Physics Letters A ••• (••••) •••–•••

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Effects of electron–electron interaction on the collinear indirect exchange coupling in graphene nanoflakes

Akram Mirehi, Ebrahim Heidari-Semiromi *

Faculty of Physics, University of Kashan, Kashan, Iran

ARTICLE INFO

Article history:
Received 1 May 2018
Received in revised form 5 July 2018
Accepted 31 July 2018
Available online xxxx
Communicated by M. Wu

Keywords:
Graphene nanoflakes
RKKY interaction
Magnetic impurities
Electron–electron interaction
Rashba spin–orbit interaction

ABSTRACT

Using the Hubbard model in the framework of the tight-bonding formulation, we studied the effects of the electron–electron (e–e) interaction on the indirect magnetic exchange coupling between the magnetic impurities embedded in triangular graphene nanoflakes. The results show that the magnitude of the coupling enhances in the presence of the e–e interaction and Rashba spin–orbit interaction (RSOI). The RKKY coupling magnitude depends on the impurity positions in nanoflake and the size of the system, as well.

1. Introduction

Carbon-based magnetic nanomaterials attracted particular attention, mainly due to their tuneable electronic structure which is dependent on its geometry, especially the edge form [1]. These nanostructures are suitable candidates for technological applications such as q-bits in quantum computers and spintronics. In general, there is not any symmetry between spin down and spin up states in magnetic materials. The polarized spins can be considered for spintronic purposes [2].

The graphene nanoflakes show peculiar magnetic behavior due to the existence of surface and edge effects, which is different from bulk graphite behavior [3,4]. The shape of the graphene nanoflake (triangular, rectangular, or hexagonal) has a strong influence on its structural, electronic, vibrational properties when the number of carbon atoms is small (< 100) [5]. Among allotropes of graphene, zigzag-edged triangular nanoflakes have peculiar electronic spectrum, containing a shell of degenerate zero-energy states at the Fermi energy [6,7]. The important role of electronic correlations and magnetization in triangular graphene quantum dots has been investigated by a combination of tight-binding, Hartree–Fock, and configuration interaction methods. It was shown that electronic correlations play a crucial role in fractionally filled degenerate shells at the Fermi level for graphene quantum dots [8]. Also, theoretical calculations show that in the presence of e–e interactions the single zigzag edge of graphene nanoribbons leads to a shell of degenerate states at the Fermi level [9]. These results can be utilized to design a strongly correlated electronic system as a function of fractional filling of the shell in the carbon-based material whose magnetic properties can be controlled by applied gate voltage [8]. Interactions between magnetic moments introduced to graphene lattice attract considerable attention. One of the most important magnetic properties is the effective interaction between magnetic moments embedded in the host material, the so-called Ruderman–Kittel–Kasuya–Yosida (RKKY) coupling [10–12]. This well-known coupling has the considerable impact on the magnetic order of the impurities and also can be useful to determine the intrinsic magnetic properties of the host [13]. The possibility of introducing magnetic impurity atoms such as Mn, Fe and Co to graphene surface has been investigated using density functional theory [14]. In particular, the coupling in nanoflakes is different from the infinite system, as the dominance of the edge in a nanoflake modifies the indirect coupling and breaks the translational symmetry. So far, the significant efforts have been performed on the calculations of RKKY coupling properties in nanosized graphene structures. Namely, the effects of e–e interaction on the RKKY coupling have been studied in the zigzag graphene nanoribbons where the zero-energy states localized at the zigzag edges significantly modify the coupling behavior [13]. However, various investigations are made for the appearance of magnetism in graphene nanostructures without introduced magnetic impurities [15]. On

* Corresponding author.
E-mail address: eb.heidari@gmail.com (E. Heidari-Semiromi).

https://doi.org/10.1016/j.physleta.2018.07.050
0375-9601/

the other hand, the main efforts have focused on the calculations of RKKY coupling properties in the graphene nanostructures with introduced magnetic impurities [16–18]. Also, the effects of e–e interaction and charge doping on the RKKY coupling in the absence of Rashba interaction have been studied in the graphene nanoflakes in the framework of the Hubbard model [19]. Recently also, the importance of RSOI in the RKKY coupling between two embedded magnetic impurities has been investigated in zig-zag graphene nanoflakes without e–e interaction. However, the results show that magnetic phase transition (from F to AF magnetic or vice versa) does not occur in such a system through the RSOI [20]. The anisotropic contribution of the indirect exchange interaction in the presence of both Hubbard and Rashba type interactions has not been studied yet.

We incorporate the Hubbard and Rashba terms in order to investigate the effects of e–e interaction in the framework of the Hubbard model on the collinear indirect exchange coupling between the magnetic impurities for the various sizes of the graphene nanoflakes. We solve mean-field Hamiltonian selfconsistently using exact diagonalization. In the presence of both Rashba and e–e interactions, the $SU(2)$ symmetry breaking leads to emerging different contributions such as collinear and non-collinear terms in the RKKY amplitude. In this work, our attention is mainly on the dependence of the collinear term on the e–e interaction and RSOI strengths for various sizes of the system. Also, the dependence of the indirect coupling on the positions of the magnetic impurities which are located in on-site and plaquette locations at the edge of the nanoflake was investigated. We conclude that the e–e interaction influences on the magnitude of an indirect interaction in the presence of the RSOI. For a fixed position of the magnetic impurities, the coupling character does not change from F to AF magnetic or vice versa in the presence of the Hubbard and Rashba terms. Recently, the efforts have been focused on the problem of the indirect exchange coupling between magnetic impurity spins in graphene mediated by charge carriers. The obtained results for triangular nanoflakes demonstrate that doping of the nanoflake with a single charge carrier in presence of the Hubbard term leads to changing sign of the coupling from an AF to F magnetic for some geometries [19].

