Going beyond skyrmions optically: Ultrafast generation of antiferromagnetic meron-antimeron pairs

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We propose a new mechanism to produce a meron-antimeron pair in a two dimensional antiferromagnet with an ultrafast laser pulse via thermal Schwinger mechanism. Unlike ultrafast skyrmion nucleation, this process conserves total topological charge. We systematically show different stages of the dynamics and define proper topological invariants to characterise the configurations. The emergent structure can retain its topological structure for up to 100 ps. By introducing a topological structure factor we show that pair formation is robust against any random choice of initial magnetic configuration and can survive against disorder. Our findings demonstrate that the rich world of spin textures, which goes beyond conventional skyrmions, can be reached optically.

In the quest for fast and efficient mechanism for manipulating magnetic order, ultrafast optical manipulation of magnetism emerged one of the most promising paradigms. Interaction between an ultrafast laser and magnetic moments takes place at a much faster timescale and consumes far less energy [1, 2] compared to electrical switching [3]. The underlying physical mechanism is, however, still in a mist. From the initial experimental demonstration of ultrafast demagnetisation [4] this effect was considered to be of thermal origin conventionally modelled with the phenomenological three temperature model. Zhang and Hübers [5] proposed a microscopic mechanism mediated by spin-orbit coupling, whereas Koopmans and co-workers proposed an alternative mechanism mediated by electron-phonon coupling [6]. These theoretical frameworks aim to understand the transition from ordered magnetic states to strongly disordered and often nonmagnetic states, which gives the impression that the governing mechanism behind the ultrafast demagnetisation is of thermal origin [7]. Based on time-dependent density functional theory approach, Dewhurst et al. recently proposed an alternative mechanism [8] for transferring angular momentum between different sites, which has been subsequently observed experimentally [9]. This mechanism relies on a coherent redistribution of spin angular momentum [10] and therefore can be exploited to drive a ferromagnet-to-antiferromagnet transition [11].

In this context, an ability to generate any desired magnetic configuration, i.e. a spin texture of desired properties, with an ultrafast optical laser, remains a challenge. Recent experimental demonstration of skyrmion nucleation with an ultrafast laser by Büttner et al. [12] has proved the feasibility of optical generation of spin textures. However, the proposed explanation of the effect relies solely on classical magnetisation dynamics which does not take into account electronic interactions. Besides, the working model contains the anti-symmetric Dzyaloshinskii-Moriya interaction which is known to drive the system into a skyrmionic state without any additional excitation [13]. Optical skyrmion generation has been also demonstrated with a tight-binding electronic Hamiltonian with spin-orbit coupling [14], which also makes its solely-optical origin somewhat ambiguous. Such topological structures are known to arise during the transition between two different magnetic configurations [15, 16], however, their transient nature makes them useless for any practical purpose. An alternative mechanism of laser induced magnetisation dynamics was recently proposed by Ghosh and co-workers [17], showing the emergence of a new chiral spin-mixing interaction which can lead to chiral formation even in absence of any intrinsic spin-orbit coupling. The emergent chirality is quite sensitive to the laser parameters which emphasizes the importance of coherent interaction of the laser with the electronic degrees of freedom for chiral state generation. This mechanism leads to a quasi-stable chiral formation which can survive for several picoseconds, and it is distinctly different from that driven by thermal excitations.

It is well-known that skyrmions are nontrivial magnetic configurations that are equivalent to magnetic monopoles which can be characterised by a skyrmion number [18]. Due to their heavy mass [19], creating isolated magnetic monopoles still remains quite challenging. An alternative paradigm would lie in producing a monopole-
antimonopole pair [20], which is also making its appearance in recent experimental observations of magnetic textures. Indeed, topological spin textures often emerge in pairs consisting of a texture and its anti-texture, keeping the total topological charge to zero. Such pair formation has been observed both at metallic interfaces [21] and predicted in two-dimensional magnets [22, 23]. These pairs can be further transmuted to a pair of different but opposite textures (for example meron to skyrmion [24] conversion by an external magnetic field) without violating the conservation of topological charge.

