Physics Letters A 378 (2014) 1036–1041

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Interaction effects near constriction of a quasi two-dimensional electron system: an exact diagonalization study

B. Szafran *, M.P. Nowak, E. Wach, D.P. Żebrowski

AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, al. Mickiewicza 30, 30-059 Kraków, Poland

ARTICLE INFO

Article history:
Received 4 December 2013
Received in revised form 27 January 2014
Accepted 29 January 2014
Available online 6 February 2014
Communicated by R. Wu

ABSTRACT

We present a systematic exact diagonalization study of a quasi two-dimensional few-electron system in a closed three-dimensional cylindrical geometry containing a constriction that models a quantum point contact formed within the two-dimensional electron gas. The calculations that are performed using the configuration interaction approach with multicenter Gaussian basis indicate that the tendency of the majority spin to gather in the area of an increased effective potential – e.g. by constriction of the quantum point contact – is distinct already for weak constrictions and low electron numbers. Opposite effects – nearly equal spin up and spin down densities – are obtained for local cavities of the confinement potential. Formation of a quasi-bound single-spin island within the constriction is also discussed.

© 2014 Elsevier B.V. All rights reserved.

1. Introduction

Properties of electron systems near constrictions formed within the two-dimensional electron gas have attracted a lot of attention [2] in the context of fractionally quantized conductance plateaux observed for quantum point contacts (QPCs) [1]. The fractional plateaux appear besides the integer ones, which are well understood on the basis of the Landauer approach [4] as due to opening of subsequent single-electron transport channels. It is generally agreed that the appearance of the fractional plateaux results from the electron–electron interaction, but the exact scenario of their formation is under discussion. The most popular – and not always mutually excluding hypotheses – include: spontaneous spin polarization of the low-density electron gas [1,3,5–14], Kondo transport mechanism [15–18], Wigner crystallization within the QPC [19–21], incoherent scattering from ferromagnetic fluctuations near the Stoner instability [22] and formation of correlated electron currents [23].

Ferromagnetic ordering of spins within QPC that is obtained for low electron gas within the density functional theory [2,5,6,8,10,11] is in an apparent contradiction with the Lieb–Mattis theorem [24]. Possible reasons [2] that the theorem could not hold for local ferromagnetic ordering within QPC include its finite length and width, connections to the reservoirs,[1] and spin–orbit interaction [26]. The only work which goes beyond the mean field theory is Ref. [27], which uses Monte Carlo techniques and indicates that the state with ferromagnetic ordering along the QPC is always higher in the energy than the spin-unpolarized state.

The dependence of fractional conductance plateaux on temperature [16] indicates the possible Kondo mechanism of the transport [15–18]. The necessary prerequisite of the Kondo mechanism is that QPC gives support to a quasi-bound single-electron-spin state [15]. Formation of this state is under debate: Refs. [18] and [28] both using local spin-density DFTs found an island of an uncompensated single-spin state quasi-bound within QPC. However, several papers using similar methodology [8,10,11,14] concluded that QPC does not support a quasi bound-state. Calculations of Ref. [29] based on the Hartree–Fock methods indicated that the quasi bound-state is formed but with zero spin. A study that goes beyond the mean field approach seems necessary for the definitive answer. Recently, a microscopic explanation for 0.7 anomaly was proposed [30] which assumes no spin polarization at zero magnetic field, and indicates that the fractional plateau results from the smeared van Hove singularity in the local density of states near the bottom of the lowest subband within QPC.

In this work we investigate the interaction effects near constrictions of the confinement potentials using the configuration-interaction approach which gives the exact solution of the Schrödinger equation for a few interacting electrons. We find (i) a distinct tendency for formation of majority spin density near confinement potential constrictions, (ii) that this tendency is triggered by

* Corresponding author.

[1] The exact diagonalization calculations indicate that for finite quasi-one dimensional systems (quantum dots) the spins of the ground-state are ordered antiferromagnetically in space: see [25]. In the low-density limit, when the Wigner crystal is formed the ground-state becomes nearly degenerate with respect to the spin. The exchange potential in the DFT approaches is then likely to promote the spin polarization.

http://dx.doi.org/10.1016/j.physleta.2014.01.052
0375-9601/© 2014 Elsevier B.V. All rights reserved.

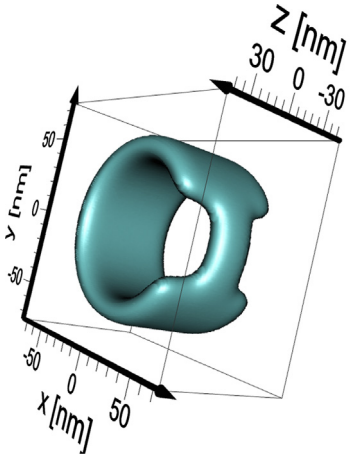

Fig. 1. Schematics of the considered geometry. The electrons are free to move within a cylindrical area of radius $R_t = 50$ nm with a finite extension along the axis and the radial direction. A constriction is formed at a side of the cylinder.

the electron–electron interaction, and (iii) that a single-spin island within the QPC is formed when it is long enough.

2. Theory

We consider a few-electron system which is confined in the cylindrical geometry given by Fig. 1. In the previous studies, the periodic boundary conditions were occasionally used for discussion of states near QPCs, in form of a strictly 1D [29], or 2D ring [27]. The present model is closer to the actual constriction present in QPC devices.

