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Multi-Meron Interactions and Statistics in Two-Dimensional Materials

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Abstract

As a fundamental type of topological spin textures in two-dimensional (2D) magnets, a magnetic meron carries half-integer topological charge and forms a pair with its antithesis to keep the stability in materials. However, it is challenging to quantitatively calculate merons and their dynamics by using the widely used continuum model because of the characteristic highly inhomogeneous spin textures. In this work, we develop a discrete method to address the concentrated spin structures around the core of merons. We reveal a logarithmic-scale interaction between merons when their distance is larger than twice their core size and obtain subsequent statistics of meron gas. The model also predicts how these properties of single and paired merons evolve with magnetic exchange interactions, and the results are in excellent agreement with the Monte Carlo simulations using the parameters of real 2D van der Waals magnetic materials. This discrete approach not only shows equilibrium static statistics of meron systems but also is useful to further explore the dynamic properties of merons through the quantified pairing interactions.

Migrating the concept of soliton from particle physics to condensed matter physics, the topological solitons, such as skyrmions and merons, have attracted tremendous interests in magnetic systems tracing back to several decades ago because of their potential applications for quantum information and storage.^{1–6} With substantial experimental advances in recent years, such types of nonlinear spin textures have been observed in various material platforms, e.g., magnetic material surfaces, disks, and thin films within a wide range of temperature.^{7–16} The formation of merons merely requires an in-plane $O(2)$ magnetic anisotropy and does not demand any specific type of interactions, such as frustrated symmetric exchange interactions or the antisymmetric Dzyaloshinskii-Moriya (DM) interaction which stabilize the skyrmions.^{17,18} Therefore, merons could be one of the common topological solitons in low-dimensional and weak spin-orbit coupling (SOC) magnetic systems.^{19–21} More recently, the newly emerging atomically thin two-dimensional (2D) magnets may work as the neat and natural playground for such topological spin textures.^{22–25} There are numerous experimental measurements detecting meron states through suppression or large fluctuations of magnetic orders especially for monolayer structures. For example, the suppressed antiferromagnetic (AFM) order of monolayer NiPS_3 was reported, and the XY features were discussed in monolayer CrCl_3 .^{26,27}

A systematic theoretical exploration is highly demanded in light of the recent experimental achievements in exploring topological spin textures. The strict 2D planar magnetic vortices and antivortices are known as the BKT physics and have been heavily studied for decades^{28,29}. For the topological merons in the natural material, the in-plane geometry of the magnetic vortices and antivortices are inherited. However, unlike the strict 2D model, the out-of-plane spin texture is presented around the core region to lower the free energy of meron in realistic materials. Current studies about meron solitons mainly focus on the structure and stability of bimerons in the frustrated ferromagnets (FM) or chiral AFM monolayers as well as their dynamical responses under external spin currents or magnetic fields within the Landau-Lifshitz-Gilbert framework.^{21,30–}

³⁴ The accurate description of the structural properties of single meron is limited, which is, however, the foundation for studying bimerons and further collective interactions. To date, most previous works followed the continuum analysis that has been successful in describing skyrmions. For example, the structure of a single meron was mimicked through the micromagnetic simulations (e.g., OOMMF package) accompanied by the continuum analysis³⁵, and its stability was also

discussed through a continuum model based on the Heisenberg Hamiltonian with the DM interaction included³⁶. However, different from skyrmions, merons typically exhibit much more compact core structures and form complicated networks in real materials. As pointed out in the seminal work of G. M. Wysin¹ about 2D easy-plane ferromagnets, the region close to the vortex geometry center cannot be described well by a continuum field. This is because the rapid variation of magnetic moments at the core represents a singularity in the continuum perspective.¹ These characters make the continuum approach contentious to describe general properties of merons. Finally, the statistical distribution of the distance between merons is another determining property of the integrative multi-meron networks in materials, whereas there has been barely rigorous investigation about this fundamental trait in realistic materials. In this regard, it is worth endeavoring to find a general model to describe the thorough profile of individual merons and their pairs.

