Strain-induced modulation of exchange interaction in monolayer zigzag nanoribbons of B$_2$S

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Keywords: Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, strain, zigzag nanoribbons of B$_2$S, electronic structure, staggered sublattice potential, near-midgap band, flat band

Abstract
In this work, the strain modulation of electronic structure and magnetic interaction in monolayer nanoribbons of B$_2$S, a recently realized monolayer system, is investigated. In the first part of our study, we focus on how the electronic structure of monolayer nanoribbons of B$_2$S is modified under uniaxial strains, then employing a tight-binding framework together with the conventional theory of elasticity, we discuss how strain-induced local deformations can be used as a means to affect Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in zigzag nanoribbons of B$_2$S. We show that breaking the inversion symmetry in the unit cell of a zigzag B$_2$S nanoribbon (ZBSNR), e.g. by introducing a staggered sublattice potential, plays a key role in the modulation of its electronic and magnetic properties. More interestingly, for the ZBSNRs belong to the group \( M = 4p \), with \( M \) the width of the ZBSNR and \( p \) an integer number, one can see that a band gap, in which a pair of near-midgap bands completely detached from the bulk bands is always observed. As a key feature, the position of the midgap bands in the energy diagram of ZBSNRs can be shifted by applying the in-plane strains \( \varepsilon_x \) and \( \varepsilon_y \). Moreover, the near-midgap bandwidth monotonically decreased with increasing strength of the strain and increases with the width of the ZBSNR. The energy gap of the ZBSNRs decreased with increasing the applied strain and ribbon width. The spatial and strain dependency of the exchange interaction in various configurations of the magnetic impurities are also evaluated. It is shown that magnetic interactions between adsorbed magnetic impurities in B$_2$S nanoribbons can be manipulated by careful strain engineering of such systems. Our results suggest that these tunable electronic and magnetic properties of ZBSNRs mean they may find applications in spintronics and pseudospin electronics based on monolayer B$_2$S nanoribbons.

1. Introduction
The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [1–3], is an indirect exchange coupling between magnetic impurity dopants mediated by a background of conduction electrons of the host material. Of fundamental interest in the field of spintronics, the RKKY interaction is the most important mechanism of the coupling between localized spins in metals and semiconductors. Depending on the spatial separation of the magnetic impurities, the magnetic coupling could be ferromagnetic [4–9] or antiferromagnetic [10, 11] and is oscillatory due to the sharpness of the Fermi surface. Another interesting phases such as spiral [12, 13] and spin-glass [14–16] are also attainable in the magnetically doped systems. Besides these practical magnetic phases, the RKKY interaction can provide information about the intrinsic properties of the material since this coupling is proportional to the spin susceptibility of the host system. A key feature of the RKKY exchange is the long-range oscillations with the Fermi wavevector originates from the Friedel oscillations, that falls off by \( R^{-3} \), where \( D \) is the dimension of the system [17, 18]. In undoped single layer graphene, the RKKY interaction has contributions that decay with \( R^{-3} \), a reflection of the vanishing density of states at the Fermi energy, while it falls off as \( R^{-2} \) in doped case. It was shown that the RKKY interaction consists of three Heisenberg, Ising, and Dzyaloshinskii-Moriya (DM)
terms on the surface of zigzag silicene nanoribbons as well as the three dimensional topological insulators \[12, 14, 19\], and the competition between them causes rich spin textures.

An additional term, namely the spin–frustrated has discovered in a three-dimensional Weyl semimetal (WSM) that along with the Dzyaloshinskii–Moriya term lies in the plane perpendicular to the line connecting two Weyl points \[20\]. A decay rate of \( R^{-3} \) for doped WSM is found, while a much faster decay rate of \( R^{-4} \) is found for half-filling band at Weyl points.

In a spin polarized system \[21\] and a material with multi-band structure \[18\], these oscillations become more complicated than a monotonous oscillation with \( \sin(2k_F R) \) behavior, where \( k_F \) is the wave vector of the electrons (holes) at the Fermi level and \( R \) is the distance of two magnetic impurities. In addition, it is important to note that the magnitude of the RKKY interaction can be severely affected by the density of states (DOS) at the Fermi level \[13, 17\]. Owing to the bipartite nature of the honeycomb sublattice, the RKKY coupling in graphene is highly sensitive to the direction of the distance vector between impurities \[17, 22\]. In materials with spin–orbit interaction of Rashba type \[23\], the exchange interaction depends on the direction of the magnetic moments and as the result the RKKY interaction becomes anisotropic \[13\]. Recently, in a detailed study it has shown that the topological phase transition in the zigzag silicene nanoribbons can be probed by using the RKKY interaction \[12\]. In another work, it has concluded that the RKKY interaction in the bulk phosphorene monolayer is highly anisotropic and the magnetic ground-state of two magnetic adatoms can be tuned by changing the spatial configuration of impurities as well as the chemical potential varying \[24\].

In the last decades, dilute semiconductors have emerged as a research hotspot due to their functionalities for application in spintronic devices and magnetic recording media \[25–27\]. In this regard, inducing magnetism in otherwise nonmagnetic two dimensional (2D) materials may lead to next generation of spintronic devices based on the spin degrees of freedom \[12, 14, 19\]. Motivated by the interaction of two dimensional lattices with magnetic objects, we have recently addressed the problem of indirect exchange coupling between localized magnetic moments mediated by the conduction electrons of 2D materials \[12, 24, 28\]. Of particular interest is the potential for zigzag nanoribbon–based spintronic devices to be realized, and thus much attention has been focused on determining the magnetic properties of 2D honeycomb nanoribbons. The RKKY interaction in nanoribbon of two dimensional lattices has attracted strong attention in condensed matter physics \[12, 24, 29, 30\].

