Spin stiffness in zigzag graphene nanoribbon under electric field

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Abstract. We considered the effect of the electric field on the spin stiffness in the zigzag graphene nanoribbon by means of first-principles calculation. To reach the intention, a fixed planar spiral structure was formed together with a spin constraint method in the antiferromagnetic edge states of the zigzag graphene nanoribbon. The spin stiffness was then obtained by fitting the total energy difference in a set of spiral vector via the Heisenberg model. We showed that the trend of the spin stiffness changes as the electric field increases up to certain value. This means that the electric field can control the spin stiffness in the zigzag graphene nanoribbon.

1. Introduction

The exploration of graphene, as well as the graphene nanoribbon (GNR), to exploit its benefit for applications of electronic devices is of interest until now [1-8]. Some theoretical and computational aspects reveal that the GNR can be considered as a strong candidate for the promising material in nanotechnology [9]. In general, the GNR can be grouped into two kinds based on the cutting way, i.e., the armchair and zigzag graphene nanoribbons, both of which show the interesting phenomena when some treatments are employed [10-16].

It has been reported that the spin stiffness in the monolayer zigzag graphene nanoribbon (ZGNR) is higher than that in 3d transition ferromagnetic metals based on the Heisenberg model. Note that the highest spin stiffness in the ferromagnetic metals is possessed by fcc nickel, which has the spin stiffness about 700 meVÅ² [17-20]. According to Yazyev and Katsnelson [21], the spin stiffness is a parameter to examine if ZGNR-based devices can be useful in the room temperature. This indicates that the spin stiffness gives an important information for the device quality beside the band gap.

Our aim is to examine the change of spin stiffness of ZGNR when the external electric field is considered by using the density functional theory (DFT) approach within the Heisenberg model. We calculate and fit the total energy difference for a set of spiral wavevectors in the self-consistent calculation. We observe that the spin stiffness initially enhances until a certain value of electric field and then reduces. We justify that the applied electric field can govern the spin stiffness in the real system.

We give our structure of the monolayer ZGNR for the ferromagnetic and antiferromagnetic configurations in section 2. The method of how to construct the spiral structure in a reliable situation and the computational method will also be presented. We present the results and the discussions based on the results in the third section. At last, the final conclusions will be presented in the last section.
2. Method

The DFT calculation for the noncollinear structure was performed by using the OpenMX code [22], which exploits the norm-conserving pseudopotentials [23] and the localized orbital basis function [24, 25]. To calculate efficiently, we utilized the generalized Bloch theorem (GBT) to replace the supercell calculation. To do so, the noncollinear Bloch wavefunction is represented with the linear combination of pseudo-atomic orbitals (LCPAO) [26]

\[ \psi_{\nu k}(r) = \frac{1}{\sqrt{N}} \sum_{\alpha} \left[ e^{i(k-q/2) \cdot R_n} C_{\nu k, \alpha}^{\dagger}(1) + e^{i(k+q/2) \cdot R_n} C_{\nu k, \alpha}^{\dagger}(0) \right] \times \phi_{\alpha}(r - \tau_i - R_n) \] (1)

where the localized function is represented by \( \phi_{\alpha} \). Meanwhile, the magnetic moments of the carbon atoms at the edges experience a continuous rotation from site to site, which is given by

\[ M_i = M_i \{ \cos(\mathbf{q} \cdot \mathbf{R}_i) \sin \theta_i + \sin(\mathbf{q} \cdot \mathbf{R}_i) \sin \theta_i + \cos \theta_i \}, \] (2)

where \( \mathbf{q} \) and \( \mathbf{R}_i \) are the spiral and lattice vectors, respectively.

A flat spiral configuration for the ferromagnetic and antiferromagnetic alignment at the edges in the ZGNR was constructed for the fixed magnetic moments of the carbon atoms with the cone angle \( \theta = 90^\circ \) and the azimuthal angle \( \phi = 0^\circ \) at one edge and \( \phi = 180^\circ \) at the other edge with an applied constraint method [27, 28], see Fig.1. Here, we choose the planar spiral instead of the conical spiral \( (\theta < 90^\circ) \) due to the stability in the self-consistent calculation, especially for \( \mathbf{q} \) very close to zero. We applied both \( \mathbf{q} \) and electric field \( \mathbf{E} \) in the periodic direction \((x\text{-axis})\), as shown in Fig. 1.

![Figure 1](image)

**Figure 1.** Crystal model of monolayer ZGNR from top view for the ferromagnetic alignment (a) and the antiferromagnetic alignment (b). The blue and white spheres refer to carbon and hydrogen atoms while the yellow dashed line represents the unit cell.

