Stacking Domain Wall Magnons in Twisted van der Waals Magnets

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Using bilayer CrI3 as an example, we demonstrate that stacking domain walls in van der Waals magnets can host one dimensional (1D) magnon channels, which have lower energies than bulk magnons. Interestingly, some magnon channels are hidden in magnetically homogeneous background and can only be inferred with the knowledge of stacking domain walls. Compared to 1D magnons confined in magnetic domain walls, 1D magnons in stacking domain walls are more stable against external perturbations. We show that the relaxed moiré superlattices of small-angle twisted bilayer CrI3 is a natural realization of stacking domain walls and host interconnected moiré magnon network. Our work reveals the importance of stacking domain walls in understanding magnetic properties of van der Waals magnets, and extends the scope of stacking engineering to magnetic dynamics.

The physical properties of two-dimensional (2D) van der Waals materials depend sensitively on the stacking arrangement between adjacent layers. Consequently, the modulation of stacking can strongly modify the local electronic properties. For example, in bilayer graphene, the stacking domain walls between the AB and BA stackings [1][2] induce a variation in the electronic Hamiltonian, which can give rise to one dimensional (1D) topologically protected electronic states [3][4][5]. Similarly, in transition metal dichalcogenides (TMD), electrons can be confined in stacking domain walls, which can be controlled experimentally via strain engineering [7].

Recently it has been realized that the stacking dependence also extends to magnetic properties. For example, in bilayer CrI3, the interlayer exchange coupling changes sign as the stacking is varied [8][13]. Therefore a stacking domain wall also induces a modulation in the spin Hamiltonian. It is thus natural to expect stacking domain walls to host 1D spin wave (magnon) channels. Previously, confined 1D magnons have been proposed to exist in magnetic domain walls [14][15]. However, magnetic domain walls are generally fragile with respect to external perturbations and may even have its own dynamics. On the other hand, stacking domain walls, whose energy scale is at least one order of magnitude larger than magnetic domain walls, provide a more stable platform to host 1D magnons.

In this work, using bilayer CrI3 as an example, we study 1D magnons in stacking domain walls in van der Waals magnets. We show that, quite generally, all stacking domain walls of bilayer CrI3 can host 1D magnons, which have lower energies than bulk magnons. The existence of these 1D magnons can be adiabatically traced back to the Goldstone modes of the spin Hamiltonian. Interestingly, we find that some magnon channels are hidden in magnetically homogeneous background and can only be inferred with the knowledge of stacking domain walls. These domain walls are naturally realized in moiré superlattices in twisted bilayer magnets with small twist angles. Moiré magnons have been recently studied in Refs. [16][18]. However, these works have ignored lattice relaxation, and the information of stacking domain walls are not utilized in the construction of the spin Hamiltonian. With a full account of lattice relaxation, we calculate the stacking and magnetic moiré pattern in small angle twisted bilayer CrI3 (Fig.3). In this system, the stacking domain walls and corresponding 1D magnon channels are interconnected, forming a magnon network, which will dominate low-energy spin and thermal transport. Our work reveals the importance of stacking domain walls in understanding magnetic properties of van der Waals magnets, and extends the scope of stacking engineering to magnetic dynamics.

Stacking domain wall.—CrI3 is a layered magnetic material in which the magnetic order can survive down to the monolayer limit [19]. The Cr atoms in a monolayer CrI3 forms a hexagonal lattice with lattice constant 6.9 Å. Monolayer CrI3 is a ferromagnet with the easy axis pointing to the out-of-plane direction. Bilayer CrI3 has two stable stackings, i.e., rhombohedral and monoclinic stackings. Both stackings have roughly the same energy, but rhombohedral stacking strongly favors interlayer ferromagnetic (FM) configuration while monoclinic stacking weakly favors interlayer antiferromagnetic (AFM) configuration [8][13].

