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Davoud Adinehloo and Morteza Fathipour
School of Electrical and Computer Engineering, University of Tehran, Tehran 14395-515, Iran

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The aim of this report is to unfold how the thermo-electric spin-polarized current in a transverse-biased zigzag graphene nanoribbon changes in the presence of uniaxial deformations and uniform perpendicular magnetic field. Employing the two-parameter Hubbard model along with the non-equilibrium Green’s function formalism, we found that both uniaxial strain and magnetic field can significantly modulate the bandgap, local distribution of edge states, and the critical transverse electric field needed to achieve the half-metallic phase in the ribbon. Our analysis shows a significant enhancement of the maximum attainable spin-polarized current as functions of both source temperature and contacts temperature difference, with increasing the magnetic field or applying any magnitude of compressive strain. Furthermore, it is shown that the magneto-resistance ratio of the device, can be drastically tuned via strain engineering, reaching values as high as $2 \times 10^4 \%$ for compressive strains of 5% magnitude.

The paper is organized as follows: The numerical models employed for computing the electronic bandstructure of ZGNRs in the presence of a perpendicular magnetic field and uniaxial deformation are explained in Sec. II. The NEGF method used to calculate the DOS and transmission coefficient are also briefly described in this section. The main results and relevant discussions on how various physical quantities of interest, including the spin-polarized current and MR ratio can be modulated with uniaxial deformations and magnetic field. Next, we address the tunability of spin-polarized current and the strain-induced variation of magneto-resistance (MR) ratio, in a transverse-biased ZGNR device driven by a temperature gradient applied across the source-drain contacts.

I. INTRODUCTION

Being the most flexible conducting material known thus far, graphene has gained tremendous attention for its use in stretchable electronics, where strain is ubiquitous and the structure is subjected to various kinds of elastic deformations. Local strain engineering is also proposed as an intriguing method for designing the essential circuit elements of all carbon-based electronics. From synthetic standpoint, for graphene on pre-strained flexible substrates, experimental evidence regarding the possibility of exerting uniform deformations of up to 25% has been reported. Furthermore, through thermal cycling and exploiting different thermal expansion coefficients of graphene and the supportive platform, it has been recently demonstrated that compressive strains of up to 2% magnitude have been reported. Graphene nanoribbons (GNRs), as quasi-1D elongated strips of graphene, experiencing uniaxial strains of up to 6% has also been synthesized recently. For zigzag-edged graphene nanoribbons (ZGNRs), theoretical investigations based on tight-binding (TB) model and density functional theory have revealed the potential of uniaxial strain as a way of tuning the electronic bandgap.

Although ballistic spin-polarized transport in a transverse-biased deformed ZGNRs, driven by a voltage gradient across the ribbon’s length, has been thoroughly studied before for thermo-spin currents in ZGNRs, previous reports employing various geometries for the device were focused solely on the undeformed structures. Given the recent advances in designing efficient experimental routes to exert elastic deformations on low-dimensional nanostructures in conjunction with the growing interest in graphene as an appealing platform for spin caloritronic applications, in this work, for the first time, including the short-range electron-electron interactions, the concurrent influences of uniaxial strain and magnetic field on the energy spectrum of ZGNRs are investigated. The mean field approximation of the two-parameter Hubbard model in conjunction with the non-equilibrium Green’s function (NEGF) formalism is employed to serve the purpose in computing the electronic bandstructure, and spin-resolved thermo-electric current. We unfold how the bandgap and spatial distribution of density of states (DOS) are affected in deformed ZGNRs subjected to various magnitudes of magnetic field. Furthermore, with a brief introduction on the achievability of half-metallic phase in the ZGNRs, through the application of a critical transverse electric field, we address its modification with uniaxial deformations and magnetic field. Next, we address the tunability of spin-polarized current and the strain-induced variation of magneto-resistance (MR) ratio, in a transverse-biased ZGNR device driven by a temperature gradient applied across the source-drain contacts.

II. NUMERICAL METHODS

Adopting the standard convention in categorizing ZGNRs, hereafter $N_x$-ZGNR is referred to a ribbon with $N_x$ zigzag chains across its width (see Fig. 1(a)). With orthogonal $p_z$ orbitals as the basis, the mean field approximation of the two-parameter Hubbard model, i.e.,

\[
\begin{align*}
H &= \sum_{\langle ij \rangle} t_{ij} c_{i \sigma}^\dagger c_{j \sigma} + \sum_{\langle \sigma \rangle} \sum_{\langle ij \rangle} \epsilon_{ij} c_{i \sigma}^\dagger c_{j \bar{\sigma}} \\
&\quad + \sum_{\langle \sigma \rangle} \sum_{i} U_{i\sigma} n_{i\sigma} (1-n_{i\sigma}) c_{i \sigma}^\dagger c_{i \sigma},
\end{align*}
\]