The detailed computation applied a 150 Ryd cutoff energy within the generalized gradient approximation (GGA) as the exchange potential [29]. In addition, a \( 90 \times 1 \times 1 \) k-point mesh was used in the periodic direction. For the carbon atoms, we used a linear combination of two \( s \) primitive orbitals and two \( p \) primitive orbitals as a basis set and the cutoff radius of 4.0 Bohr while a linear combination two \( s \) primitive orbitals and one \( p \) primitive orbital are used for the hydrogen atoms with the cutoff radius of 6.0 Bohr. In addition, a lattice constant of 2.46 Å in the x-axis (periodic direction) and a vacuum area of 50 Å in the non-periodic direction were also assigned.

Before calculating the spin stiffness, we calculate the magnon energy, which is obtained from the subtraction of total energy difference with the relationship [30]

\[ \hbar \omega_\mathbf{q} = \frac{1}{M} \left( E(\mathbf{q}) - E(\mathbf{q} = 0) \right), \] (3)
where \( \hbar \omega_q \) is the magnon energy and the right-hand side denotes the total energy difference per magnetic moment obtained from the self-consistent calculation. The spin stiffness \( D \) is thus evaluated by using the quadratic dispersion relation \( \hbar \omega_q = Dq^2 \).

3. Results and Discussions
Figure 2. shows the dispersion relation, from which the spin stiffness can be obtained. We see that the magnon energy increases as the ribbon width \( N \) increases, thus the spin stiffness increases. It is also deduced that the spin stiffness in the antiferromagnetic alignment is higher than that in the ferromagnetic alignment. Because the antiferromagnetic alignment has a lower energy (more stable state) than the ferromagnetic alignment, we can deduce the spin stiffness in the antiferromagnetic alignment for the monolayer ZGNR is always higher than that in the ferromagnetic alignment.

![Figure 2](image-url)

**Figure 2.** Dispersion relation of magnon energy in the case of \( E = 0 \) for ferromagnetic alignment (a) and antiferromagnetic alignment (b) for several ribbon widths \( N \).

As observing Fig. 3, we see the different critical electric field both in the ferromagnetic alignment and in the antiferromagnetic alignment. For the tendency, as the ribbon width of the ZGNR increases, the spin stiffness, as well as the magnetic moment, initially increases up to a certain critical electric field and then decreases. A critical electric field were also obtained with different tendency in Ref. [31], which used the Hubbard model. In Ref. [31], the spin stiffness initially reduces as the electric field enhances until a certain critical electric field along \( y \) direction, the spin stiffness starts to increases and then reduces again. This difference occurs may be determined by the on-site Coulomb repulsion and the direction of the electric field, which were used by Ref. [31]. In the density functional theory, this on-site Coulomb repulsion is treated by the so-called LDA+U, which is not used in our calculation.

The interesting case occurs when the electric field is employed along the \( y \)-direction. While the spin stiffness always reduces for the antiferromagnetic alignment with the same ground state, the spiral ground state does exist for the ferromagnetic alignment [32]. However, the energy scale of the spiral state is very low, thus getting a difficulty to observe at the room temperature. This means that the property is very subtle for the implementation in the spintronic devices.

For the last comment, as mentioned in Ref. [30], the increase of the spin stiffness due to the increase of the ribbon width indicates that the energy to make an excitation of magnon in the ZGNR also increases. This is related to the separated length of the magnetic carbon atoms at the two edges, which is determined by the ribbon width. This distance represents the exchange coupling constant, which is
responsible to measure how large spin stiffness can be obtained. Therefore, we can conclude that the spin stiffness can be supervised by the electric field. For the additional information, we also justify that the highest spin stiffness always belongs to the most stable configuration, see Ref. [33].

Figure 3. Dependence of spin stiffness on electric field for ferromagnetic alignment (a) and antiferromagnetic alignment (c), and dependence of magnetic moment on electric field for ferromagnetic alignment (b) and antiferromagnetic alignment (d) in ZGNR. The boxes, filled circles, and triangles denote the ribbon width of 12, 10, and 6, respectively.

4. Conclusions
We obtain a critical electric field, at which both the spin stiffness and magnetic moment change the trend. As the ribbon width increases, the spin stiffness increases with the same tendency when the electric field is taken into account, thus requiring the energy so much to excite the magnon for the large ribbon width in the ZGNR. We also show that the larger spin stiffness is possessed by the antiferromagnetic alignment. It indicates that the most stable state must have the largest spin stiffness.

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