In this paper, we develop a discrete model to study the equilibrium meron properties based on a Heisenberg Hamiltonian that takes the onsite anisotropy and nearest neighbor (NN) exchange interactions into account. By constructing the soliton profile of both single and paired merons based on discrete lattices, we obtain the optimal core size, pair interaction, meron distance distribution and their evolution with the characteristic exchange interaction strength. The Above model results agree well with the non-interfering Monte-Carlo (MC) simulations. Thus, this discrete soliton method gives rise to a general way to study merons in practical materials and provide a comprehensive picture of low temperature meron statistical properties

Hamiltonian and simulation setup. We consider the following XXZ-type Heisenberg Hamiltonian with the NN exchange interaction (J) and effective onsite anisotropy (A) to describe 2D magnets:

$$\mathcal{H} = A \sum_i (m_i^z)^2 + \frac{J}{2} \sum_{\langle i,j \rangle} \vec{m}_i \cdot \vec{m}_j \quad (1),$$

where $\vec{m}$ represents the magnetic moment. Our previous study shows that the NN approximation produces a good agreement with the experiment and can predict the characteristic transition temperature of monolayer chromium trihalides within an error bar of several Kelvin.³⁷ Hexagonal lattices are utilized in this study because most currently synthesized 2D magnets belong to this space group. To mimic realistic materials, we initially set these parameters close to the effective

values of monolayer CrCl_3 : the values of the effective onsite anisotropy A and Heisenberg exchange constant J are $35 \mu\text{eV}$ and $-790 \mu\text{eV}$, respectively, which are obtained by first-principles calculations²⁰. We have to address that the effective anisotropy A takes into account both the magneto-crystalline anisotropy and the shape anisotropy (magnetic dipolar interactions), and its positive sign results in the in-plane $O(2)$ symmetry which is crucial for realizing merons while prohibiting the formation of long-range magnetic orders at finite temperature. This approximation can capture the essential meron physics while dramatically simplify the model and corresponding MC simulations. Utilizing monolayer CrCl_3 as the starting point, we will keep A fixed while scanning J within a reasonable range to predict the meron properties in general 2D magnets. In other words, we mainly focus on the exchange interaction and the ratio of J/A , to avoid scanning a vast parameter space while grasping the essential physics.³⁹

Based on the Hamiltonian in Eq (1), we perform MC simulations via the Metropolis algorithm on 2D hexagonal lattices with a size of 240×240 hexagonal unit cells (if not particularly specified), which contains 115,200 magnetic moments. The periodic boundary condition is implemented in the MC simulations. A MC step consists of an attempt to assign a new random direction in three-dimensional (3D) space to one of the random magnetic moments in the lattice, and the acceptance ratio is setting via the vanilla Metropolis method. All magnetic moments are set to point along the out-of-plane direction at the initial stage to mimic the experimental cooling condition with the help of an external field.^{22,23} Such initial setting warrants the overall zero topological numbers of system. The temperature of MC is setting to $k_B T = J_0/36$ to get a unclouded meron profile from thermal blurring. We run 2.304×10^6 MC steps in total (averaged 2×10^5 steps per magnetic atom) to ensure the equilibrium state is reached.

Single meron. We start from the merons in monolayer CrCl_3 , a 2D magnet expected to be promising to hold in-plane magnetic polarizations and merons.^{19–21,27} Figures 1 (a) and (b) present the schematic top and side views of merons obtained from MC simulations of monolayer CrCl_3 using the DFT-calculated J and A as mentioned above.^{20,37} These figures reveal a few fundamental characters of merons. First, the spin texture has a wave-pocket-like core with the $\pm \hat{z}$ direction spin components, while the easy-plane spin components form the vortex or anti-vortex swirling around the core.^{11,14,16,40,41} Secondly, under ideal conditions, the in-plane swirling of a meron/anti-meron

extends to infinity until it is terminated by the system boundary or anti-meron/meron. These features are different from many other widely studied topological spin textures, such as skyrmions or magnetic bubbles which are self-contained.^{5,42} For example, a general studied skyrmion can be decomposed into an inner core, an outer domain, and a domain wall separating the core and outer domains as plotted in the inset of Figure 1 (b).^{6,38,43}