where $t_{ij}$ is the hopping integral between nearest neighbor sites, $\epsilon_{ij}$ is the on-site energy, $U_{i\sigma}$ is the Hubbard U parameter, and $n_{i\sigma} = c_{i \sigma}^\dagger c_{i \sigma}$ is the occupation number of an electron with spin $\sigma$. The Hamiltonian is solved for the ground state using a density matrix renormalization group method, and the electronic bandstructure, and spin-resolved thermo-electric current are obtained as functions of magnetic field and temperature.

The NEGF method is employed to calculate the DOS and transmission coefficient. The main results and relevant discussions on how various physical quantities of interest, including the spin-polarized current and MR ratio can be modulated with uniaxial deformations and magnetic field. Next, we address the tunability of spin-polarized current and the strain-induced variation of magneto-resistance (MR) ratio, in a transverse-biased ZGNR device driven by a temperature gradient applied across the source-drain contacts.
is employed in this report to model the relevant energy bands of interest for electronic transport properties. In Eq. (1), $c_{i\sigma}^\dagger$, $c_{i\sigma}$ and $n_i$ are the creation, annihilation, and occupation number operators, respectively, for an electron with spin $\sigma = \uparrow, \downarrow$ located at the $i$-th atomic site in the ZGNR. $t_{ij}$ is the undeformed hopping element between sites $i$ and $j$, is assumed to be $-3$ eV (Ref. 16) and $\langle i,j \rangle$ stands for the nearest-neighbor pairs of atoms. $U$, the Hubbard parameter, represents the on-site Coulomb repulsion and is set to be 3 eV.\(^\text{17}\) $\langle n_i \rangle$ given by

$$\langle n_i \rangle = \int_{-\infty}^{+\infty} dE D_{i,\sigma}(E)f(E)$$

is the average spin-resolved electron density, where $f$ is the Fermi-Dirac distribution function and $D_{i,\sigma}$ is the local density of states (LDOS) with spin $\sigma$ at $i$-th carbon site. We incorporate the NEGF formalism to obtain the physical quantities of interest, namely, LDOS and transmission probability. In accordance with this approach, the LDOS can be obtained via

$$D_{i,\sigma}(E) = -\frac{1}{2\pi} \text{Im}[G_{\sigma}^{i\sigma}(E) - G_{\sigma}^{\sigma i}(E)]_{ii},$$

where $G_{\sigma}^{i\sigma}(E)$ is the spin-dependent retarded/advanced Green’s function of the channel, defined as

$$G_{\sigma}^{i\sigma}(E) = \left[ E I - H - \Sigma_{S,\sigma}^{i\sigma}(E) - \Sigma_{D,\sigma}^{i\sigma}(E) \right]^{-1},$$

$I$ is the unity matrix and $\Sigma_{S,\sigma}^{i\sigma}$ and $\Sigma_{D,\sigma}^{i\sigma}$ are the spin-dependent retarded/advanced self-energies for the source and drain, respectively. Only for computational purposes, Eq. (1) is decoupled into two spin-dependent terms $(H_{\sigma=\uparrow,\downarrow})$, linked via the spin-resolved electron density. With an anti-ferromagnetic initial condition, a self-consistent field procedure (Eqs. (1)–(4)) is then used to obtain the electronic properties of the ribbon.\(^\text{15}\)

The Landauer-Büttiker formula is adopted to calculate the spin-polarized current, through

$$I_\sigma = \frac{q}{\hbar} \int_{-\infty}^{+\infty} dE T_\sigma(E) \Delta f(E, T_\sigma, T_s + \Delta T),$$

where $\Delta f$ is the source-drain Fermi functions difference,\(^\text{18}\) $T_s$ and $T_s + \Delta T$ ($\Delta T$ denoting the temperature difference) are assumed to be the operating absolute temperatures of source and drain, respectively. $T_\sigma$ is the spin-dependent transmission coefficient given by $T_\sigma = \text{Tr}[G_{\sigma}^{\uparrow\uparrow}G_{\uparrow\downarrow}G_{\downarrow\uparrow}G_{\downarrow\downarrow}]$, where $\Gamma_{S(D)}$ is the broadening function for the source (drain) contact and is defined as $\Gamma_{S(D)} = -\text{Im}\{[\Sigma_{S(D),\sigma}^{\sigma\sigma} - \Sigma_{S(D),\sigma}^{\sigma\sigma}]\}$.