All these studies so far have been done on ferromagnetic materials which naturally raises an alluring question — is it possible to combine the aforementioned ideas and stimulate such pair production in an antiferromagnet via an optical excitation? Antiferromagnets are favorable materials due to their natural abundance and faster response as compared to ferromagnets. Besides, they are immune to any external magnetic field and also demonstrate rich and topologically nontrivial electronic properties. However, regarding the nontrivial real space textures in antiferromagnets, reported studies are restricted to a narrow domain of skyrmions only [25]. Here, we demonstrate that it is indeed possible to go beyond skyrmions and nucleate meron-antimeron pairs in an antiferromagnet with an ultrafast laser pulse. We present a systematic study of the different stages of nucleation and demonstrate the gradual formation of meron-antimeron pair starting from a collinear antiferromagnetic state. We analyze different physical observables at different stages of the dynamics and define a proper topological invariant to characterize their dynamical evolution. Finally we reveal the robustness of the overall process versus disorder.

Result and Discussion: We define a two-dimensional antiferromagnet on a square lattice with a time dependent double-exchange Hamiltonian [17, 26, 27]

\[ H = -J \sum_{i,j,\mu} c_{i,\mu}^\dagger (\hat{\mathbf{m}}_i \cdot \mathbf{\sigma})_{\mu \nu} c_{j,\nu} - \sum_{i;j,\mu} \tau_{ij}(t) c_{i,\mu}^\dagger c_{j,\mu}, \]

where \( c_{i,\mu}, c_{i,\mu}^\dagger \) are the creation (annihilation) operators of an electron at site \( i \) with spin \( \mu \). \( \hat{\mathbf{m}}_i \) is a unit vector at site \( i \) denoting the direction of the magnetisation and \( \mathbf{\sigma} \) is the vector of Pauli spin matrices. \( J \) denotes the coupling between the local magnetic moment and the itinerant moment, which, following Hund’s rule is kept positive [27] and set to 1 eV. \( \tau_{ij}(t) \) is the time-dependent hopping parameter between site \( i \) and site \( j \). The action of the laser is defined as a time varying electric field with a Gaussian envelope modelled as a time varying vector potential

\[ \mathbf{A}(t) = -E_0 e^{-(t-t_0)^2/2\sigma^2} (\cos(\omega(t-t_0))\hat{x} + \sin(\omega(t-t_0))\hat{y}), \]

where \( E_0 \) is the peak amplitude of laser occurring at time \( t = t_0 \) and \( \omega \) is the angular frequency. \( \sigma \) denotes the broadening of the pulse which we kept at 5 fs. In this work we keep \( E_0 = 0.1 \text{eV}a_0^{-1} \) (\( a_0 \) being the lattice constant), and \( \omega = 2.02 |J|/\hbar = 3.07 \times 10^{13} \text{Hz} \). This is incorporated in the Hamiltonian (Eq.1) via Pierel’s substitution \( \tau_{ij}(t) = \tau e^{i(e/\hbar)A(t) \cdot r_{ij}} \), where \( r_{ij} \) is the vector connecting site \( i \) to site \( j \). The static value of the hopping parameter is kept at \( \tau = 0.4 \) eV. For our study we consider a super-cell of dimension 20 \( \times \) 20 with periodic boundary condition.

The ground state is constructed by filling half of the lowest eigenvalue states which in our case are all the states with negative eigenvalues. For our choice of parameters, this corresponds to an antiferromagnetic alignment [17, 26]. We simulate the thermal equilibrium at finite temperature by adding a small random fluctuation (0.1\( \tau \)) to the polar angle while the azimuthal angle is chosen randomly between 0 and 2\( \pi \). This randomness is crucial to initiate the magnetisation dynamics by generating initial spin-mixing interaction [17]. Note that our initial configuration does not posses any spin-orbit coupling or any specific non-collinear order and therefore constitutes a trivial antiferromagnetic insulator. At any instance of time \( t \) any quantum state \( |\psi(t)\rangle \) can be expressed as the linear combination of instantaneous eigenstates \( |n(t)\rangle \) of the Hamiltonian which is evolved within Schrödinger pic-
This allows us to evaluate the instantaneous effective field for any site $i$ as $\frac{1}{\hbar} \sum_{\nu} \langle \psi_i | - \nabla_{m_i} H | \psi_i \rangle$, $\mu_B$ being the Bohr magneton. This effective field is used in a set of Landau-Lifshitz-Gilbert equations [17, 27, 28]