To quantitatively describe a single meron, we have calculated its topological charge that has been widely employed to characterize the topological properties of spin textures.⁵ The topological charge is defined as $Q = \int q(\vec{r}) = \int \frac{1}{4\pi} \vec{n} \cdot \left(\frac{\partial \vec{n}}{\partial x} \times \frac{\partial \vec{n}}{\partial y} \right)$,^{44,45} where $\vec{n}$ is the unit vector of local magnetic moment $\vec{m}$. The schematic topological charge distribution $q(\vec{r})$ of a meron in monolayer CrCl_3 is shown in Figure 1 (c). In this study, the integrated topological charge of the considered merons and anti-merons belongs to the half integer class ($\pm 1/2$). The half integer topological charge supports the idea that merons have to form pairs to stabilize in an integer topology number form, which agrees with previous studies and observations.^{12,16} Moreover, the most topological charge is condensed around the small core region. As shown in Figure 1 (c), the diameter of the 5% isoline of the maximum value of local topological charge is about 4 nm, which is the length of 6 lattice constants because the in-plane lattice constant of CrCl_3 is about $6.01 \text{ \AA}$.²⁰ This is much smaller than the skyrmions observed in $\text{Fe}_{0.5}\text{Co}_{0.5}\text{Si}$, in which the core size is around 90 nm.⁹ In addition to the topological charge, we have also calculated the magnetic energy distribution based on the Heisenberg Hamiltonian (Eq. 1). In Figure 1 (d), the magnetic energy profile shows the similar features as the topological charge distribution: most magnetic energy is condensed around the core region within a diameter of 7 nm. These results conclude that a manifest character of merons is their highly inhomogeneous spin texture around the core. The condensed core dominates most their energetic and topological properties of the single meron texture. This feature distinguishes merons from the skyrmion, in which the topological charge is allocated around domain wall far away from the soliton center. Interestingly, such highly inhomogeneous spin textures of meron are suitable to carry binary information based on the out-of-plane spin direction of cores and can be manipulated by external field pulse, which is not achievable for the strict 2D planar vortexes.¹⁵ On

the other hand, as we will show in the following, such highly inhomogeneous spin textures also bring difficulties in describing and quantifying merons through the traditional continuum analysis.

The first step is to build a modeled profile function to describe the spin texture of a single meron. Inspired by the hyperbolic secant form of the optic solitons⁴⁶, we construct the profile function to describe the meron geometry:

$$\Phi(\phi) = v\phi + \delta \quad (2)$$

$$\Theta(r) = \frac{\pi}{2} - \arctan \left[\frac{1}{\sinh \left(\frac{r}{w} \right)} \right] \quad (3)$$

where $\Phi(\phi)$ and $\Theta(r)$ are the azimuthal and polar angles, respectively, which describe the direction of a magnetic moment $\vec{m}$ on the polar coordinate $r(r, \phi)$ (illustrated in Figure 1 (a)), i.e., $\vec{m} = m_0(\sin(\Theta)\cos(\Phi), \sin(\Theta)\sin(\Phi), \cos(\Theta))$. In Eq. (2), δ is the phase factor varying from 0 to 2π describing the swirling. We refer positive vorticity v to a meron and negative v to an anti-meron. In this work, we restrict the discussion to $|v| = 1$, which is the most common and fundamental meron state with $\pm \frac{1}{2}$ topological charge, although $|v| > 1$ can still exist if considering specific exchange interactions beyond NN.⁴⁷ In Eq. (3), a_0 is the lattice constant of magnetic lattices. w is the scale size of the meron core region, and it is the only tunable parameter in this model. We can compare w with the widely used full width at half maximum (FWHM) marked in Figure 1 (b). For the soliton form in Eq. (3), $\text{FWHM} = 2 \ln(2 + \sqrt{3}) w \approx 2.63 w$.