The stacking configuration is described by the relative in-plane displacement \( b \) between the top and bottom layer [Fig. 1(a)], which is only defined modulo lattice translations. All possible values of \( b \) constitutes the stacking space, which coincides with the unit cell of CrI3. Stacking domain walls are described by a continuous variation of the stacking vector \( b \). In our study of each domain wall, we choose our coordinates such that the domain wall always lies in the \( z \) direction at \( x \sim 0 \). The \( y \) axis points to the out-of-plane direction. \( x \ll 0 \) is the left stacking domain, described by \( b(\sim \infty) = -b_{\text{left}} \). Similarly, \( b(\sim \infty) = b_{\text{right}} \) is the stacking vector of the right stacking domain. Around \( x = 0 \), \( b(x) \) changes rapidly from \( b_{\text{left}} \) to \( b_{\text{right}} \), passing through a series of unstable stackings. In CrI3, there are three types of stacking domain walls: domain walls
The elastic energy $E_{\text{str}}$ can be minimized by solving the Euler-Lagrangian equation $\delta E_{\text{str}} / \delta b = 0$. For the RM domain wall, $V$ is roughly reflection symmetric with respect to the line connecting rhombohedral and monoclinic stackings (yellow line in Fig. 1[a]), and we can safely assume $b(x)$ simply takes this straight path $[b^x(x) = 0]$. Furthermore, $V$ can be approximated as a cosine function on the path of the stacking vector: the two minimums of the cosine function at $\pm \pi$ correspond to rhombohedral and monoclinic stackings (the endpoints of the yellow line); the maximum of the cosine function is in the middle between the two stable stackings. With this assumption, the Euler-Lagrangian equation admits a solution:

$$b^z = 2(b^z_{\text{right}} - b^z_{\text{left}}) \arctan[x/w]/\pi + b^z_{\text{left}}. \quad (2)$$

The characteristic width $w = |b_{\text{left}} - b_{\text{right}}| \sqrt{G/V_0}/\pi$ is roughly $8.8 \, \text{Å}$, where $V_0$ is the barrier of $V$ along the path of $b(x)$. Notice that the range of $x$ for which $\arctan[x/w]$ varies significantly is roughly $6w$.

In contrast, for the RR and MM domain walls, $b(x)$ has to bypass a high energy barrier [AC stacking denoted by the brown dot in Fig. 1(a)], and analytic solutions cannot be obtained. We instead numerically solve the Euler-Lagrangian equation and present $b(x)$ as the red line and cyan line in Fig. 1[a] for the two types of domain walls. Nevertheless, it is possible to fit $b^z$ to Eq. (2) to obtain an estimation of the domain wall width. The characteristic widths for the RR and MM domain walls are $9.5$ and $7.5 \, \text{Å}$, respectively. All three types of stacking domain walls are plotted in Fig. 1[c]. Note that we are studying shear domain walls and therefore $b_{\text{left}} - b_{\text{right}}$ is always along the domain wall direction.

**1D magnon channel.—**The variation of the stacking vector $b$ induces a variation in interlayer exchange coupling. In Fig. 1(b), we plot interlayer exchange couplings for different stackings together with paths of $b(x)$ for the three types of stacking domain walls. To study the magnetic properties of the domain walls, we again take the continuous limit and adopt the following micromagnetics energy functional

$$E_{\text{mag}} = \int \left[ \sum_{\alpha, \beta, l} \frac{A}{2} (\partial_\alpha m^\beta_l)^2 - \sum_l \frac{K}{2} (m^l)^2 - \sum_{\alpha} J m^\alpha_1 m^\alpha_2 \right] \, dx, \quad (3)$$

where $\alpha, \beta$ are Cartesian indices, $l$ is layer index and $m$ is the unit vector pointing in the direction of magnetization. The first term and the second term in $E_{\text{mag}}$ is intralayer FM coupling and magnetic anisotropy, where $A \approx 5.3 \, \text{meV}$ and $K \approx 0.032 \, \text{meV} / \text{Å}^2$ for monolayer CrI$_2$. The last term describes the interlayer exchange coupling, where $J$ depends on $x$ and is plotted in Fig. 1[d] for different domain walls.