On the other hand, strain engineering, a key strategy for manipulating the magnetic coupling in 2D nanostructures \[30\], has a perfect platform for its implementation in the atomically thin materials. Motivated by the search for materials for spintronics, a huge number of works have been performed to examine the effectiveness of mechanical strain in modulating the magnetic properties of 2D layered materials \[30–37\].

Very recently, a new 2D anisotropic Dirac cone material, B\(_2\)S monolayer, appears in the research field by using global structure search method and first principles calculation combined with tight-binding model \[38, 39\]. B\(_2\)S monolayer, showing a Fermi-velocity of 106m/s in the same order of magnitude as that of graphene, was found to be mechanically, thermally and dynamically stable. It is the first pristine honeycomb lattice with a tilted anisotropic Dirac cone structure, stabilized by sulfur atoms in free standing condition. Since, boron atom has one electron less than carbon all the reported 2D boron-based Dirac cone materials, have much more complicated geometries in comparison with the pristine honeycomb structure of graphene. Both theoretical and experimental studies have shown that the pristine honeycomb geometry of 2D boron sheet is unstable in its freestanding form which can be stabilized by adding two electrons to each boron hexagonal ring via doping metal atoms \[40, 41\].

In this paper, based on the Green’s function technique, within the tight-binding model we investigate the RKKY interaction between two magnetic impurities placed on the surface of the B\(_2\)S nanoribbons. In the first part of the study, we focus on how the electronic structure of monolayer nanoribbons of B\(_2\)S is modified under uniaxial strains as well as by introducing staggered sublattice potentials, then employing a tight-binding approach together with the conventional theory of elasticity, we discuss how strain-induced local deformations can be used as a means to affect magnetic exchange interaction in zigzag nanoribbons of B\(_2\)S. Moreover, we show that for the ZBSNRs belong to group \( M = 4p \), with \( M \) the width of the ZBSNR (\( M \) atoms wide) and \( p \) an integer number, a band gap in which a pair of near-midgap bands completely detached from the bulk bands, is always observed.

This paper is organized as follows: In section 2, we introduce the system under consideration, i.e. a monolayer zigzag B\(_2\)S nanoribbon under the influence of strain and staggered potential applied to it. A tight-binding model Hamiltonian for monolayer B\(_2\)S is presented and then the band spectrum of ZBSNR under a staggered potential is calculated. Then we introduce the theoretical framework which will be used in calculating the RKKY interaction from the real space Green’s function. After that, we discuss our numerical results for the proposed magnetic doped ZBSNR in the presence of an in-plane strain. Finally, our conclusions are summarized in section 3.
2. Theory and model

As previously mentioned, the most stable atomic configuration of the B$_2$S monolayer, as a strained graphene, has a honeycomb structure in which each hexagonal ring is distorted with the bond angles ranging from 114° to 123°, because B and S atoms have different covalent radii and electronegativities [38, 39]. The geometry structure of a monolayer zigzag nanoribbon of B$_2$S, laid in the xy plane, is depicted in figure 1. As shown, each hexagon consists of four B atoms and two S atoms, with an orthogonal primitive cell with a space group of Pbam and a point group D$_{2h}$. In this structure there are two kinds of bonds with 1.62 Å and 1.82 Å bond lengths for B-B and B-S connections, respectively [38].

For better strain engineering in 2D layered materials, a deeper understanding of how the geometry and electronic structure change by imposing lattice strains on the samples is crucial. To verify the role of strain on the magnetic exchange interaction, the understanding of changes in the band structure and bandgap transformation is critical. For B$_2$S monolayer, it is shown that the bands near the Fermi level are originated from the magnetic exchange interaction, the understanding of changes in the band structure and bandgap transformation can be mapped from the real space tight-binding model given by equation (1) [38].

\[
H_{B,S} = \sum_i U_i c_i^\dagger c_i + \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j,
\]

where $c_i^\dagger$ ($c_i$) represents the creation (annihilation) operator of electrons at site $i$ ($j$), $U_i$ ($i = B, S$) is the onsite energy of the $i$-th atom and $t_{ij}$ is the nearest-neighbors hopping amplitude between $i$-th atom and $j$-th atom. $\langle \rangle$ denotes the nearest neighbors. The suggested values of these hopping integrals are specified as $t_1 = 0.8$ eV and $t_2 = 1.7$ eV [38]. However, it has been found that the onsite energies for S and B atoms are 6.4 eV and 5.4 eV, respectively which means that the sulfur atom is more electronegative than boron atom.

Having an accurate tight-binding model, as presented in the previous equation, we can numerically calculate the momentum space dispersion of a monolayer zigzag nanoribbon of B$_2$S, directly. To do so, we assume the periodic boundary condition along the ribbon in the x-direction.

Owing to the translational invariant along the ribbon direction (x), the momentum in the x-direction is a good quantum number thus the k-dependent band structure of ZBSNR, from the tight-binding model, is obtained from $\sum_k \psi_k^\dagger H_k \psi_k$. In order to obtain the k-space Hamiltonian $H_k$, one can, e.g. perform the Fourier transformation along the x-direction to the real space Hamiltonian:

\[
H_k = H_{00} + H_{01} e^{-ik_xa} + H_{11} e^{ik_xa}
\]

in which $a$ is the unit-cell length along the x-axis. Moreover, Hamiltonian matrices $H_{00}$ and $H_{01}$ describe coupling within a principal unit cell (intra-unit cell) and between the adjacent principal unit cells (inter-unit cell), respectively which can be mapped from the real space tight-binding model given by equation (1).
\( H_{00} \) is a \( 3M \times 3M \) Hamiltonian matrix representing the hopping terms between sites within a cell:

\[
H_{00} = \begin{pmatrix}
H_{AA} & H_{AB} & H_{AC} \\
H_{BA} & H_{BB} & H_{BC} \\
H_{CA} & H_{CB} & H_{CC}
\end{pmatrix},
\]

and \( H_{01} \) is a \( 3M \times 3M \) Hamiltonian matrix connecting the sites between neighboring cells, which can be written in the form

\[
H_{01} = \begin{pmatrix}
H_{A_1A_2} & H_{A_1B_1} & H_{A_1C_1} \\
H_{B_1B_2} & H_{B_1B_1} & H_{B_1C_1} \\
H_{C_1A_2} & H_{C_1B_1} & H_{C_1C_1}
\end{pmatrix},
\]

where \( H_{AA}, H_{BB} \) and \( H_{CC} \) are three-diagonal \( M \times M \) matrices, as shown in appendix, and the \( H_{01} \) Hamiltonian matrix, has all elements equal to zero except for element (cell) \( \{3,1\} \) which is equal to \( H_{C_1A_2} \), shown in the appendix.