The electrons are confined within a cylindrical area of central radius $R_t = 50$ nm (see Fig. 1). The area has a finite extension along the axis ($\simeq 80$ nm). The cylindrical confinement of electrons is implied by a choice of the multicenter Gaussian basis for single-particle wave functions, according to the procedure used previously for description of transport in two-dimensional semiconductor nanochannels [31,32]. Namely, we consider basis functions

$$f_k(x,y,z) = \left(\frac{\alpha}{2\pi}\right)^{3/4} \exp\Big[-\frac{\alpha}{4}\big((x-X_k)^2 + (y-Y_k)^2 + (z-Z_k)^2\big)\Big], \tag{1}$$

with the centers of Gaussians (X_k, Y_k, Z_k) forming a uniform mesh on the surface of the cylinder. The mesh contains 11×48 centers with 11 locations along the axis of the cylinder (see Fig. 2), and 48 along the circumference. We use the localization parameter of the Gaussians $\alpha = 0.023$ [1/nm^2], which allows for a smooth tunneling of electrons between the neighbor centers and imply localization of wave functions in the direction from the axis of the order of $2/\alpha \simeq 13$ nm (see Fig. 1). Thus the region occupied by electrons in the radial direction is of the order of the one present in the growth direction of the two-dimensional electron gas.

We consider the following single-electron Hamiltonian

$$h = -\frac{\hbar^2}{2m^*}\nabla^2 + V(x,y,z) + \frac{1}{2}\mu_B g B \sigma_z, \tag{2}$$

where $m^* = 0.067 m_0$ is the GaAs conduction band effective mass, $V(x,y,z)$ is the potential which is introduced to tailor a constriction within the cylinder (see Fig. 2), μ_B is the Bohr magneton, $g = -0.44$ is the GaAs Landé factor, and B is the value of the magnetic field oriented along the axis of the cylinder. In this work we consider a small value of the magnetic field $B = -0.01$ T, which is

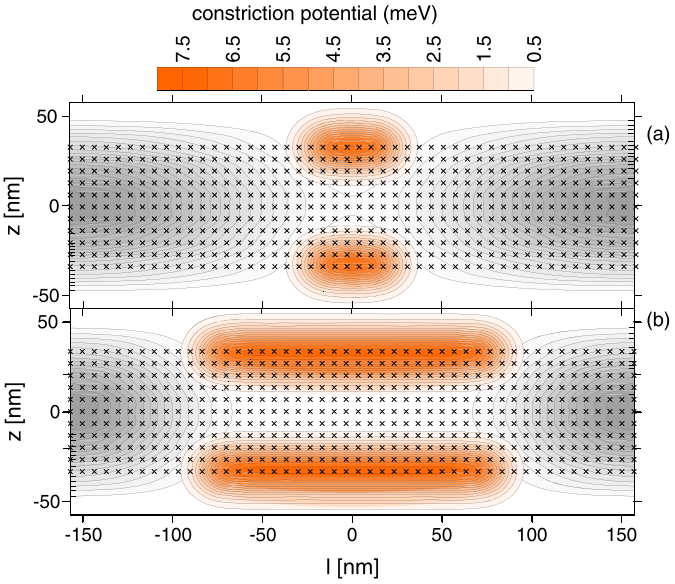

Fig. 2. The orange-colored contours show the potential forming the constriction at the central cross-section of the cylinder (distance of the axis $\rho = R_t$, where l stands for the coordinate along the circumference of the cylinder). The gray contour lines in the background show the single-electron ground-state charge density, and the crosses – the centers of the Gaussian functions of the basis (1). Plots (a) and (b) correspond to the constriction of a length of 46 nm and 164 nm, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

introduced to residually split the degeneracies of the few-electron spectra with respect to the spin (the difference of spin-up and spin-down single-electron energies is then 0.25 μeV). For the applied value of B the orbital effects of the magnetic field can be neglected. The eigenequation of operator (2) is diagonalized in the basis

$$\psi_\mu(x,y,z,\sigma) = \chi(\sigma)\sum_k c_k^\mu f_k(x,y,z), \tag{3}$$

where χ is one of the eigenstates of the σ_z Pauli matrix.

The N-electron Hamiltonian

$$H = \sum_{i=1}^{N} h_i + \frac{e^2}{4\pi\epsilon\epsilon_0}\sum_{i=1,\,j=i+1}^{N}\frac{1}{r_{ij}} \tag{4}$$

is diagonalized according to the standard procedure of configuration interaction (CI) approach in the basis of antisymmetrized products (Slater determinants) of the single-electron spin-orbitals

$$\Psi(\mathbf{r}_1,\sigma_1,\mathbf{r}_2,\sigma_2,\ldots,\mathbf{r}_N,\sigma_N) = \sum_l d_l \mathcal{A}\big\{\psi_{l_1}(\mathbf{r}_1;\sigma_1)\psi_{l_2}(\mathbf{r}_2;\sigma_1)\ldots\psi_{l_N}(\mathbf{r}_N;\sigma_N)\big\}, \tag{5}$$

where $\mathcal{A}$ is the antisymmetrization operator and d_l is determined by diagonalization of the Hamiltonian (4). We use GaAs dielectric constant of $\epsilon = 12.4$.

The CI calculation requires evaluation of Coulomb matrix elements. In this work we use the approach applied previously for the three-dimensional description of states localized in quantum dots [33]. Instead a large number of six-dimensional integrations, we perform sequentially two operations in three-dimensional space [34]. We first solve the Poisson equation for the Coulomb potential generated a product of single-particle wave functions for one electron [33,34], and next integrate it with the product of wave functions of the other electron.

The few-electron basis (5) is constructed using 28 lowest-energy single-electron spin-orbitals which ensures convergence of

Download English Version:

https://daneshyari.com/en/article/8205426

Download Persian Version:

https://daneshyari.com/article/8205426

Daneshyari.com