We start with the magnetic properties of the RR domain wall. Rhombohedral stacking strongly favors interlayer FM configuration. In the domain wall, the stacking vector passes through an region favoring interlayer AFM configuration [Fig. 1[b, d]]. However, this interlayer AFM tendency is punished by both intralayer FM coupling ($\propto A$) and the magnetic anisotropy ($\propto K$). To quantitatively characterize the competition, we carry out simulations of the Landau-Lifshitz-Gilbert equation with the damping term. Our simulation shows that...
the weak interlayer AFM coupling within the domain wall does not change the direction of the magnetization and the ground state is simply described by a uniform, out-of-plane \( \mathbf{m} \).

The variation of interlayer exchange coupling, although not manifested in the magnetic ground state, will enter the equation of motion of magnetization dynamics, \( \delta \mathbf{m}_i = -\gamma \mathbf{m}_i \times \mathbf{H}_i \), where the effective magnetic field is proportional to the functional derivative of \( E_{\text{mag}} \) with respect to \( \mathbf{m}_i \) (\( i = 2 \) and \( \bar{i} = 1 \))

\[
\mathbf{H}_i = AV^2 \mathbf{m}_i + K m_i^z \mathbf{y} + J m_{\bar{i}},
\]

where \( \gamma \) is the gyromagnetic ratio. Since \( \mathbf{m} \) is a unit vector, the first order variation of magnetization is written as \( \delta \mathbf{m}_i = \delta m_i^x \hat{x} + \delta m_i^y \hat{y} + \delta m_i^z \hat{z} \). The ground state respects mirror symmetry in the \( y \) direction (\( M_\gamma \)), so it is natural to decouple the mirror eigenspaces by defining \( \delta \mathbf{m}_\pm = (\delta \mathbf{m}_1 \pm \delta \mathbf{m}_2)/2 \). With the notation \( \delta m_i^x = \delta m_i^y + i\delta m_i^z \), the Landau-Lifshitz equation can be transformed to two decoupled Schrödinger type equations:

\[
i\gamma^{-1} \partial_t \delta m_i^+ = [-A \partial_x^2 + K + Ak_z^2] \delta m_i^+, \\
i\gamma^{-1} \partial_t \delta m_i^- = [-A \partial_x^2 + K + 2J(x) + Ak_z^2] \delta m_i^-,
\]

where we have assumed \( \mathbf{m} \), behaves like a plane wave in the \( z \) direction with wave vector \( k_z \). We see that \( \delta \mathbf{m}_z \) is blind to the interlayer coupling. For \( \delta \mathbf{m}_z \), since the variation of \( J(x) \) serves as a trapping potential [Fig. 1(a)], despite the magnetization of the ground state is uniform across the RR domain wall, a 1D magnon solution generally exists and is confined in the domain wall. In Fig. 2(a) we present the profile of this 1D magnon. It is a circular motion isotropic in the \( x-z \) plane and the magnon profile is independent of \( k_z \). The frequency of this 1D magnon channel at \( k_z = 0 \) is calculated to be smaller than the bulk magnon excitation gap \( \gamma K \). Therefore, the low energy magnon transport should be dominated by this 1D magnon channel.

To gain more insights into the existence of this 1D magnon channel, we assume the width and depth of the trapping potential \( J(x) \) can be artificially tuned. For a weak trapping potential \( J(x) \), the magnetic ground state is a uniform interlayer FM configuration across the RR domain wall, which is the case for CrI\(_3\). The degree of freedom \( \delta \mathbf{m}_z \) describes the deviation from interlayer FM configuration and the frequency of the corresponding magnon is determined by the energy cost of such deviation. Since in the domain wall the interlayer exchange coupling \( J(x) \) becomes smaller, such energy cost is lower in the domain wall. Therefore, a confined mode should exist in the domain wall, which is manifested as a bound state due to the trapping potential \( J(x) \) in Eq. (5). The weak trapping potential scenario is plotted in Fig. 2(a). For increasingly stronger trapping potential, there will be a critical point where the frequency of this 1D magnon at \( k_z = 0 \) becomes zero. Beyond this critical point, the magnetic ground state deviates from the interlayer FM configuration [Fig. 2(c)] in the domain wall. However, the 1D magnon mode does not disappear. The magnetic energy described by Eq. (5) is actually invariant under a global (independent of \( x \)) rotation along the \( y \) direction. This continuous symmetry immediately gives rise to a Goldstone magnon mode, which costs no energy at \( k_z = 0 \) and is still localized in the domain wall [Fig. 2(c)].