To achieve a spin-polarized current, a transverse electric field which changes the on-site potentials along the $y$-axis is employed. To model this effect, the following term should be added to the system’s Hamiltonian in Eq. (1):

$$H_E = \sum_{i,\sigma} qE_{ext} \langle n_i \rangle_{i,\sigma}$$

FIG. 1. (a) The atomic structure of an undeformed $N_z$-ZGNR. $a = 2.41$ Å is the ribbon’s lattice constant. Grey (white) filled circles denote carbon atoms which belong to sublattice A (B). $x$-axis is chosen in a way that it passes through the middle of the ribbon. (b) The electronic bandstructure of an $8$-ZGNR calculated from the TB method and Hubbard model. (c) Spatial profile of the spin-resolved probability for $k_x = 0.78$ and 0.9 (labeled as 1 and 2, respectively, in (b)) in the first conduction and valance bands. Blue/red color circles denote spin up/down. The radius of each circle is proportional to the amplitude of probability on each atomic site.
where $E_{\text{ext}}$ is the applied external electric field and $y_i$ is the transverse position of the $i$-th carbon atom.$^{19}$

To model the electronic bandstructure of a deformed structure, we have adopted the model outlined in Ref. 8, in which the bonding lengths of undeformed ($r$) and deformed ($r'$) structures are related, through

$$r' = \sqrt{[(1 + \varepsilon)\cos(\alpha)]^2 + [(1 - \nu\varepsilon)\sin(\alpha)]^2}r,$$  

(7)

where $\varepsilon$ is the uniaxial strain, with its positive/negative value, which denotes a tensile/compressive strain. $\nu$ is the Poisson’s ratio, relating the subsequent shrinkage (stretching) in the direction perpendicular to the pulling (compressing) axis (here, $y$- and $x$-axes, respectively) and is set to be 0.165 for ZGNR.$^{20}$ $\alpha$ is the angle between undeformed bonding length ($r$) and $x$-axis. Bonding length dependency of the hopping parameters can be described by the Harrison’s model which suggests that: $t'_{ij} = \xi^{-2}t_{ij}$, where $\xi$ is a dimensionless parameter, defined as $\xi = r'/r$ and $r'$ is the hopping amplitude in the presence of uniaxial strain.$^{21}$

Peierls phase approximation is invoked to compute the ribbon’s energy spectrum under a uniform perpendicular magnetic field.$^{16}$ The acquired phase and the modified hopping elements can be expressed by

$$t'_{ij} = t_{ij} \exp \left(\frac{i q}{h} \int_{r}^{r'} A \cdot dl\right),$$  

(8)

where $r_{ij}$ is the undeformed coordinate of atom $i/j$ and $t'_{ij}$ is the modified hopping parameter in the presence of magnetic field. $A$ is the vector potential, assumed to be $A = (-\phi, 0, 0)/\xi S$, where $\phi$ is the magnetic flux passing through each hexagon ring (with area $S$ for an undeformed ribbon) of the honeycomb lattice.

As a final remark, Eq. (8) with some minor modifications can also be used in the concurrent presence of magnetic field and uniaxial strain to modify the hopping elements. These changes include replacing $t_{ij}$ with $t'_{ij}$ (obtained from Harrison’s Model), inserting coordinates of deformed structure instead of those for undeformed ribbon, and changing the area of a hexagon to $S \times (1 + \varepsilon)(1 - \nu\varepsilon)$.

### III. RESULTS AND DISCUSSION

In this section, we present our main numerical results and related discussions. The section is divided into three segments, covering the separate effects of uniaxial strain and perpendicular magnetic field in the first two parts, followed by Sec. III C on the concurrent impacts of both perturbations.

In each part, we first explore how the ribbon’s electronic bandstructure is changed by a specific type of perturbation, and then we address how the device performance is affected by it. In our numerical treatment, $N_z$ is chosen to be 8. Furthermore, in all calculations, both channel and contact regions of the device experience the uniaxial deformation, magnetic field, or the transverse electric field, if applied.

#### A. Variation of spin current with uniaxial strain

The electronic bandstructures of an 8-ZGNR, obtained from both tight-binding method (Eq. (1) with $U = 0$) and Hubbard model are depicted in Fig. 1(b). The unique feature of the energy spectrum in zigzag-edged GNRs, as reported previously in literature, is the emergence of edge states, defined as the electronic states localized in the ribbon’s edges, while being extended along the periodic direction.$^{22,23}$

To quantitatively distinguish the electronic states localized at the edges from those with the bulk nature, we define a critical wave-vector, $k_c$:

$$k_c = 2 \cos^{-1}\left(\frac{0.13 + 0.38(1 + \varepsilon)}{1 - \nu\varepsilon}\right) \times \frac{N_z}{N_z + 1},$$  

(9)

which restricts edge states to be in the first conduction/valance band (CB/VB) with the pertaining wave-vector in the range, $k_c < |k_{\text{edge}}| < 1$. We stress that the above analytical form for $k_c$, including the effect of uniaxial strain, is reported here for the first time, and is obtained by extending the detailed procedure outlined previously in Ref. 24 for the undeformed ribbons.