Next, we employ the meron-soliton profile in Eqs. (2) and (3) to tune the parameter w for obtaining the ground state (lowest) energy based on the Hamiltonian in Eq. (1). One popular way to evaluate such energy is to use the continuum approximation:^{2,36,43,48}

$$E = \int \int \left(A' m_z^2 + \frac{J'}{2} |\nabla \vec{m}|^2 \right) dS \quad (4).$$

1 A' and J' are treated as the continuous effective coefficients related with Eq. (1), and a normalized
 2 coefficient is necessary to ensure the proper unit of those micromagnetic anisotropy and exchange
 3 constants since the second exchange term has a real-space gradient square. That gradient square
 4 needs a factor of the area of a unit cell, which is $\sqrt{3}/2$ in hexagonal lattices (the lattice constant
 5 can be chosen as one since the ratio is relevant). Moreover, there are two magnetic Cr atoms (spins)
 6 in one unit cell, which gives another factor of 2. As a result, we need a normalized coefficient of
 7 $1/\sqrt{3}$ to A'/J' . This approach has provided gratifying results for describing skyrmions.⁴³ (See
 8 section 1 of the Supplemental Information for the detailed analysis of Eq. (4) and corresponding
 9 boundary effect) In Figure 2 (a), we present the radial profile of merons in monolayer CrCl_3 from
 10 the continuum model (the dash line) and the MC simulation (the dots). Unfortunately, compared
 11 with the MC result, the core size calculated by the continuum model is apparently underestimated.
 12 This deviation is from the fact that the main structures of merons, such as the topological charge
 13 distribution and the out-of-plane spin texture, are highly concentrated and dramatically varied
 14 around the center of the soliton within a few nm close to the singularity point of the continuum
 15 treatment. This can be seen from Figure 1 (b), in which sharp variations of the spin texture are
 16 observed within a small-sized core.

17
 18 To overcome such deviation induced by the singularity at the meron core, we can deal with the
 19 discrete degrees of freedom of the meron in hexagonal lattices applying the profile function,
 20 without the continuum approximations.¹¹ Following this idea, we discretize the single meron profile
 21 function (Eqs (2) and (3)) based on magnetic Bravais lattices and obtain the corresponding energy
 22 by directly following the Heisenberg Hamiltonian in Eq. (1). Via the procedure of energy
 23 optimization, the discretized approach provides a very good portrait for the meron comparing with
 24 the observed meron instance in the low-temperature ($k_B T = J_0/36$) MC simulation of monolayer
 25 CrCl_3 evidenced by the agreement between the red solid line and dots in Figure 2 (a). Meanwhile,
 26 such a good agreement also corroborates the validation of our proposed soliton formula in Eq. (3)
 27 for describing merons.

28
 29 Then we go beyond monolayer CrCl_3 to check this discrete approach for general materials. We
 30 have calculated the single-meron profile by changing the exchange interaction J within a
 31 reasonable range of natural materials, such as chromium trihalides, (from $0.5 J_0$ to $4J_0$, where J_0 is

the exchange interaction strength of monolayer CrCl_3). The results are summarized in Figure 2 (b). The model based on the discrete soliton solution (Eq. 3) always provides satisfactory agreements with MC results within such a wide range of magnetic interactions. Moreover, Figure 2 (b) reveals the trend of merons core associated with the exchange interaction. For example, a larger exchange interaction will increase the core size of merons. This is similar to the characteristic length scale increase as $\sqrt{J/A}$ in common magnetic domain wall structures. Such a trend is consistent with the understanding that a larger exchange interaction J (in principle, J/A) increases the energy cost of forming in-plane swirling at the core region and makes the spins prefer to the $\hat{z}$ direction. Consequently, the soliton favors a broader span of the spin variations along $\hat{z}$ and thus a larger core size. It is worth mentioning that this trend is opposite to overall size shrinkage against the increasing J in skyrmions. When the exchange J increases the size decrease of the inner region of skyrmions overlays the thickness increase of the domain wall involving the DM interaction, resulting in an overall decreased size of skyrmions.⁴¹

Figure 2 (c) summarizes the FWHM of merons calculated by the three approaches, i.e., simulated from MC, optimized from the continuum and the discrete approaches based on profile function, for a wide range of exchange interaction J . As explained above, the continuum approach neglects the lattice discretization effect around the core even truncated with a_0 avoiding the singularity and consequently underestimates the size of the meron soliton. In contrast, by introducing the lattice discretized profile function, the theoretical prediction of meron size is in good agreement with the MC simulation which is non-interfered method with the model.