To explain the band structure of the nanoribbons, the eigenvalues of the Hamiltonian \( 2 \) must be solved. Furthermore, corresponding wave function for a given energy and wave vector can be used in order to evaluate the site-resolved local density of states (LDOS) in the ribbons as \( \rho(r, E_{nk}) = \sum_{m} |\psi_{nmk}(r)|^2 \delta(E_{nk} - E_{nmk}) \), where \( n, m \) are band indexes and \( r \) is the sublattice position.

2.1. Inclusion of strain

In this subsection, the effect of strain on the band structure and magnetic exchange interaction is analyzed and discussed. We first consider a zigzag B\(_2\)S nanoribbon in the \( xy \)-plane, in the presence of uniaxial strains \( \epsilon_x \) and \( \epsilon_y \). As is known, the strain modulates the band structure by modifying the hopping parameters and hence a significant influence on the magnetic exchange interaction is expected. As it has been shown, the strength of the hopping parameter \( t \) between \( s \) and \( p \) orbitals depends strongly on the bond length \( r \) and can be written as \( t \propto \frac{1}{r} \) [42–44]. It is worthwhile to note that since it has been assumed that the principal directions of the two neighboring Wannier orbitals keep their orientation along the bond vector of the two neighbor sites, the angular dependence of the mechanical strain is negligible. Moreover, the applied mechanical strain can affect the electronic structure significantly by modifying the hopping parameters in the tight-binding model.

Let the \( x \)-axis be in the direction of the zigzag edge of B\(_2\)S nanoribbon and the \( y \)-axis in that of the armchair edge, as seen in figure 1. Within the context of continuum mechanics and in the linear deformation regime, application of a uniaxial strain will cause the following change of the bond length \( r \) in terms of strain components \( \epsilon_x \) and \( \epsilon_y \)

\[
\begin{pmatrix}
x' \\
y'
\end{pmatrix} = \begin{pmatrix}
1 + \epsilon_x & \gamma \\
\gamma & 1 + \epsilon_y
\end{pmatrix} \begin{pmatrix}
x \\
y
\end{pmatrix},
\]

where \( r = x + y \) and \( r' = x' + y' \) denote the positions of an atom before and after deformation, respectively.

In the linear deformation regime, an expansion of the norm of \( r \) to first order in strains \( \epsilon_x \) and \( \epsilon_y \) can be expressed as

\[
r' \simeq (1 + \alpha_x \epsilon_x + \alpha_y \epsilon_y) r,
\]

where \( \alpha_x = (x/r)^2 \) and \( \alpha_y = (y/r)^2 \) are the strain-related geometrical coefficients in zigzag B\(_2\)S nanoribbon. By invoking the relationship between the hopping parameter and the bond length, we get the following geometrical strain effect on the hopping parameter,

\[
t = t_0 \left(1 - \frac{2}{r} \alpha_x \epsilon_x - \frac{2}{r} \alpha_y \epsilon_y\right).
\]

Here, we examine the dependence of band gaps of ZBSNRs on the uniaxial strain and ribbon’s width (see figure 2). From the evaluated electronic band structures, we find that the magnitude of the bandgap in each type of the zigzag B\(_2\)S nanoribbon is reduced as the applied strain increases. Instead, the bandgap is a linear function of the applied strain. This is consistent with previous first principles calculations of graphene nanoribbons and other 2D layered materials [45, 46].

It is noteworthy to mention that to further explore the width dependence of the band structures and magnetic couplings, the ZBSNRs are classified into two different family structures, the \( M = 4p \) and \( M = 4p + 2 \), with \( p \) as an integer number.

The associated band structures of the zigzag B\(_2\)S nanoribbons with width of \( M = 62 \) (an example for the group \( M = 4p + 2 \)) and \( M = 64 \) (an example for the group \( M = 4p \)), are plotted in figures 3(a) and (b), respectively. Interestingly, for the ZBSNRs belong the \( M = 4p \) group one can see that a band gap in which a pair
of near-midgap bands (green and red curves) completely detached from the bulk bands, is always observed. As is known, these near-midgap energy bands are due to the edge states whose wave functions are confined near the ZBSNR edges \([41, 47, 48]\). As shown in the figure 3, for ZBSNRs with width of \(M = 4p\), only one pair of near-midgap edge modes is formed but for ZBSNRs with width of \(M = 4p + 2\). In addition to the edge states (near-midgap bands), there are other detached bulk states in the energy gap (see figure 3(a)).
It seems promising for zigzag nanoribbons to modulate the midgap energy bands, for the next generation of semiconductor devices \[41, 47, 48\]. Thus, it is interesting to look at the bandgap and midgap states modulation in ZBSNRs. As shown in figure 4, as a key feature, the position of the midgap bands in the energy diagram of ZBSNRs can be shifted by applying the in-plane strains \( \varepsilon_x \) and \( \varepsilon_y \). Particularly, the near-midgap energies move up under positive strains, while shift down with negative strains. Moreover, the near-midgap bandwidth (MBW) monotonically decreases with increasing strength of the strain and increases with the width of the ZBSNR (see figure 5). It is worthwhile to note that the bandwidth is generally defined as the energy difference between the upper and lower band edges. Degeneracy of the near-midgap bands, which are always degenerate at \( k_x a = 0 \), is increases dramatically with increasing the width of the ZBSNR. As suggested by Soleimanikahnoj et al these tunability of near-midgap bands in ZBSNRs can pave the way for their potential application in pseudospin electronics based on nanoribbons \[49\].