The energy spectrums obtained from both methods, as shown in the figure, are distinct only in the energy regions pertaining to edge states, in which the TB approach predict a metallic ground state, while the Hubbard model suggests a semiconducting behavior (with a bandgap, $\Delta_0$). The discrepancy is mainly attributed to the presence of a large number of states (an immediate consequence of the flat bands appeared in the electronic bandstructure, see the TB energy spectrum in Fig. 1(b)) in the vicinity of Fermi level, each with a highly localized spatial profile. This in turn increases the significance of electron-electron interactions, as a large number of carriers, with energies close to Fermi level, will be localized in an extremely confined spatial region.$^{19,25}$

The other property of edge states is the wave-vector dependent decay rates, i.e., for the range $k_c < k_{\text{edge}} < 1$, as we increase the $k_{\text{edge}}$, the corresponding edge state penetrates less into the ribbon, manifesting a more localized behavior, see Fig. 1(c), where the spatially resolved probability pertaining to two cases of $k_{\text{edge}} =$ 0.78 and 0.9 is plotted. Although both CB and VB are spin degenerate, for both bands, states with opposite spins are localized at different edges of the ribbon.

Moreover, the spin-dependent spatial profile of edge states reverts as one moves from the CB to VB, i.e., while states with $\sigma = \uparrow$ in the CB are mostly localized on the upper edge, the up-spin states in the VB have non-zero DOS on the lower edge and vice versa for $\sigma = \downarrow$.

In Fig. 2(a), the electronic bandstructures of an undeformed ribbon are compared with those structures compressed or stretched by 10%. In all the calculations, the applied strain is limited to $\pm 10\%$, to ensure that the structural integrity of the ribbon is preserved.$^{26,27}$ As seen in the figure, upon the application of uniaxial strain, the low energy spectrum undergoes two major changes: (1) Compressive (tensile) strains tend to decrease (increase) the band gap. (2) The range of $k_{\text{edge}}$ corresponding to edge-states increases (decreases) with tensile (compressive) strains. The latter is further verified by
the monotonic reduction of \( k_s \) (obtained from Eq. (9)), as the strain changes from compressive to tensile (see the inset). To assess the spatial variation of edge states, the relative square amplitudes of electronic wave functions at sites \( 2A \) and \( 1A \) as a function of \( k_s \), for various magnitudes of strain are plotted in Fig. 2(b). This quantity can be regarded as a rough estimation of damping factor in edge states, i.e., a qualitative measure of edge localization for a state with wave-vector \( k_s \). Clearly, for a constant \( k_s \), tensile (compressive) strain decreases (increases) the damping factor, forcing the edge state to penetrate more (less) into the ribbon.

The energy-resolved DOS for both up and down spins as a function of transverse electric field are depicted in Fig. 3(a). As shown, increasing the \( E_{\text{ext}} \) decreases (increases) the bandgap for carriers with \( \sigma = \uparrow (\downarrow) \), with nearly similar slopes. At a critical magnitude of electric field (\( E_{\text{ext}}^{\text{crit}} \)), system acquires a half-metallic state, i.e., the ribbon behaves as a metal for up-spin carriers, while being an insulator for down-spin electrons. The origin of this half-metallic phase has been explored previously, attributing the semiconductor-half metallic transition to opposite energy shifts of spatially separated spin-ordered edge states.\(^{28} \) The applied electric field is restricted to be in the range \( [0, E_{\text{ext}}^{\text{crit}}] \) V/nm, for which the accuracy of the Hubbard model has been verified.\(^{10} \) In Fig. 3(b), we compare the variation of the bandgap for both up- and down-spin carriers with electric field at various strain magnitudes. According to the figure, for a constant \( E_{\text{ext}} \), compressive (tensile) strain decreases (increases) the bandgap for both types of spin and the ascending (descending) trend of \( \Delta \sigma_1 (\Delta \sigma_2) \) with transverse electric field occurs almost with the same slope, irrespective of the strain magnitude. Furthermore, \( E_{\text{ext}}^{\text{crit}} \) increases (decreases) as the ribbon is compressed (stretched) (see the inset).