Finally, it is worth mentioning that the meron core size is relatively robust against the distance between them. Figure 2 (d) displays the MC results of merons' the out-of-plane ($\hat{z}$) spin component under the different pair distances ranging from 10 to 40 nm observed in simulations of monolayer CrCl_3 . The soliton profiles are nearly the same within the wide range of distance. Notable, the persistence of meron core structure against the pair distance emphasizes the importance of the discrete model in capturing the meticulous structure of the meron core region and verifies the feasibility of studying the interactions among merons through the rigid particle supposition, which will be realized in the following bimeron profile and multi-meron statistics.

Bimeron profile. Unlike a skyrmion which maintains an integer topological charge itself, a single meron only carries half-integer topological charge and shows up in pairs, so-called bimeron states, to ensure the system belongs to the integer topological class. Hence, their pairing properties are worth being studied. Based on the in-plane geometry of vortex and anti-vortex swirling^{11,29}, the spin moment ($m(\theta, \phi)$) of a bimeron can be written as Eq. (5) based on the single meron profiles illustrated in Figure 3 (a):

$$\begin{cases} \theta = z^+ \theta^+(r - r^+) + z^- \theta^-(r - r^-) \\ \phi = \gamma^+ \phi^+(r - r^+) + \gamma^- \phi^-(r - r^-) + \delta \end{cases} \quad (5)$$

where we label the meron and anti-meron via the superscripts by their in-plane swirling type: $\gamma^+ = 1$ for vortex and $\gamma^- = -1$ for anti-vortex, the corresponding vorticities are contained in angles $\phi^\pm$. r^+ and r^- are the core locations of meron and anti-meron, $z^\pm$ indicates the spin direction of the meron (anti-meron) core along the positive (+1) or negative (-1) z-axis. The overall sign of the integrated topological charge of a single meron (anti-meron) is decided by the product of its core region spin direction z and in-plane swirling vorticities γ , which is $N = \frac{1}{2} \gamma z = \pm \frac{1}{2}$.^{14,16} For the bimerons discussed in this work, there are three classes of the overall topological index (0 and ± 1). To corroborate results with experiments and MC simulation conveniently, we mainly focus on the class 0 configurations (as illustrated in Figure 1 (b)) where the spin z-direction of the cores in meron and anti-meron are the same. This configuration can be smoothly transferred from the field-induced FM state that could be easily realized in experiments and MC simulations because the conservation of the topological number and the initial setups of the perfect FM order in simulations. Since we only consider the isotropic exchange and onsite anisotropy, the phase factor δ can be an arbitrary value between $(0, 2\pi)$ that gives the same degenerated energies. For example, in Figure 3(b) we present the structure appearance of meron pairs with four typical values of δ , i.e., $0, \frac{1}{2}\pi, \pi$, and $\frac{3}{2}\pi$, which are observed in the MC simulations.^{11,16}

With the above meron pair profile function, we can evaluate the pair interaction energy against the distance ($|\vec{r}^+ - \vec{r}^-|$) between meron and anti-meron by using the discrete method established in the bimeron profile Eq.5. First, we begin with merons in monolayer CrCl_3 . Figure 3 (c) presents the results obtained by the discrete (dots) approach. An attractive interaction is observed between meron and anti-meron. A logarithm curve (dashed line) excellently fits the results for $d > 2r_0$.

1 Interestingly, the Yang-Mills equations, which originally proposed meron-pair quasiparticles in
2 high-energy physics, derives the similar logarithm-scale energy variation.^{3,4}

3
4 Such a logarithm scale can be understood by analyzing the asymptotic behavior far away from the
5 center ($|r| \gg |d|$) via the continuum analysis which is well established in the BKT physics.^{28,29}

6 Due to the highly concentrated meron profile, the corresponding asymptotic interaction between
7 meron and anti-meron mainly comes from the region far from the cores. Thus, it is dominated by
8 the exchange interaction of in-plane swirling of local magnetic moments since the highly localized
9 core region does not contribute to the interaction between meron and antimeron instances by the
10 short-range Heisenberg exchange. To capture the primary scaling of interaction, the energy can be
11 estimated as $E = \frac{J'}{2} \iint \nabla \vec{m} \cdot \nabla \vec{m} dS$. Combined with the meron profile (Eq (5)), we could get the
12 asymptotic energy expression as: (The details can be found in Section 2. of the Supplemental
13 Information)

$$14 \quad E = J' \pi [(\gamma^+ + \gamma^-)^2 \ln \left(\frac{L}{a_0} \right) - 2\gamma^+ \gamma^- \ln \left(\frac{d}{a_0} \right)] \quad , (6)$$

15 where L is the system size. For bimeron states, $\gamma^+ + \gamma^- = 0$ and $\gamma^+ \gamma^- = -1$. Therefore, the first
16 term is zero, and the residual second term contributes to a logarithm-scale energy between meron
17 and anti-meron.