2. Model and Hamiltonian

We consider a triangular graphene nanoflake with the zigzag edge in which two magnetic impurities are embedded in on-site or plaquette positions. The total Hamiltonian for the graphene nanoflake can be written as:

$$H = H_0 + H_R + H' + H_{imp}. \tag{1}$$

Here, H_0 is the nearest-neighbor tight-binding Hamiltonian, with hopping integral t (usually taken as 2.8 eV) [21]:

$$H_0 = -t \sum_{<i,j>,\sigma} (c^{\dagger}_{i,\sigma}\, c_{j,\sigma} + c^{\dagger}_{j,\sigma}\, c_{i,\sigma}), \tag{2}$$

where $< i, j >$ denotes that the summation is taken over all the pairs of nearest-neighbor atoms. Here, $c^{\dagger}_{i,\sigma}$ and $c_{j,\sigma}$ are creation and annihilation field operators of electrons at the nearest-neighbor sites i and j in the nanoflake, while $\sigma = \uparrow, \downarrow$ is the electron spin.

H_R is the Rashba Hamiltonian that is given by [22]:

$$H_R = \frac{i\alpha}{a} \sum_{<i,j>} \sum_{\sigma=\uparrow,\downarrow} c^{\dagger}_{i,\sigma}\, [\sigma \times d_{ij}]_z c_{j,\sigma}, \tag{3}$$

where α is the Rashba strength, a is the carbon–carbon bond length, $d_{i,j}$ is the displacement vector between the nearest-neighbor sites from j to i, and σ is the Pauli matrix.

Also, the effects of the e–e interaction are described using the Hubbard term, in which a mean-field approximation in a self-consistent way is applied [15]:

$$H' = U \sum_i (n_{i\uparrow} < n_{i\downarrow} > + < n_{i\uparrow} > n_{i\downarrow}) - U \sum_i < n_{i\uparrow} >< n_{i\downarrow} >, \tag{4}$$

where $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ is the electron number operator at site i; the effective parameter $U > 0$ defines the Hubbard on-site repulsion. In this expression, $< n_{i\uparrow>}$ ($< n_{i\downarrow>}$) is the electron density of the number operator for an electron with spin-up (spin-down) which is calculated by a self-consistent solution. The values of the electron density are determined by iteration, starting from the initial guess of $< n_{i\sigma} >$ which can be chosen randomly. The Hubbard term appears only in the diagonal elements of the Hamiltonian matrix.

In equation (1), H_{imp} describes interaction between the magnetic impurity spins (S_a and S_b) and spins of the conduction electrons (s_a and s_b), the so-called Anderson–Kondo term [1]:

$$H_{imp} = \frac{J_0}{2}(S_a.s_a + S_b.s_b), \tag{5}$$

where J_0 is the constant potential showing coupling between on-site impurity spins S_a and S_b and the electron spins (s_a and s_b) at the same sites. In all the results the value of $J_0/t = 0.1$ was accepted. The selected value of J_0/t is based on the calculations (by first principle approach) of strength of the hybridization between atomic orbitals of the magnetic impurities in one hand and $2p_z$ orbital of the carbon at the other hand.

The operator of the spin of the electron for both orientations σ and σ' in the second-quantization representation can be written as:

$$s_a = \sum_{\sigma,\sigma'=\uparrow,\downarrow} < \sigma |s_a| \sigma' > c^{\dagger}_{a,\sigma} c_{a,\sigma'}. \tag{6}$$

After the substitution the operator of the spin of the electron into the Eq. (5), the Anderson–Kondo interaction in the second-quantization representation is achieved:

$$H_{imp} = \frac{J_0}{2} \sum_{\alpha=x,y,z} S^{(\alpha)}_a \sum_{\sigma,\sigma'=\uparrow,\downarrow} < \sigma |s^{(\alpha)}_a| \sigma' > c^{\dagger}_{a,\sigma} c_{a,\sigma'} + \frac{J_0}{2} \sum_{\alpha=x,y,z} S^{(\alpha)}_b \sum_{\sigma,\sigma'=\uparrow,\downarrow} < \sigma |s^{(\alpha)}_b| \sigma' > c^{\dagger}_{b,\sigma} c_{b,\sigma'}. \tag{7}$$

In the absence of spin-dependent interactions such as intrinsic or Rashba spin–orbit interactions, the system under consideration is rotational-invariant in spin vector space. In this situation, the RKKY interaction has only the collinear contributions such as Heisenberg or Ising types. In other words, the tensor of the RKKY interaction is diagonal, and the off-diagonal elements of this tensor which are related to the noncollinear contributions are zero. The $SU(2)$ symmetry in the spin vector space is broken by considering the intrinsic or Rashba type spin–orbit interactions. Therefore, the contributions which are related to the diagonal elements of the tensor such as Ising and Heisenberg would change. Moreover, the contributions of the off-diagonal elements of the tensor would appear. If all of the diagonal elements of the tensor are equal, we have Isotropic Heisenberg indirect exchange. If only the first component of the tensor, S_xS_x, is none zero, we have the Ising exchange interaction in the x direction. Otherwise, if the two components of the tensor are none zero, then $2D$ Ising exchange interaction appears in the x and y directions.

Please cite this article in press as: A. Mirehi, E. Heidari-Semiromi, Effects of electron–electron interaction on the collinear indirect exchange coupling in graphene nanoflakes, Phys. Lett. A (2018), https://doi.org/10.1016/j.physleta.2018.07.050