Next, we focus on the effect of uniaxial strain on the device’s current. Figures 4(a) and 4(b) show the current as a function of \( T_s \) and \( \Delta T \), respectively. As shown, \( I_1 \), regardless of \( T_s \) and \( \Delta T \), is nearly zero, which can be readily explained by referring to the ascending trend of \( \Delta \sigma_1 \) with \( E_{\text{ext}} \) and the negligible overlap between \( \Delta \sigma_1 \) and \( T_s \) (see the inset of Fig. 4(b)). It should be emphasized that the Fermi functions difference, plotted in the inset of Fig. 4(b), is attained for the highest values of \( T_s \) and \( \Delta T \) considered in this study. Thus, it presents the maximum possible overlap, still not adequate for generating any flux of spin-down carriers. For up-spin current, however, strong modulation of current with both \( T_s \) and \( \Delta T \) can be observed.

From Fig. 4(a), for a constant \( \Delta T \), with increasing \( T_s \), \( I_1 \) is nearly zero till a threshold temperature, \( T_s^{\text{th}} \) is reached. For \( T_s > T_s^{\text{th}} \), the current increases rapidly to a maximum value at \( T_s^{\text{max}} \) and then decreases gradually with further increasing the source temperature. According to Fig. 4(b), \( I_1 \) increases with \( \Delta T \) and then saturates for temperature differences above \( \Delta T^{\text{sat}} \). When uniaxial strain is applied, as shown in Figs. 4(a) and 4(b), the up-spin current experiences the following changes: (1) Compressive (tensile) strain decreases (increases) both the \( T_s^{\text{th}} \) and \( T_s^{\text{max}} \). (2) The maximum attainable current as a function of \( T_s \) increases (decreases) as the ribbon compressed (stretched). (3) Compressive (tensile) strain tends to increase (decrease) the \( \Delta T^{\text{sat}} \) and the saturated current also. To further explain these trends for the up-spin current, similar to Ref. 13, we employ a simplified version of Eq. (5) with the form

\[
I_1 = \frac{q k_B T_s}{h} \left[ h_1(T_s) + (1 - \eta)h_2(T_s, \Delta T) \right],
\]

where \( h_1 \) and \( h_2 \) are defined as

\[
h_1(T_s) = \ln \left[ 1 + \frac{e^{E_{\text{crit}}/(k_B T_s)}}{1 + e^{E_{\text{crit}}/(k_B T_s)}} \times \left( 1 + \frac{e^{E_{\text{crit}}/(k_B T_s)}}{1 + e^{E_{\text{crit}}/(k_B T_s)}} \right)^2 \right],
\]

\[
h_2(T_s, \Delta T) = \ln \left[ 1 + \frac{e^{E_{\text{crit}}/(k_B T_s(1-\eta))}}{1 + e^{E_{\text{crit}}/(k_B T_s(1-\eta))}} \times \left( 1 + \frac{e^{E_{\text{crit}}/(k_B T_s(1-\eta))}}{1 + e^{E_{\text{crit}}/(k_B T_s(1-\eta))}} \right)^2 \right],
\]

where \( \eta \) is the relative temperature difference, defined as the \( \Delta T / T_s \). \( E_{\text{crit}} \) and \( E_{\text{crit}}^{\text{up}} \) are the corresponding energies for the first two steps occurring in the \( T_s \); at energies above the Fermi level. \( E_{\text{crit}} \) and \( E_{\text{crit}}^{\text{up}} \) have the same definition as \( E_{\text{crit}}^{\text{up}} \) and \( E_{\text{crit}} \), respectively, for energies below the Fermi level (for better visualization, see the inset of Fig. 4(b)). Inserting the
modified energies of deformed structure, the effect of strain is accounted for, accordingly. Hereafter, we focus on two limits: (I) when $T_s$ and $D_T$ are comparable ($\eta \to 1$) and (II) when the temperature difference $D_T$ is much smaller compared to $T_s$, and thus $\eta \to 0$. For these extreme cases, employing Eq. (5), one can readily derive the slope of current versus $T_s$ as:

$$\frac{\partial I_t}{\partial T_s} = \frac{q k_B}{h} \left[ h_1(T_s) + T_s \frac{dh_1(T_s)}{dT_s} \right],$$

(13)

$$\frac{\partial I_t}{\partial D_T} = \frac{q k_B}{h} \left[ 2 \frac{dh_1(T_s)}{dT_s} + T_s \frac{d^2h_1(T_s)}{dT_s^2} \right].$$

(14)

The corresponding curves are plotted in the left and middle panels of Fig. 5. Comparing these analytical results with the numeric curves presented in Fig. 4(a), one can see that, irrespective of strain magnitude for both low and high source temperatures, the model can accurately predict the variation of current versus $T_s$, as

current dependence on $\Delta T$. It should be mentioned that for case I, regardless of strain’s magnitude, $\partial I_t/\partial \Delta T$ is zero, an explicit proof of saturation behavior of current at high values of $\Delta T$. For case II, the slope of $I_t$ versus $\Delta T$ has a similar analytical form as in Eq. (13) (see the results presented in the right panel of Fig. 5). As seen, the prediction of a constant positive slope, which increases (decreases) with compressive (tensile) deformation is consistent for the variation of $I_t$ with $\Delta T$ at low temperature differences.