One of the fascinating properties of the new families of 2D layered materials is their possibility to use a staggered potential to manipulate their electronic properties. Motivated by this important problem, we further examine the effect of staggered sublattice potential on the electronic structure, by breaking the discrete sublattice symmetry of this honeycomb structure. Here, we investigate the band dispersion of the ZBSNRs of infinite length \( L (N \rightarrow \infty) \) under the influence of the staggered potential.

The calculated band structure of the zigzag nanoribbons of \( \text{B}_2\text{S} \) for two different ribbon widths \( M = 16, 18 \) are shown in figure 6. The top panels (a)–(d) are for \( M = 16 \) and the bottom ones (e)–(h) are for \( M = 18 \). The staggered sublattice potentials are as \( U_5 = 0, U_6 = 5.4 \) (a), (e), \( U_5 = 6.4, U_6 = 0 \) (b), (f), \( U_5 = 0, U_6 = 0 \) (c), (g) and \( U_5 = 6.4, U_6 = 5.4 \) (d), (h), all in units of eV. As can be seen, the resulting band structures are completely different at various values of the strength of the staggered potential.

Figure 4. Shift of the midgap energy bands under both positive and negative uniaxial strains \( \varepsilon_x \) (a) and \( \varepsilon_y \) (b), for ZBSNRs with \( N = 150, M = 16 \) (an example for the group \( M = 4p \)).
As is known, understanding the sublattice-dependent of local density of states (LDOS) is essential to assess the configuration-dependent magnetic interaction. Figure 7 illustrates the LDOS of the ZBSNRs, (a), (b) for the edge sites and (c), (d) for the bulk sites, in which (a), (c) are for ZBSNRs with \( N = 150, M = 16 \), while (b), (d) are for ZBSNRs with \( N = 150, M = 18 \). As shown, the LDOSs are effectively modulated in the ZBSNRs, for the three groups of \( n = 3p, n = 3p + 1 \) and \( n = 3p + 2 \), where \( p \) is an integer. In figure 7, looking at the LDOS corresponding to the various lattice sites, it is clear that the higher values of LDOS appear on the edges.

2.2. The RKKY interaction

We are here focusing on the indirect exchange interaction in well-defined pairs of magnetic impurities with different configurations and distances on a B\(_2\)S surface. The carrier-mediated exchange coupling between the spin of itinerant electrons and two magnetic impurities located at positions \( r \) and \( r' \), with magnetic moments \( S_1 \) and \( S_2 \), is given by

\[
V = -\lambda (S_1 \cdot s(r) + S_2 \cdot s(r')), \tag{8}
\]

As is known, understanding the sublattice-dependent of local density of states (LDOS) is essential to assess the configuration-dependent magnetic interaction. Figure 7 illustrates the LDOS of the ZBSNRs, (a), (b) for the edge sites and (c), (d) for the bulk sites, in which (a), (c) are for ZBSNRs with \( N = 150, M = 18 \), while (b), (d) are for ZBSNRs with \( N = 150, M = 16 \). As shown, the LDOSs are effectively modulated in the ZBSNRs, for the three groups of \( n = 3p, n = 3p + 1 \) and \( n = 3p + 2 \), where \( p \) is an integer. In figure 7, looking at the LDOS corresponding to the various lattice sites, it is clear that the higher values of LDOS appear on the edges.
where \( s(\mathbf{r}) \), \( s(\mathbf{r}') \) are the conduction electron spin densities at positions \( \mathbf{r} \) and \( \mathbf{r}' \) and \( \lambda \) is the coupling between the impurity spins and the itinerant carriers.

In the linear response regime, the interaction energy between the two localized magnetic moments, derived from second-order perturbation theory, may be written as a Heisenberg form

\[
E(\mathbf{r}, \mathbf{r}') = J(\mathbf{r}, \mathbf{r}') S_1 \cdot S_2,
\]

Using the charge susceptibility for a crystal

\[
\chi(\mathbf{r}, \mathbf{r}') \equiv \frac{\delta n(\mathbf{r})}{\delta V(\mathbf{r}')},
\]

where \( \delta V(\mathbf{r}') \) is a spin-independent perturbing potential and \( \delta n(\mathbf{r}) \) is the induced charge density, the RKKY interaction \( J(\mathbf{r}, \mathbf{r}') \) is written as

\[
J(\mathbf{r}, \mathbf{r}') = \frac{\lambda^2}{4} \chi(\mathbf{r}, \mathbf{r}').
\]

The static spin susceptibility can be written in terms of the integral over the unperturbed Green’s function

\[
\chi(\mathbf{r}, \mathbf{r}') = -\frac{2}{\pi^2} \int_{-\infty}^{\infty} d\varepsilon \Im [G^0(\mathbf{r}, \mathbf{r}', \varepsilon) G^0(\mathbf{r}', \mathbf{r}, \varepsilon)],
\]

where \( \varepsilon_F \) is the Fermi energy. The expression for the susceptibility may be obtained by using the spectral representation of the Green’s function

\[
G^0(\mathbf{r}, \mathbf{r}', \varepsilon) = \sum_{n,s} \psi_{n,s}(\mathbf{r}) \psi_{n,s}^*(\mathbf{r}'),
\]

where \( \psi_{n,s} \) is the sublattice component of the unperturbed eigenfunction with the corresponding energy \( \varepsilon_{n,s} \). For a crystalline structure, \( n, s \) denotes the band index and spin. In other words, it just denotes a complete set of quantum states. Substituting equation (13) into equation (12), after integration over energy, we will get the result for the RKKY interaction.

