Physica B 481 (2016) 179–184

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Effects of impurity on the energy spectra of quantum-dot lithium

Z.D. Vatansever [a,b,*], S. Sakiroglu [a], K. Akgungor [a], I. Sokmen [a]

[a] Department of Physics, Faculty of Science, Dokuz Eylül University, 35390 İzmir, Turkey
[b] Dokuz Eylül University, Graduate School of Natural & Applied Sciences, 35390 İzmir, Turkey

ARTICLE INFO

Article history:
Received 9 January 2015
Received in revised form
17 September 2015
Accepted 3 November 2015
Available online 10 November 2015

Keywords:
Quantum dot
Impurity
CI method

ABSTRACT

In this work, the effects of an off-center attractive Gaussian impurity on the ground-state energy and spin properties of parabolic quantum-dot lithium are investigated with Configuration Interaction Method. Phase transition between spin-1/2 and spin-3/2 states of the system is obtained for various strengths of the impurity potential and the electron–electron interaction. Charge densities of the system are studied in different interaction regimes. Numerical results reveal that the gap between two spin states is increased by the impurity which consequently yields to the suppression of the polarization.

1. Introduction

Owing to the rapid development in semiconductor technology, it is possible to create quantum dots (QDs) with few-electrons by laterally confining two-dimensional electron gas in semiconductor heterostructures [1,2]. The shape of the QDs can be designed such as rectangular, triangular and elliptic but two-dimensional disk-shaped QDs, whose confinement potential can be modeled as parabolic potential, are mostly considered [3]. Because of the circular symmetry of the parabolic confinement, clean QDs have single-particle energy spectrum with two-dimensional shell structure and degeneracies at zero magnetic field. Also, in some single-electron transport measurements of QDs, lifted degeneracies and some anticrossings are observed that is interpreted as the existence of both attractive and repulsive type impurities, which breaks the circular symmetry of the system [4,5].

QDs have attracted much attention due to their applications in optoelectronic device technology, such as photo-dedectors, QD-based lasers, solar cells [6]. From the theoretical point of view, the competition between external confinement and the electron–electron interaction leads to a complicated many-body problem. Thus, the accurate description of electronic properties of these systems depends strongly on the theoretical method being used. Mean-field approaches such as Hartree–Fock [7,8] and Density Functional Theory (DFT) [9–11] have been widely used especially, for QDs with large number of electrons. However, energy and charge density distribution obtained from mean-field approaches cannot accurately describe the system in strongly correlated regime [1]. Configuration Interaction (CI) method is extensively applied to obtain the ground and also excited state energies and wave functions of QDs [12–17]. Since the dimension of the Hamiltonian matrix grows rapidly with the electron number (N) in the system, this method is applied to quite symmetric systems with small N ($N \leq 8$) [16]. Besides, Quantum Monte Carlo (QMC) method is proved to be very powerful when treating the many-electron systems in a wide range of electron–electron interaction strength [18–21]. In comparison with CI method, larger quantum dot systems can be examined with QMC methods despite the fermion sign problem.

Parabolic QDs exhibit various properties for different values of the ratio λ between the electron–electron interaction and the strength of the confining potential, which can also be varied experimentally. When the electron density decreases, the correlation effects become strongly dominant and the system passes from a Fermi-liquid (small λ) to Wigner molecule (large λ) behavior [7–9]. According to QMC calculations, in impurity-free parabolic QDs, Wigner molecule forms below certain critical value of electron density by showing a shell-structure and ground-state spin transitions [18]. The presence of an impurity can cause substantial effects on electronic structure of few-electron QDs together with increasing electron–electron interaction in the absence of magnetic field. The influence of an attractive Gaussian-type impurity on the addition energies and electron densities of the parabolic QDs for $N \leq 10$ in the incipient Wigner molecule regime has been investigated within the framework of Path Integral Monte Carlo (PIMC) [22]. Hirose and Wingreen [23] studied the ground-state energy and spin of a parabolic quantum dot at zero magnetic field considering multiple Gaussian-type impurity potentials for $N = 10, 11$ by using spin DFT in the weak and intermediate

* Corresponding author at: Department of Physics, Faculty of Science, Dokuz Eylül University, 35390 İzmir, Turkey, fax:+90 232 4534188.
E-mail address: zeynep.demir@deu.edu.tr (Z.D. Vatansever).

http://dx.doi.org/10.1016/j.physb.2015.11.004
0921-4526/

interaction regime. In the above mentioned symmetry broken few-electron quantum dot systems, in order to treat the electron–electron interaction with highly accurate numerical analysis, CI method stands as a powerful tool with its simplicity in comparison with QMC method.

So far, to our best knowledge, despite the electronic structure of parabolic QD-lithium (three-electron QD) at zero magnetic field is investigated in literature [13,24], we are not aware of any previous works on energetics and spin configurations of QD-lithium with impurity. In this paper, the effects of an attractive Gaussian-type impurity on the ground state and spin properties of three-electron parabolic quantum dot are presented. Using CI method, the ground-state spin transitions for varying electron–electron interaction strengths have been investigated in detail at zero magnetic field case. The charge densities of the system are given in Fermi-liquid and Wigner-molecule states to analyze electron localization in different interaction regimes.

The paper is organized as follows. The model quantum dot system and computational details of CI method are given in the next section. In Section 3 we give our numerical results and our conclusions are presented in Section 4.