$$\frac{dm_i}{dt} = -\gamma (m_i \times B_i) - \lambda m_i \times (m_i \times B_i), \quad (2)$$

where $\gamma = \frac{g_e \mu_B}{\hbar \nu_e}$, $\lambda = \frac{g_e \mu_B \alpha}{\hbar}$, with $g_e$ being the gyromagnetic ratio, $\mu_i$ is the onsite magnetic moment which we keep at $1 \mu_B$ and $\alpha$ is the dimensionless damping coefficient which we keep fixed at 0.2.

After the action of the ultrafast laser, one can observe three different phases of dynamics originated from complex interactions between electronic and magnetic degrees of freedom (Fig. 2). The peak amplitude of the laser occurs at $t = 25$ fs (Fig. 2b), marked by the left edge of the gray area in Fig. 2. This triggers a redistribution of occupation of quantum states (Fig. 2a) which in turns start building the torque. An initial randomness is imperative to start this process which also determines how fast the system can respond to the pulse [17]. In our present setup after a latency period of approximately 100 fs (right edge of gray region in Fig. 2) the magnetic moments start re-organising themselves causing the fast relaxation phase [17] that lasts for approximately 0.5 ps (Fig. 2b). The system then enters into the slow relaxation phase which eventually leads to the final texture shown in Fig. 1. Note that the energy absorption takes place only during the short duration defined by the Gaussian envelope of the pulse (green segment in Fig. 2c). The steady state can be characterised by evaluating the average torque [29] defined as $\langle \tau_s \rangle = \frac{1}{N} \sum_{ij} \nu_{ij} (m_{ij} \times B_{ij})$, where the index $i, j$ correspond to the position, $\nu_{ij} = \pm 1$ is the sublattice index, and $N$ is the total number of sites. Note that the optical excitation predominantly produces the out of plane component of the torque (Fig. 2d) leading to the final in-plane texture. Assuming that the average energy gain per site is $\sim 0.1$ eV with the dissipation rate being $10^{-6}$ eV fs$^{-1}$, it would take the system about 100 ps to dissipate the excess energy and regain its initial configuration.

**Dynamical evolution of topological charge:** From Fig. 1 one can see that the final configuration contains a pair of antiferromagnetic meron and anti-meron. This is reminiscent of Schwinger mechanism which produces a particle and anti-particle. Similar mechanism can also generate monopole-antimonopole pairs [30] that can survive even in presence of a thermal bath [31]. Such pair nucleation for topological defects was also predicted in the context of bubble collision [32] following Kibble mechanism [33]. To characterise the pairs we choose their skyrmionic charge. On a ferromagnetic background, each meron can be characterised by a skyrmion number $\pm \frac{1}{2}$, resulting in a total zero skyrmion number for the whole configuration. For an antiferromagnet, one can define a skyrmion number for each sublattice [16], however it does not take the inter-sublattice interaction properly into account. To avoid this, we define a staggered skyrmionic charge (Fig. 3)

$$S_{ij}^{s} = \nu_{ij} [m_{ij} \cdot (\partial_x m_{ij} \times \partial_y m_{ij})], \quad (3)$$

where $\nu_{ij} = \pm 1$ for the opposite sublattices and $\partial_x m_{ij} = (m_{i+1,j} - m_{ij})$. Since the total skyrmionic charge of the complete cell is zero, we use an absolute skyrmion density $S_{Tot}^{s} = \sum |S_{ij}^{s}|$ to characterise the configuration. For a well-isolated meron-antimeron pair this number should be 1. However due to the finite size there is always some overlap between the different regions causing a deviation of the total absolute skyrmion charge from 2 for the whole super-cell (Fig. 3b). For a proper topological characterisation in this case, we evaluate the winding number [34] for all four meron/antimeron centres defined as