It is worth noting that \( J(x) \) does not need to become negative to trap a 1D magnon. For arbitrarily weak trapping potential, this 1D magnon solution exists. However, if \( J(x) \) never takes negative value, the frequency of the 1D magnon will be larger than the bulk magnon excitation gap \( \gamma K \). The bulk magnon with the frequency \( \gamma K \) is contributed by \( \delta \mathbf{m}_x \), which is unaffected by the interlayer exchange coupling.

Similar to the RR domain wall, the MM stacking domain wall appears between two magnetically identical (AFM) domains. However, since the AFM interlayer coupling strength in CrI\(_3\) is much weaker than FM interlayer coupling, the magnetization now tilts away from the \( y \)-axis in the MM stacking domain wall. We parameterize the magnetization of the
top layer $\mathbf{m}_1(x)$ in spherical coordinates $\theta$ (polar angle) and $\phi$ (azimuth angle) and present the magnetic ground state in Fig. 2(b). The Goldstone mode argument discussed above immediately gives rise to a zero energy 1D magnon mode trapped in the MM domain wall. Nevertheless, it is instrumental to write down the magnetic dynamical equations. We expand $\delta \mathbf{m}_1$, as $\delta \mathbf{m}_1 = \delta \mathbf{m}_1^\theta \mathbf{e}_\theta + \delta \mathbf{m}_1^\phi \mathbf{e}_\phi$, where $(\mathbf{e}_\theta, \mathbf{e}_\phi)$ is the local unit vectors associated with $\mathbf{m}_1$ [Fig. 2(b)]. Instead of $M$, the ground state now respects two fold rotation symmetry in the $x$ direction ($C_{2x}$). We decouple the eigenspaces of $C_{2x}$ by defining $\delta \mathbf{m}_\pm = (\delta \mathbf{m}_1^\theta \pm \delta \mathbf{m}_2^\theta)/2$. The dynamical equation for $\delta \mathbf{m}_\pm$ is

$$
\gamma^{-1} \partial_t \delta \mathbf{m}^\theta = (A\partial_x^2 - U^\theta - A\kappa_x^2) \delta \mathbf{m}_\pm^\theta,
$$

$$
\gamma^{-1} \partial_t \delta \mathbf{m}_+^\phi = (-A\partial_x^2 + U^\theta + A\kappa_x^2) \delta \mathbf{m}_-^\phi,
$$

where $U^\theta = -K \cos(2\phi)$ and $U^\theta = -A(\partial_x \phi)^2 + K \sin^2(\phi) - J[1 - \cos(2\phi)]$. Every term in $U^\theta$ and $U^\phi$ is a trapping potential, which is a combined effect of varying magnetization and varying $J(x)$. These trapping potentials serve as an alternative explanation for the 1D Goldstone magnon mode in the MM domain wall. The profile of the 1D magnon of $\delta \mathbf{m}_\pm$ is shown in Fig. 2(a). For $k_\parallel = 0$, the magnon is perfectly polarized: $\delta \mathbf{m}_\pm^\phi = 0$, consistent with the Goldstone mode oscillating around the $y$ axis. This perfect polarization is reduced by finite $k_\parallel$ [Fig. 2(a)]. Equation (6) shows that even when $\phi = \pi/2$ across the domain wall [for example, for weaker variation of $J(x)$] and the Goldstone mode argument fails. MM domain walls can still support 1D magnons due to the variation of $J(x)$ alone.

In the Supplementary Materials [20], we presented the dynamical equation for $\delta \mathbf{m}_-$. Whether the variation of $J$ and $\phi$ serves as a trapping potential depends on the specific parameters. Nevertheless, for bilayer CrI$_3$, $\delta \mathbf{m}_-$ also has a 1D magnon solution with energy slightly higher than the 1D magnon mode of $\delta \mathbf{m}_+$, but lower than the bulk magnons.