The analytical background of this approach has been already described, in details, in previous works \([12, 24]\) and will not be rediscussed here. We only extract from these theoretical considerations, the following desired result

\[
\chi(\mathbf{r}, \mathbf{r}') = 2 \sum_{n,s} \frac{f(\varepsilon_{n,s}) - f(\varepsilon_{n,s}')}{\varepsilon_{n,s} - \varepsilon_{n,s}'} \times \psi_{n,s}(\mathbf{r}) \psi_{n,s}^*(\mathbf{r}') \psi_{n,s}'(\mathbf{r}) \psi_{n,s}'^*(\mathbf{r}),
\]

where, \( f(\varepsilon) \) is the Fermi function. This is a well-known formula in the linear response theory that is the main equation in this work.

Figure 7. Local density of states of ZBSNRs (a), (b) for edge lattices and (c), (d) for bulk lattices. (a), (c) are for ZBSNRs with \( N = 150, M = 18 \) (example for the group \( M = 4p + 2 \)), while (b), (d) are for ZBSNRs with \( N = 150, M = 18 \) (example for the group \( M = 4p \)).
2.3. Numerical results for the RKKY interaction in zigzag B\textsubscript{2}S nanoribbons

Here we numerically calculate the RKKY exchange interaction (equation (14)) for the zigzag B\textsubscript{2}S nanoribbons, based on the tight-binding model (equation 1). Note that for simplicity, all obtained data for the RKKY interaction are multiplied by 10\textsuperscript{3}.

Figures 8 and 9 show the effective exchange interaction for doped ZBSNRs ($E_F = 2$ eV) with $N = 300$, $M = 16$ for different strain strengths $\varepsilon_x$, (a), (b) and $\varepsilon_y$, (c), (d), for the case when both the impurities are located on the same edge, one impurity is fixed at the edge site with coordinate $(10,1)$ and the other can be located on lattice points $(n,1)$ with $n = 11, 12, \ldots$.

![Image](image-url)

Figure 8. The variation of $\chi$ versus distance between two impurities, for doped ZBSNRs ($E_F = 2$ eV) with $N = 300$, $M = 16$ for different strain strengths $\varepsilon_x$, (a), (b) and $\varepsilon_y$, (c), (d), for the case when both the impurities are located on the same edge, one impurity is fixed at the edge site with coordinate $(10,1)$ and the other can be located on lattice points $(n,1)$ with $n = 11, 12, \ldots$.

Figures 8 and 9 show the effective exchange interaction for doped ZBSNRs ($E_F = 2$ eV), as a function of the distance between the impurities for different strain strengths $\varepsilon_x$ and $\varepsilon_y$ for various spatial configurations of the two magnetic impurities, as shown in the figure 1. Figure 8 shows the results for the case when both the impurities are located on the same edge, one impurity is fixed at the edge site with coordinate $(10,1)$ and the other can be located on lattice points $(n,1)$ with $n = 11, 12, \ldots$ The panels (a) and (b) are for different positive and negative strains $\varepsilon_x$, respectively and the panels (c) and (d) are for for different positive and negative strains $\varepsilon_y$, respectively.

What the figure 9 shows is the same as figure 8 but for the case when both the impurities are located in the interior of the ZBSNR, one spin is fixed at the lattice site with coordinate $(10,8)$ and the other can be located on lattice points $(n,8)$. First of all, the general feature of the exchange coupling, oscillatory behavior with distance between the two impurities, is seen in these figures. As an important result, the RKKY coupling for the edge impurities is about two order of magnitude larger than when both impurities are in the bulk due to the existence of edge states at the edge of the ZBSNR. In addition, the oscillatory nature as well as the amplitude of the exchange interaction are highly sensitive to the strain. We observe that for small separation between the two impurities ($R/a_x > 10$) when impurities are located inside the edge, two magnetic impurities become ferromagnetically coupled, as shown in figure 9(a).

The strain engineering of the magnetic ground state in dilute semiconductors and 2D materials is a perfect platform for their implementation in nano devices. To gain further insight into this practical mechanism, the role of strain on the magnetic interaction of ZBSNRs is also explored. To this end, we have shown that the magnetic properties of the ZBSNRs can be effectively tuned by mechanical strains, as shown in figures 10 and 11. In the panels (a), (b) both the impurities are located on the same edge, such that the one of the spins is fixed at the edge site with coordinate $(10,1)$ and another can be located on lattice points $(n,1)$, while in panels (c), (d) both the impurities are located within the bulk of ZBSNR, such that the one of spins is fixed at the lattice site with coordinate $(10,8)$ and another can be located on lattice points $(n,8)$.  

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**Figure 8.** The variation of $\chi$ versus distance between two impurities, for doped ZBSNRs ($E_F = 2$ eV) with $N = 300$, $M = 16$ for different strain strengths $\varepsilon_x$, (a), (b) and $\varepsilon_y$, (c), (d), for the case when both the impurities are located on the same edge, one impurity is fixed at the edge site with coordinate $(10,1)$ and the other can be located on lattice points $(n,1)$ with $n = 11, 12, \ldots$. The panels (a) and (b) are for different positive and negative strains $\varepsilon_x$, respectively and the panels (c) and (d) are for for different positive and negative strains $\varepsilon_y$, respectively.

