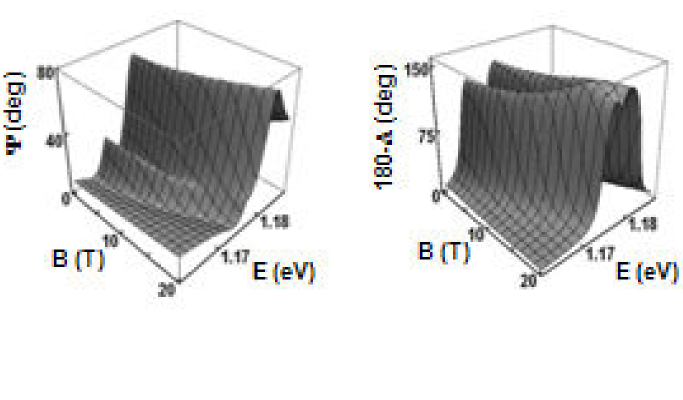

Fig. 5. Ellipsometric angles of a layer of quantum dot molecules.

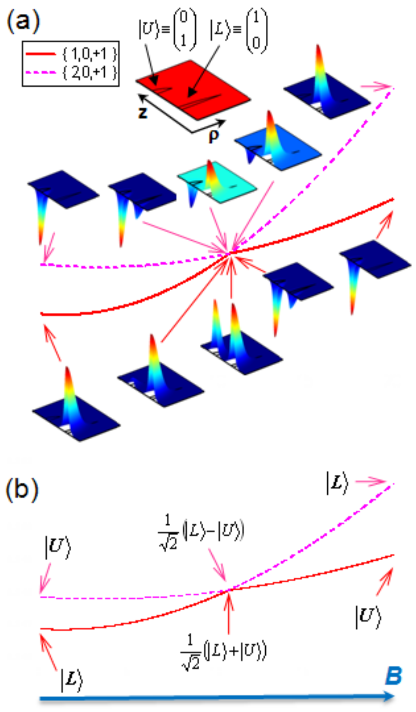

Fig. 6. Schematic of the dynamic coherent manipulation of (a) the electronic wave functions and (b) magnetic qubit in the asymmetrical quantum dot molecule.

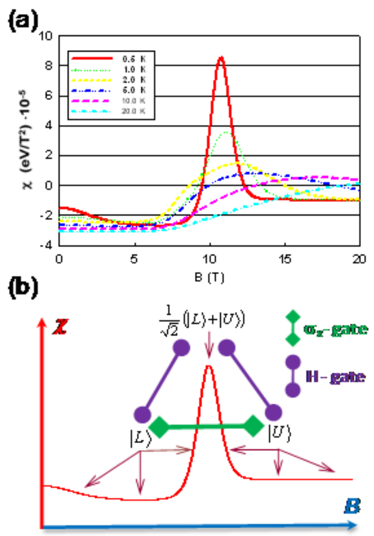

Fig. 7. Schematic of the quantum gate's realization in the asymmetrical quantum dot molecule: (a) magnetic susceptibility of the single electron asymmetrical double dot molecule at different temperatures; (b) quantum gate's control.

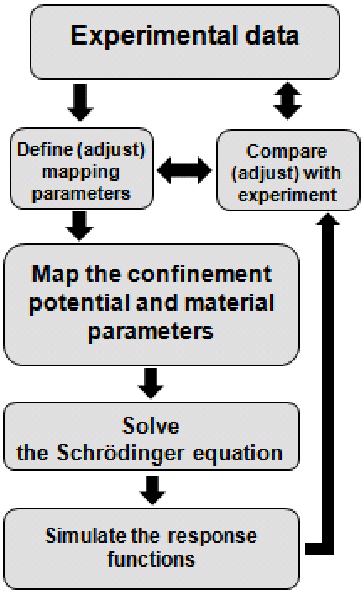

Fig. 8. Flow diagram of the mapping procedure.

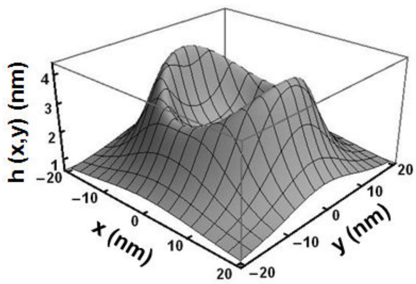

Fig. 9. Geometry of an asymmetrical nano-ring.

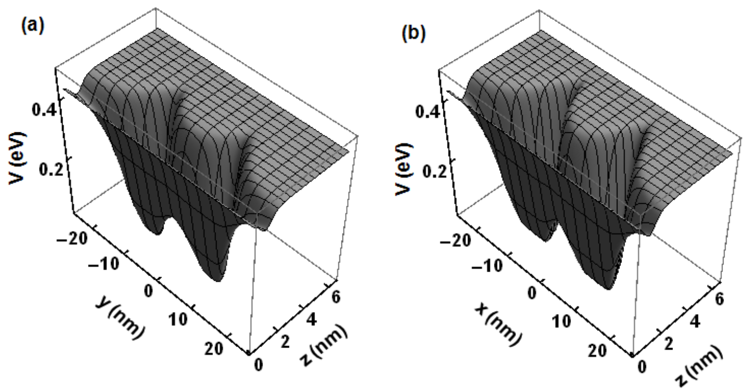

Fig. 10. Two projections of the confinement potential on (a) (0,y,z) and (b) (x,0,z) planes