Our discussion so far for Figs. 4 and 5 is all restricted to a specific case of $E_{ext} = 0.3 \text{ V/nm}$. To assess how changing the magnitude of applied electric field can affect the device’s current, in Figs. 6(a)–6(c), we depict the mesh plots of $T_s$, $T_{max}$, and $\Delta T_{sat}$, respectively, as functions of $\epsilon$ and $E_{ext}$. It can be inferred that increasing the transverse electric field has a similar effect to that previously explained for compressive strains, indicating the possibility of reaching even higher magnitudes of spin-polarized current, by more compressing the structure, and increasing the transverse bias voltage.

B. Magneto-induced variation of spin current

Figure 7 shows the electronic bandstructures of a 8-ZGNR in the two cases of $\varphi = 0$ and $\varphi = 0.005$. For the magnitudes of $\varphi$ in the range $[0, 0.005]$, the magnetic field only changes the energy spectrum in the range attributed to edge states. As shown in the four magnified views on the
FIG. 4. Spin-dependent current as a function of (a) source temperature ($T_s = 200$ K) at various strain magnitudes. The inset in (b) shows the energy dependence of spin-resolved transmission probabilities and source-drain Fermi functions difference at $T_s = 500$ K and $T_T = 200$ K. $E_{ext}$ is set to be 0.3 V/nm.

right side of Fig. 7(a), the spin-degeneracy is no longer preserved in the range corresponding to edge states. For the CB and positive $k_x$, the spin-up subband experiences an upward energy shift, while the corresponding spin-down subband moves downward in energy. Moreover, magnetic field also breaks the time-reversal symmetry, i.e., the corresponding energy-shifts of spins up and down is reversed when we move from the positive $k_x$ to its negative values. For edge states in the VB with $k_x > 0$ ($k_x < 0$), similar trends can be observed as those previously explained for the CB with the same wave-vector. As a consequence, the spin-resolved bandgaps do not possess a direct nature, as it was in the presence of uniaxial strain or transverse electric field and the bandgaps for both up- and down-spin carriers tend to decrease with $\varphi$. To illustrate how the magnetic field changes the spatial distribution of edge states, the occupation probabilities for four values of $k_x = \pm 0.74$ and $\pm 0.88$ in both CB and VB, as a function of site index are plotted in Fig. 7(b). As shown in these figures, magnetic field does not change the qualitative features of edge states, i.e., the edge state, irrespective of the spin type penetrates more into the ribbon, with decreasing $|k_x|$, and carriers with opposite spins are still accumulated at different edges. The main difference, however, is that in the presence of a magnetic field, damping factors will be changed, i.e., the edge state depending on its wave-vector and energy can decay more or less rapidly into the ribbon in comparison to the case where no magnetic field is applied. Nonetheless, for any edge state of spin $\sigma = \uparrow, \downarrow$, if the edge localization increases with $\varphi$, the corresponding subband will be shifted away from the Fermi energy (for CB/VB the energy shift is upwards/downwards).

In Figs. 8(a) and 8(b), the electronic bandstructures in the concurrent presence of a transverse electric field ($E_{ext} = 0.37$ and 0.41 V/nm, respectively) and perpendicular magnetic field (both with $\varphi = 0.005$) are depicted. In general, $E_{ext}$ tends to push the up-spin subbands in the conduction and valence towards each other, drifting the down-spin subbands further apart. The monotonic descending (ascending) trends of $\Delta_{\uparrow\uparrow}$ ($\Delta_{\downarrow\downarrow}$) versus $E_{ext}$ is plotted in the inset of Fig. 8(a). As shown in Fig. 8(b), for a magnetic flux of magnitude 0.005, increasing the electric field to 0.41 V/nm, closes the indirect bandgap for up-spin subbands, forcing the ribbon to fill the half-metallic state. Moreover, increasing the magnetic field, decreases the bandgap, thereby decreasing the electric field needed to induce the semiconductor to half-metal transition (see the inset of Fig. 8(b)).