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**Figure 9.** The variation of $\chi$ versus distance between two impurities, for doped ZBSNRs ($E_F = 2$ eV) with $N = 300$, $M = 16$ for different strain strengths $\varepsilon_x$, (a), (b) and $\varepsilon_y$, (c), (d), for the case when both the impurities are located in the interior of the ZBSNR, one spin is fixed at the lattice site with coordinate $(10,8)$ and the other can be located on lattice points $(n,8)$. First of all, the general feature of the exchange coupling, oscillatory behavior with distance between the two impurities, is seen in these figures. As an important result, the RKKY coupling for the edge impurities is about two order of magnitude larger than when both impurities are in the bulk due to the existence of edge states at the edge of the ZBSNR. In addition, the oscillatory nature as well as the amplitude of the exchange interaction are highly sensitive to the strain. We observe that for small separation between the two impurities ($R/a_x > 10$) when impurities are located inside the edge, two magnetic impurities become ferromagnetically coupled, as shown in figure 9(a).
It is shown that the RKKY coupling between adsorbed impurities at a fixed distance on the ZBSNR has an oscillatory behaviour versus strains, due to the strain dependence of the Fermi wave vector. The sign-changing oscillations of the exchange coupling, which appear in terms of strains $\varepsilon_x$ and $\varepsilon_y$, are very interesting and may have significant implications for strain engineering of the magnetic ground state in ZBSNRs.

The quenching of the short-distance RKKY interaction at and below a certain strain is seen in these figures. It is clear that the position configuration of the magnetic impurities has a very significant impact on the strain engineering of magnetic coupling in 2D ZBSNRs. For instance, for ZBSNRs with $M = 18$ (the $M = 4p + 2$ family of ZBSNRs), top panels (a), (b) are for two impurities placed on the same edge and bottom panels (c), (d) are for both the impurities are within the bulk of ZBSNR.
Magnetic properties of ZBSNRs mean they may of the exchange interaction are highly sensitive to the strain. Our results suggest that these tunable electronic and the existence of edge states at the edge of the ZBSNR. In addition, the oscillatory nature as well as the amplitude versus strains, due to the strain dependence of the Fermi wave vector. As an important result, the RKKY coupling between adsorbed impurities at a

impurities located on a zigzag B2S nanoribbon, a recently realized monolayer, as a strained graphene. In the

To summarize, in this work we numerically investigate the RKKY exchange coupling between two magnetic impurities in B2S nanoribbons can be manipulated by careful strain engineering of such systems. We found that magnetic impurities are also evaluated. It is shown that that magnetic interactions between adsorbed magnetic

ZBSNR family), whether the impurities are on the edge or inside the ZBSNR, when the first moment is pinned on a n = 3p family site (here n = 69), if the second one is seated on a n = 3p + 1 family site (here n = 79), the observed peaks of the RKKY oscillations are stronger.

For the case of the ZBSNR of width M = 20 (a M = 4p family) (see figure 11), in the case when both the impurities are placed at the same edge, if the first moment is pinned at a n = 3p family site (here n = 69), when the second one is seated on a n = 3p family site (here n = 79), the observed peaks of the RKKY oscillations are stronger. But in the case when both the impurities are away from the edge (when both the impurities are inside the bulk, along the line m = 10), the strongest peaks are related to the n = 3p family site (here n = 78).

3. Summary

To summarize, in this work we numerically investigate the RKKY exchange coupling between two magnetic impurities located on a zigzag B2S nanoribbon, a recently realized monolayer, as a strained graphene. In the first part of our study, we focus on how the electronic structure of the monolayer nanoribbons of B2S is modified under uniaxial \( \varepsilon_x \) and \( \varepsilon_y \), then employing a tight-binding approach together with the conventional theory of elasticity, we discuss how strain-induced local deformations can be used as a means to affect Ruderman-Kittel-Kasuya-Yosida interaction in the zigzag nanoribbons of B2S. We show that breaking the inversion symmetry in the unit cell of a zigzag B2S nanoribbon, e.g. by introducing a staggered sublattice potential, plays a key role in the modulation of their electronic properties. More interestingly, for the ZBSNRs belong to the group M = 4p, with M the width of the ZBSNR and p an integer number, one can see that a band gap, in which a pair of near-midgap bands completely detached from the bulk bands, is always observed. As a key feature, the position of the midgap bands in the energy diagram of the ZBSNRs can be shifted by applying the in-plane strains \( \varepsilon_x \) and \( \varepsilon_y \). Moreover, the near-midgap bandwidth monotonically decreases with increasing the strength of the strain and increases with the width of the ZBSNR. The energy gap of the ZBSNRs decreases with increasing the applied strain and ribbon’s width. The spatial and strain dependency of the exchange interaction in various configurations of the magnetic impurities are also evaluated. It is shown that that magnetic interactions between adsorbed magnetic impurities in B2S nanoribbons can be manipulated by careful strain engineering of such systems. We found that the RKKY coupling between adsorbed impurities at a fixed distance on the ZBSNR has an oscillatory behaviour versus strains, due to the strain dependence of the Fermi wave vector. As an important result, the RKKY coupling for the edge impurities is about two order of magnitude larger than when both impurities are in the bulk due to the existence of edge states at the edge of the ZBSNR. In addition, the oscillatory nature as well as the amplitude of the exchange interaction are highly sensitive to the strain. Our results suggest that these tunable electronic and magnetic properties of ZBSNRs mean they may find applications in spintronics and pseudospin electronics based on monolayer B2S nanoribbons.

**Figure 11.** The variation of \( \chi \) with strain \( \varepsilon_x \) (a), (c) and \( \varepsilon_y \) (b), (d), for different distance configurations, for \( N = 150, M = 20 \) (the \( M = 4p \) family of ZBSNRs), (a), (b) for two impurities placed on the same edge and (c), (d) for both the impurities are within the bulk of ZBSNR.
Appendix. Explicit form of the matrix elements of the intercellular and intracellular part of Hamiltonian

In this appendix, we want to show the form of the intercellular and intracellular part of Hamiltonian. We employed the tight binding model to obtain the sublattice energy values and corresponding wave functions.