2. The model and method

We consider a two-dimensional quantum dot with parabolic confinement of frequency ω_0 at zero magnetic field. We assume that due to the strong confinement along the z-direction, only the lowest state is occupied so that electrons move on $x-y$ plane. Thus, in the effective mass approximation, the Hamiltonian of N-electron quantum dot system is :

$$H = \sum_{i=1}^{N} h_i + \frac{1}{2}\sum_{i\neq j}^{N} \frac{e^2}{4\pi\epsilon^*}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{1}$$

where e, ϵ^* and $\mathbf{r}$ are electron charge, dielectric constant of the host semiconductor and position of the electron, respectively. h_i is the single-particle Hamiltonian given as :

$$h_i = \frac{\mathbf{p}_i^2}{2m^*} + \frac{1}{2}m^*\omega_0^2\mathbf{r}_i^2 + V_{imp}(\mathbf{r}_i) \tag{2}$$

where $\mathbf{p}$ and m^* are the momentum and effective mass of the electron, respectively.

We model the off-center impurity as Gaussian potential which breaks the circular symmetry of the system [22,23]:

$$V_{imp}(\mathbf{r}) = -V_0 \exp\left[-\frac{(\mathbf{r}-\mathbf{r}_0)^2}{2\sigma_0^2}\right]. \tag{3}$$

Here V_0 is a measure of the strength of impurity potential whereas σ_0 determines the spatial stretch of the impurity potential. $\mathbf{r_0}$ describes the location of the impurity.

It is practical to use second quantization formalism when studying the many-particle systems. On the basis of selected complete and orthonormal single-particle orbitals $\{\phi_i(\mathbf{r})\}$, the second quantization form of the N-electron Hamiltonian in Eq. (1) is written as:

$$\mathcal{H} = \sum_{i,j,\sigma} \epsilon_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} + \frac{1}{2}\sum_{i,j,k,l}\sum_{\sigma,\sigma'} U_{ijkl}\, a_{i\sigma}^{\dagger} a_{j\sigma'}^{\dagger} a_{k\sigma'} a_{l\sigma} \tag{4}$$

with one-body integral

$$\epsilon_{ij} = \int \phi_i^*(\mathbf{r}) h(\mathbf{r}) \phi_j(\mathbf{r})\, d\mathbf{r} \tag{5}$$

and two-body integral

$$U_{ijkl} = \frac{e^2}{4\pi\epsilon^*}\int\int \frac{\phi_i^*(\mathbf{r})\phi_j^*(\mathbf{r}')\phi_k(\mathbf{r}')\phi_l(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}\, d\mathbf{r}\, d\mathbf{r}'. \tag{6}$$

Here $a_{i\sigma}^{\dagger}$ ($a_{i\sigma}$) is the creation (annihilation) operator belonging to the spin orbital $\phi_i(\mathbf{r})\sigma(s)$ where $\sigma(s)$ is the eigenfunction of z component of the spin operator with eigenvalue $\pm 1/2$. Single-particle states $\{\phi_i(\mathbf{r})\}$ are chosen as eigenfunctions of the single-particle Hamiltonian. In our work single-particle states, one- and two-body integrals are calculated numerically by using the OCTOPUS code [25].

In CI method the variational wave function $|C\rangle$ of the system is taken as a linear combination of Slater determinants [26]:

$$|C\rangle = \sum_{k=1}^{N_{SD}} C_k |k\rangle \tag{7}$$

where C_k are the expansion coefficients to be determined and $|k\rangle$ are the Slater determinants (SDs). N_{SD} is the number of SDs which are obtained by moving electrons from occupied to unoccupied states in the given orthonormal spin orbital basis. In this work, full CI (FCI) is employed i.e. all the possible SDs generated are included in the linear expansion. Inserting the variational wave function into the time-independent Schrödinger equation yields the matrix-eigenvalue problem $\mathbf{HC}=E\mathbf{C}$ where $\mathbf{H}$ is the Hamiltonian matrix and $\mathbf{C}$ is the vector which includes the expansion coefficients. We have calculated the Hamiltonian matrix elements between SDs, $\langle k|H|j\rangle$, analytically by using the anti-commutation relations of creation and annihilation operators.

Since the Hamiltonian of the system is spin-free, alternatively one can use Configuration State Functions (CSFs) instead of Slater determinants in Eq. (7). SDs are eigenfunctions of projected spin operator $\hat{S}_z$ only but CSFs are simultaneously eigenfunctions of the total spin $\hat{S}^2$ and $\hat{S}_z$ operator with eigenvalue S^2 and S_z, respectively. CSFs can be obtained by taking proper linear combination of Slater determinants with the same eigenvalue S_z. (See Ref. [26,27] for more detail.) We have generated CSFs by constructing the $\hat{S}^2$ matrix in the basis of SDs with S_z eigenvalue. After diagonalization of the resulting $\hat{S}^2$ matrix, the proper linear combinations are found. In three-electron case, we keep the projection spin as $S_z = 1/2$ (two spin-up and one spin-down electron), to get all the eigenstates of total spin ($S=1/2, 3/2$).

In our model system, the total angular momentum does not conserve since the impurity breaks the circular symmetry of the system. Therefore for a system with fixed number of electrons, comparing with the pure system, the Hamiltonian matrix becomes larger because one cannot select one-particle states with certain angular momentum. In order to improve the accuracy of the calculations and decrease the execution time, we have parallelized our CI code by means of Message Passing Interface (MPI). Calculation of the Hamiltonian matrix elements, which is the kernel of the code, is done in parallel by the present processors in the system. Because the Hamiltonian matrix is symmetric and sparse, nonzero elements of the lower triangular matrix are stored with compressed sparse row format. The Hamiltonian matrix is diagonalized with Implicitly Restarted Lancozs Algorithm by using PARPACK library [28]. Obtained eigenvalues and eigenvectors are stored to be used later.

3. Results

In this section, we present our numerical results for three-electron parabolic quantum dot with an attractive impurity defined by a Gaussian potential. Dimensionless interaction parameter $\lambda = l_0/a_B^*$ is used to measure the electron–electron