Finally, we investigate the properties of the RM domain wall. Since interlayer exchange couplings of rhombohedral and monoclinic stackings have opposite signs, the RM domain wall is both a stacking domain wall and a magnetic domain wall. The magnetic ground state is presented in Fig. 2(d). The top layer generally maintains FM state, but the magnetization slightly tilts away from $+y$ direction in the domain wall; the bottom layer still roughly maintains the Walker profile $\phi_0 = -2 \arctan[\exp(x/s - x_0/s)] + \pi/2$, where the characteristic width $s \approx 9.4$ Å, $s$ is smaller than the magnetic domain width $\sqrt{A/K} \approx 12.9$ Å of monolayer CrI$_3$ since the interlayer exchange coupling favors such a domain wall. The Goldstone mode argument is also applicable to RM domain wall and we have also verified numerically such a 1D magnon channel exists. Therefore, we conclude that all three types of stacking domain walls in bilayer CrI$_3$ support 1D magnon channels.

The magnetic energy functional Eq. (3) is oversimplified in the sense that it does not include all symmetry-allowed magnetic interactions. Especially, weak Dzyaloshinskii-Moriya interaction [21, 22] (DMI) is possible in this system. With DMI, the magnons in Fig. 2(a) will be generally reflection $(x \rightarrow -x)$ asymmetric, which is a new degree of freedom and can be utilized in device designing [15, 23].

Moiré magnon network.—A natural realization of stacking domain walls is by twisting the magnetic bilayer. Twisted bilayer materials create a moiré pattern, which is a periodic modulation of stackings. After being twisted, the structure will generally relax to lower its energy. For large twist angle, lattice relaxation can be ignored, and novel spin textures may appear in this range [16]. For small twist angles, the stable stackings will grow and form domains, and unstable stackings will shrink and eventually only appear around the domain walls.

To understand at which twist angles large domains of rhombohedral and monoclinic stackings appear and to obtain a real space pattern of these domains, we calculate the lattice relaxations of the twisted bilayer CrI$_3$. Lattice relaxation of moiré superlattices is determined by the competition between the interlayer potential energy and the intralayer elastic energy. This competition can be characterized by the incommensurate sampling method introduced in Ref. [24]. We present the results of lattice relaxation for several twisting angles in the Supplementary Materials [20] and estimate large stacking domains emerge for twist angle smaller than 1.3°. Figure 3 shows the stacking and magnetic domain patterns in the small angle limit. Since the AFM monoclinic stacking is actually slightly energetically higher than the FM rhombohedral stacking (by about 15 meV), the magnetic domain pattern consists of isolated AFM domains and interconnected FM domains. These domains are useful by itself. For example, using twisted bilayer CrI$_3$ as the substrate, electrons experience periodic exchange couplings in the real space and accumulate Berry phase as they move along, which may be useful to realize the topological Hall effect [23].

Figure 3 shows that all three types of stacking domain walls appear in small angle twisted bilayer CrI$_3$. Since all stacking domain walls support 1D magnon channels, the interconnected stacking domain wall gives rise to a magnon network, which will dominate the low-energy spin and thermal transport.
In summary, we propose stacking domain walls in van der Waals magnets can support 1D magnon channels. These channels can live on uniform magnetic ground states and are robust against external perturbations. They can be realized in naturally occurring stacking faults or through careful strain engineering. We show that a realistic and highly tunable playground of such 1D magnons is twisted bilayer magnets with small twist angles, where their implications in spin and thermal transport phenomena are yet to be uncovered.

We acknowledge useful discussions with Héctor Ochoa and Wenguang Zhu. This work is supported by AFOSR MURI 2D MAGIC (FA9550-19-1-0390). The understanding of moiré magnon network is partially supported by DOE de-sc0012509. Y.G. and H.L. also acknowledge partial support from China Scholarship Council (No. 201906340219 and No. 201904910165). Computing time is provided by BRIDGES at the Pittsburgh supercomputer center (Award No. TG-DMR190080) under the Extreme Science and Engineering Discovery Environment (XSEDE) supported by NSF (ACI-1548562).

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