In Fig. 9, we address how feasible, using a perpendicular magnetic field, is to increase the spin-polarized current. Current as a function of $T_s$ and $\Delta T$ is shown in Figs. 9(a) and 9(b), respectively. According to Fig. 9(a), for low source temperatures, increasing the magnetic flux increases the current, while at high $T_s$ the current decreases with increasing $\varphi$. The applied magnetic field also decreases $T_s^{th}$ and $T_s^{max}$ while increasing the maximum current attainable with sweeping $T_s$. Increasing $\varphi$ also increases both $\Delta T_{ext}$ and the saturation current (see Fig. 9(b)). These results can be further verified using the same approach, we employed previously for the case of uniaxial strain, i.e., the variation of current with $T_s$ and $\Delta T$ can be described with Eq. (10), redefining $h_1$ and $h_2$ as

FIG. 5. $\partial I_s / \partial T_s$ versus $T_s$ for the two cases of $\eta \rightarrow 1$ (left panel, vertical axis in units of nA/K) and $\eta \rightarrow 0$ (middle panel, vertical axis in units of pA/K), at various strains and $\Delta T = 30$ K. Right panel shows the $\Delta T$ dependence of $\partial I_s / \partial T_s$ (in units of nA/K) for $\eta \rightarrow 1$, $T_s = 200$ K, and different values of strain. $E_{ext}$ is set to be 0.3 V/nm.
FIG. 6. Mesh plot of (a) $T^0$, (b) $T^{\text{max}}$, and (c) $\Delta T^{\text{sat}}$ at data points ($E_{\text{ext}}$, $\varepsilon$). In (a) and (b), $\Delta T = 30$ K, and in (c), $T = 200$ K.

FIG. 7. (a) The electronic bandstructure of an 8-ZGNR for two values of magnetic flux. Right panel shows the magnified views of the energy spectrum for the energy ranges labeled as I–IV, specified by circles in the left panel. (b) Spin-resolved probability as a function of site index, for the first conduction and valance subbands at $k_x = \pi/0.74$, and $k_x = \pi/0.88$, labeled as 1–4 in (a).

FIG. 8. Energy bands of an 8-ZGNR with (a) $E_{\text{ext}} = 0.37$ V/nm and (b) 0.41 V/nm, both in $\varphi = 0.005$. Inset in (a) shows the $E_{\text{ext}}$ dependence of the bandgap for $\sigma = \uparrow$, $\downarrow$ at two values of magnetic flux. Inset in (b) plots the $\varphi$ dependence of $E_{\text{ext}}$. 
FIG. 9. Spin-dependent current as a function of (a) source temperature ($T_s = 30$ K) and (b) contacts temperature difference ($T'_s = 200$ K) at various magnetic fields. (c) The energy dependence of spin-resolved transmission probabilities. $E_{\text{ext}}$ is set to be $0.34$ V/nm.

$$h_1(T_s) = \ln \left[ 1 + \frac{e^{E_{c1}/(k_b T_s)}}{1 + e^{E_{c1}/(k_b T_s)}} \times \frac{1 + e^{E_{c2}/(k_b T_s)}}{1 + e^{E_{c2}/(k_b T_s)}} \times \frac{1 + e^{E_{c3}/(k_b T_s)}}{1 + e^{E_{c3}/(k_b T_s)}} \right],$$

$$h_2(T_s, \Delta T) = \ln \left[ 1 + \frac{e^{E_{v1}/(k_b T_s(1-\eta))}}{1 + e^{E_{v1}/(k_b T_s(1-\eta))}} \times \frac{1 + e^{E_{v2}/(k_b T_s(1-\eta))}}{1 + e^{E_{v2}/(k_b T_s(1-\eta))}} \times \frac{1 + e^{E_{v3}/(k_b T_s(1-\eta))}}{1 + e^{E_{v3}/(k_b T_s(1-\eta))}} \right],$$

where $E_{c1,2,3}$ and $E_{v1,2,3}$ are defined as the energies where the first three steep steps occurs in the up-spin transmission function for energies above and below the Fermi energy, respectively (see Fig. 9(c)). To capture the effect of magnetic field, one can simply insert the modified energies obtained from the numerical result.

Comparing the mesh plots presented in Figs. 10(a)–10(c), with those in Figs. 6(a)–6(c), the results indicate that increasing the magnetic field changes the characteristic temperatures, similar to the case where compressive strain is applied.

C. Thermally tunable MR effect in deformed ZGNRs

A contour plot of the bandgap as functions of $\varepsilon$ and $\varphi$ is shown in Fig. 11(a). In the concurrent presence of a uniform perpendicular magnetic field and uniaxial compressive deformations, the bandgap decreases more rapidly compared to the case where we solely increase the $\varphi$ or the magnitude of compressive strain. This in turn reduces the critical transverse electric field needed for inducing the half-metallic state more effectively (see Fig. 11(b)).