In equations (3) and (4) $H_{AA}, H_{BB}$ and $H_{CC}$ are three-diagonal matrices with the following form

$$H_{AA} = \begin{pmatrix}
    U_B & t_2 & 0 & 0 & 0 & 0 \\
    t_2 & U_B & t_2 & 0 & 0 & 0 \\
    0 & t_2 & U_B & t_1 & 0 & 0 \\
    0 & 0 & t_1 & U_A & t_1 & 0 \\
    0 & 0 & 0 & t_1 & U_B & t_2 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \vdots 
\end{pmatrix}_{M \times M}$$

$$H_{BB} = \begin{pmatrix}
    U_B & t_1 & 0 & 0 & 0 & 0 \\
    t_1 & U_B & t_2 & 0 & 0 & 0 \\
    0 & t_1 & U_B & t_2 & 0 & 0 \\
    0 & 0 & t_2 & U_B & t_2 & 0 \\
    0 & 0 & 0 & t_2 & U_B & t_1 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \vdots 
\end{pmatrix}_{M \times M}$$

$$H_{CC} = \begin{pmatrix}
    U_A & t_1 & 0 & 0 & 0 & 0 \\
    t_1 & U_B & t_1 & 0 & 0 & 0 \\
    0 & t_1 & U_A & t_1 & 0 & 0 \\
    0 & 0 & t_1 & U_B & t_1 & 0 \\
    0 & 0 & 0 & t_1 & U_A & t_1 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \vdots 
\end{pmatrix}_{M \times M}$$

and $H_{AB}, H_{BC}$ are defined as

$$H_{AB} = \begin{pmatrix}
    0 & t_1 & 0 & 0 & 0 & 0 \\
    t_1 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \vdots 
\end{pmatrix}_{M \times M}$$

$$H_{BC} = \begin{pmatrix}
    0 & t_2 & 0 & 0 & 0 & 0 \\
    t_2 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \vdots 
\end{pmatrix}_{M \times M}$$

The $H_{01}$ Hamiltonian matrix, has all elements equal to zero except for element $[3, 1]$ which is equal to $H_{CA}$, given by

$$H_{CA} = \begin{pmatrix}
    0 & t_1 & 0 & 0 & 0 & 0 \\
    t_1 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \vdots 
\end{pmatrix}_{M \times M}$$

For a finite size nanoribbon of width $M$ and length $L = N$, the Hamiltonian matrix is a three-diagonal $(M \times N) \times (M \times N)$ matrix as

$$H = \begin{pmatrix}
    H_{AA} & H_{AB} & 0 & 0 & 0 & 0 \\
    H_{AB} & H_{BB} & H_{BC} & 0 & 0 & 0 \\
    0 & H_{BC} & H_{CC} & H_{CA} & 0 & 0 \\
    0 & 0 & H_{CA} & H_{AA} & H_{AB} & 0 \\
    0 & 0 & 0 & H_{AB} & H_{BB} & H_{BC} \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \vdots 
\end{pmatrix}_{[M \times N] \times [M \times N]}$$
References