$$\mathcal{W} = \frac{P_s}{2\pi} \oint \mathcal{C} d\ell \cdot \nabla \phi \quad (4)$$

where $P_s$ is the sub-lattice polarisation, given by $\text{sgn}(m_{ij}) \cdot \nu$ with $m_{ij}$ being the out of plane component.
of the magnetisation at the centre and \( \nu = \pm 1 \) for the sub lattices. \( \phi \) is the azimuthal angle and the contour \( C \) encircles the winding centre in anticlockwise direction passing through only one type of sublattice. We choose four centres (Fig. 3a), each specifying a meron/antimeron pair in a checker board pattern. This formation is fairly robust against scalar impurity averaged over 32 different configurations and scaled with its average value at \( V_0 = 0 \). For each configuration we consider the mean value at \( q = 0.1(\pm \hat{x} \pm \hat{y})\pi \).

The evolution of absorption of conventional nontrivial structures such as skyrmions or hopfions. This establishes the emergence of a pair of meron and antimeron in a checker board pattern. We show that on average the system is more likely to form a pair of meron and antimeron via thermal Schwinger mechanism. The laser excited system moves into a spin-spiral configuration process which would be helpful for its physical realisation.

**Conclusions:** In this work we present a new paradigm for generating non-trivial magnetic textures in antiferromagnets. We show that when excited by an ultrafast laser a two-dimensional antiferromagnet can host meron-antimeron pairs via thermal Schwinger mechanism. The topological texture can survive for up to 100 ps which makes it possible to observe experimentally. The process is independent of initial helicity of the laser and responsive within a moderate range of frequency and peak amplitude of the laser. We define a staggered skyrmionic charge, winding number and topological structure factor to demonstrate the formation of topological charge and show that on average the system is more likely to form a pair of meron and antimeron in a checker board pattern. This formation is fairly robust against scalar impurity which makes it easier to observe experimentally. Since the total topological charge of a texture/anti-texture pairs is always zero, pairs of different genera can be connected smoothly allowing more flexibility in exploring topological objects of higher genus. Our results thus open a new route to generate out-of-equilibrium topological features which remain inaccessible in their ground state configuration. This takes us beyond the generation of conventional nontrivial structures such as skyrmions and domain walls, and paves the way to generating more exotic higher-order topological objects such as chiral bobbers [35] or hopfions [36].

where \( \mathcal{N} = \sum \langle S^z_j \rangle^2 \) is the normalisation constant. One can readily see from Fig. 4a that the topological structure factor is reminiscent of a checker-board pattern (Fig. 4a inset) which is consistent with the skyrmionic charge distribution (Fig. 3). However, it is also possible that the laser excited system moves into a spin-spiral configuration or a combination of random clusters with no global long range order. To verify that this is not the case, we consider 70 different configurations with the same normalisation constant and evaluate the average distribution of the topological structure factor (Fig. 4). The obtained maxima in the distribution occur for \( q = 0.1(\pm \hat{x} \pm \hat{y})\pi \) which establishes the emergence of a meron-antimeron pair in our \( 20 \times 20 \) super cell.

We finally study the robustness of these emergent configuration against disorder. For that, we introduce random “impurities” modelled by on-site energy deviations ranging from \(-V_0\) to \(V_0\), and measure the topological structure factor at points \( q = 0.1(\hat{x} \pm \hat{y})\pi \) (Fig. 4). One can readily see that the structure manages to retain its basic features for fairly strong values of the impurity potential, and then gradually collapses into a featureless distribution. Note that a small random impurity can enhance the formation as denoted by the initial rise in average topological structure factor which is consistent with the behaviour against small random fluctuations of magnetic moment. This establishes the robustness of the pair formation process which would be helpful for its physical realisation.

**Topological structure factor:** The evolution of absolute staggered skyrmion charge and winding number ensures the emergence of topological objects with opposite charges coming in pairs, however it does not yet specify the distribution of the topological charge. To determine that we define a topological structure factor

\[
S_q = \frac{1}{\mathcal{N}} \sum_{ij} S^s_{ri} S^s_{rj} e^{iq \cdot (r_i - r_j)} \tag{5}
\]
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