The variation of MR ratio, defined as

$$MR = \frac{I_I(\varphi, \varepsilon) - I_I(\varphi = 0, \varepsilon)}{I_I(\varphi = 0, \varepsilon)} \times 100,$$

as a function of $T_s$ and various magnitudes of $\varphi$ and $E_{\text{ext}}$ are presented in Fig. 12. The trends observed in the figures can be explained in the following way: as $\varphi$ increases, the corresponding $T_s^{th}$ decreases, i.e., with increasing the $\varphi$, the ascending trend versus $T_s$, $I_I(\varphi, \varepsilon)$ begins at lower source temperatures. For $I_I(\varphi, \varepsilon)$, however, the pertaining $T_s^{th}$, which can be tuned via strain’s magnitude, occurs at higher temperatures, rendering the $I_I(\varphi, \varepsilon)$ for the temperatures below this threshold to be nearly zero. Therefore, increasing the $T_s$ between these two thresholds significantly enhances the device MR ratio, reaching values as high as $2 \times 10^4\%$ for $\varphi = 0.0042$ and $\varepsilon = -5\%$. Increasing the $T_s$ above the strain-induced threshold temperature, although both currents show an ascending trend versus $T_s$, $I_I(\varphi = 0, \varepsilon)$ increases with a steeper slope, thereby decreasing the MR ratio. Furthermore, increasing the transverse electric field or the magnitude of compressive strain, increases the maximum attainable MR ratio and decreases the source temperature at which MR ration is maximized.

In Fig. 13, the $\Delta T$ dependence of MR ratio for various magnitudes of $\varphi$ and $E_{\text{ext}}$ are plotted. As shown, MR ratio changes with $\Delta T$ in a similar manner as $I_I$ changes with $\Delta T$, i.e., it increases with $\Delta T$ and then saturates at a maximum value. According to these figures, although, with changing the magnitude of transverse electric field, magnetic field, or applied strain, the MR ratio as a function of $\Delta T$ can be tuned, the attainable variation is much smaller compared to the

FIG. 11. Contour plot of the (a) bandgap and (b) $E_{\text{ext}}^{\text{cm}}$ for an 8-ZGNR as functions of magnetic flux and uniaxial strain.

FIG. 10. Mesh plot of (a) $T_s^{th}$, (b) $T_s^{mn}$, and (c) $\Delta T^{th}$ at data points ($E_{\text{ext}}$, $\varphi$). In (a) and (b), $\Delta T = 30$ K, and in (c), $T_s = 200$ K.
previous case in Fig. 12, where we changed the source temperature at a fixed $\Delta T$.

IV. CONCLUSION

In this work, the concurrent influence of uniaxial deformation and perpendicular magnetic field on the thermoelectric spin-polarized current in a transverse-biased ZGNR device, employing the mean field approximation of the two-parameter Hubbard model in conjunction with the non-equilibrium Green’s function formalism, has been investigated. Inspecting the energy spectrum of deformed ZGNRs or ribbons subjected to various magnitudes of magnetic flux, we found that the critical transverse electric field, needed to trigger the half-metallic phase, decreases as the ribbon is compressed or as the magnetic field increases. With the simultaneous application of both, we have shown that the critical transverse field decreases with a steeper slope, compared to the case where we solely increase the magnetic flux or the magnitude of compressive strain.

From the device’s perspective, our calculations show a significant enhancement of the maximum attainable spin-polarized current as functions of both source temperature and leads temperature difference, with increasing magnitudes of compressive strain or magnetic field. We further report that both magnetic field and compressive deformations tend to decrease the threshold source temperature needed to generate a spin-polarized current and the source temperature at which the current versus $T_s$ is maximized. Furthermore, as the ribbon is compressed or as it experiences higher magnetic fields, the saturation of the current with the variation of source-drain temperature difference, appears at higher temperatures. Our results also reveal that with the concurrent application of a uniform perpendicular magnetic field and uniaxial deformation, one can considerably tune the magneto-resistance ratio of the device. In particular, it is suggested that with experimentally feasible magnitudes of compressive strain, MR ratios as high as $2 \times 10^4$ can be achieved at the magnetic flux of 0.005.

In conclusion, our results demonstrate the prospect of exploiting strain engineering, as a feasible method to generate near-ideal spin-polarized currents in the ZGNR-based devices, rendering zigzag-edged ribbons to manifest remarkably high room temperature MR ratios.

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