[1] Ruderman M A and Kittel C 1954 Indirect exchange coupling of nuclear magnetic moments by conduction electrons Phys. Rev. 96 99
[2] Kasuya T 1956 A theory of metallic ferro- and antiferromagnetism on zener’s model Prog. Theor. Phys. 16 45
[3] Yosida K 1957 Magnetic properties of cu-rn alloys Phys. Rev. 106 893
[4] Vozmediano M A H, Lopez-Sancho M P, Stauber T and Guinea F 2005 Local defects and ferromagnetism in graphene layers Phys. Rev. B 72 155121
[5] Brey L, Fertig H A and Das Sarma S 2007 Diluted graphene antiferromagnet Phys. Rev. Lett. 99 116802
[6] Priour D Jr., Hwang E H and Das Sarma S 2004 Disordered rkkk lattice mean field theory for ferromagnetism in dilutated magnetic semiconductors Phys. Rev. Lett. 92 117201
[7] Matsukura F, Ohno H, Shen A and Sugawara Y 1998 Transport properties and origin of ferromagnetism in (ga,rm)as Phys. Rev. B 57 2037[8]
[8] Ko K T et al. 2011 Rkkk ferromagnetism with ising-like spin states in intercalated fe$_3$al$_2$ Phys. Rev. Lett. 107 247201
[9] Ohno H 1998 Making nonmagnetic semiconductors ferromagnetic Science 281 951
[10] Minamitani E, Dino W A, Nakanishi H and Kasai H 2010 Effect of antiferromagnetic rkkk interaction and magnetic field in a two-impurity kondo system Phys. Rev. B 82 153203
[11] Hsu C-H, Stano P, Klinovaja J and Loss D 2015 Antiferromagnetic nuclear spin helix and topological superconductivity in $^{33}$c nanotubes Phys. Rev. B 92 235435
[12] Zare M, Parhizgar F and Asgari R 2016 Topological phase and edge states dependence of the rkkk interaction in zigzag silicene nanoribbon Phys. Rev. B 94 045403
[13] Shiranaz M, Cheraghchi H and Parhizgar F 2017 Effect of the rashba splitting on the rkkk interaction in topological-insulator thin films Phys. Rev. B 96 024413
[14] Abadin D A and Pesin D A 2011 Ordering of magnetic impurities and tunable electronic properties of topological insulators Phys. Rev. Lett. 106 136802
[15] Eggenkamp P J T, Swagten H J M, Story T, Litvinov V I, Swüste C H W and de Jonge W J M 1995 Calculations of the ferromagnet-to-spin-glass transition in diluted magnetic systems with an rkkk interaction Phys. Rev. B 51 15250
[16] Liu F-S, Roshen W A and Ruvalds I 1987 Resistivity from magnetic impurity pairs in metallic alloys Phys. Rev. B 36 492
[17] Parhizgar F, Sherafati M, Asgari R and Satpathy S 2013 Ruderman-kittel-kasuya-yosida interaction in biased bilayer graphene Phys. Rev. B 87 165429
[18] Parhizgar F, Rostami H and Asgari R 2013 Indirect interaction between magnetic adatoms in monolayer mos $\_2$ Phys. Rev. B 87 125401
[19] Zhu J-J, Yao D-X, Zhang S-C and Chang K 2011 Electrically controllable surface magnetism on the surface of topological insulators Phys. Rev. Lett. 106 097201
[20] Hosseini M V and Askari M 2015 Ruderman-kittel-kasuya-yosida interaction in wyl semimetalas Phys. Rev. B 92 224435
[21] Parhizgar F, Asgari R, Abedinpour S and Zareyan M 2013 Anisotropic rkkk interaction in spin-polarized graphene Phys. Rev. B 12 125402
[22] Sherafati M and Satpathy S 2011 Rkkk interaction in graphene from the lattice green’s function Phys. Rev. B 83 165425
[23] Shiranaz M, Parhizgar F, Fransson J and Cheraghchi H 2017 Impurity scattering on the surface of topological-insulator thin films Phys. Rev. B 95 235429
[24] Zare M, Parhizgar F and Asgari R 2018 Strongly anisotropic rkkk interaction in monolayer black phosphorus J. Magn. Magn. Mater. 456 307–15
[25] Zutic I, Fabian J and Sarma S D 2004 Spintronics: fundamentals and applications Rev. Mod. Phys. 73 323
[26] Babar R and Kabir M 2016 Transition metal and vacancy defect complexes in phosphorene: a spintronic perspective J. Phys. Chem. C 120 27
[27] Han W, Kawakami R K, Gmitra M and Fabian J 2014 Graphene spintronics Nat. Nano 9 794–807
[28] Zare M and Saidgehi E 2018 Exchange interaction of magnetic impurities in a biased bilayer phosphorene nanoribbon Phys. Rev. B 98 205401
[29] Klinovaja J and Loss D 2013 Rkkk interaction in carbon nanotubes and graphene nanoribbons Phys. Rev. B 87 045422
[30] Duan H, Li S, Zheng S-H, Sun Z, Yang M and Wang R-Q 2017 Anisotropic rkkk interaction and modulation with mechanical strain in phosphorene New J. Phys. 19 103010
[31] Pereira V M and Neto A H Castro 2009 Strain engineering of graphene’s electronic structure Phys. Rev. Lett. 103 046801
[32] Liu F, Ming P and Li J 2007 Ab initio calculation of ideal strength and phonon instability of graphene under tension Phys. Rev. B 76 064120
[33] Pereira V M, Castro Neto A H and Peres N M R 2009 Tight-binding approach to uniaxial strain in graphene Phys. Rev. B 80 045401
[34] Power S R, Gorman P D, Duffy J M and Ferreira M S 2012 Strain-induced modulation of magnetic interactions in graphene Phys. Rev. B 86 195423
[35] Peng F and Hongbin W 2012 Strain enhanced exchange interaction between impurities in graphene Phys. B (Amsterdam) 407 3434
[36] Guinea F, Katsnelson M I and Geim A K 2010 Energy gaps and a zero-field quantum hall effect in graphene by strain engineering Nat. Phys. 6 30
[37] Sharma A, Kotov V N and Castro Neto A H 2013 Effect of uniaxial strain on ferromagnetic instability and formation of localized magnetic states on adatoms in graphene Phys. Rev. B 87 155431
[38] Zhao Y, Li X, Liu J, Zhang C and Wang Q 2018 A new anisotropic dirac cone material: a b2l honeycomb monolayer J. Phys. Chem. Lett. 9 1815–20
[39] Li P, Li Z and Yang J 2018 Rational design of two-dimensional anode materials J. Phys. Chem. Lett. 9 4852–6
[40] Zhang L-Z, Wang Z F, Du S X, Gao H J and Liu F 2014 Prediction of a dirac state in monolayer Tjbs, Phys. Rev. B 90 161402(R)
[41] Zhang H, Li Y, Hou J, Du A and Chen Z 2016 Dirac state in the feb2 monolayer with graphene-like boron sheet Nano Lett. 16 6124–9
[42] Harrison W A Elementary Electronic Structure (Singapore: World Scientific)
[43] Tang H, Jiang J W, Wang B S and Su Z B 2009 A full spd tight-binding treatment for electronic bands of graphitic tubes Solid State Commun. 149 82
[44] Jiang J W and Park H S 2015 Phys. Rev. B 91 235118
[45] Lu Y and Guo J 2010 Band gap of strained graphene nanoribbons Nano Res. 3 189–99
[46] Zhang Y, Wu X, Li Q and Yang J 2012 Linear band-gap modulation of graphene nanoribbons under uniaxial elastic strain: a density functional theory study J. Phys. Chem. C 116 9356–9
[47] Carvalho A, Rodin A and Neto A C 2014 Phosphorene nanoribbons Europhys. Lett. (EPL) 108 47005
[48] Guo H, Lu N, Da J, Wu X and Zeng X C 2014 Phosphorene nanoribbons, phosphorus nanotubes, and van der waals multilayers J. Phys. Chem. C 118 14051
[49] Soleimanikahnoj S and Knezevic I 2017 Pseudospin electronics in phosphorene nanoribbons Phys. Rev. Appl. 8 064021
[50] Imamura H, Bruno P and Utsumi Y 2004 Twisted exchange interaction between localized spins embedded in a one- or two-dimensional electron gas with rashba spin–orbit coupling Phys. Rev. B 69 121303(R)