18
19 We must emphasize that, although the continuum treatment is helpful in understanding the
20 asymptotic behavior, it cannot provide an accurate description for the strength of pair interaction.
21 As discussed in the single meron case, the center region of merons cannot be described by the
22 continuum model, and the derivation of Eq. (6) is only asymptotically valid at the large r limit.
23 Therefore, a discrepancy between the continuum model and discrete model should be expected.
24 As shown in Figure 2 (c) the continuum analysis gives an overestimated interaction strength
25 compared with the results from the discrete model, although both exhibit a logarithm scale.

26
27 When we study meron interactions, the potential is truncated at $2r_0$, where r_0 is the FWHM of the
28 single meron. Such a rigid core treatment for studying medium and long-range interactions at
29 equilibrium state is supported by the MC simulations (Figure 2 (d)) which shows that the meron
30 core properties are barely affected by other merons that are apart larger than $2r_0$.

The attractive interaction between meron and antimeron is not directly associated with the pairing stability. The observed meron-antimeron pairs are essentially thermodynamic results at finite temperature. Beside the ferromagnetic ground state at zero temperature, at finite temperature, these quasi-orders with weak attractive interaction emerges from the Goldstone modes.²⁸ In other words, we can imagine that some meron-antimeron pairs annihilate (disappear) while other pairs emerge due to thermal fluctuations.

On the other hand, we must clarify that we constrain our study to the static profile of meron. Therefore, our approach is not able to describe the meron interaction when their cores overlap ($r < 2r_0$), because the static profile model cannot grasp the dynamic process such as the creation and annihilation of meron pair when they are nestling each other. In that situation, the meron profiles no longer follow the assumed soliton formula (Eq. 3) while they are merging.

To expand our model and discussion to general materials, we have calculated the meron/anti-meron interactions with a range of exchange interaction (J), as shown in Figure 3 (d). For all the studied values of exchange interactions, the interaction energy retains the logarithm scale. Importantly, Figure 3 (d) shows that, as the exchange interaction J increases, the meron/anti-meron attractive interaction is enhanced. Because the total energy is proportional to the exchange interaction as seen from the Hamiltonian in Eq. (1).

Finally, the scaling law of meron pairing energy vs the system size is known to be important as it provides a scale guidance for the experimental realization of meron solitons in the magnetic domains in natural materials.^{42,49,50} Unfortunately, the continuum solution confirms the energy convergence of the system as mentioned in Eq. (6) but it cannot provide the asymptotic behavior with varying system size. On the contrary, our discrete model reveals that the energy of a pair of merons with a fixed distance d converges as $1/L^2 (\sim 1/N)$ to the system size, as shown in Figure 3 (e), and a system size of 240x240 unit cells are utilized in the study.

1 It is worth mentioning that the interaction between the same type merons or antimerons is repulsive.
 2 However, without imperfections, such as magnetic defects, the conservation of the topological
 3 number will forbid the instance of a single pair of the same type merons or antimerons. In real
 4 materials, more than one pair of meron/antimerons can be thermally excited, which bring us to the
 5 complex networks of merons/antimerons discussed in the following section.

6
 7 **Nearest neighbor (NN) distance of merons in materials.** With the dispersion of interaction
 8 energy shown in Figure 3 (d), more general meron behaviors, e.g., the response to the external
 9 field and current induced torques^{5,30,31,34} can be studied through the subsequent macro soliton
 10 effective models. In the following, we focus on the statistical properties of equilibrium meron pairs
 11 in materials. Merons in materials can form complicated structures, such as the hierarchic structures
 12 from “dipole like” to “quadrupole like” or even more complicated networks.^{12,20,30,51} These
 13 topological defects networks were observed in MC simulations of monolayer CrCl_3 , as shown in
 14 Figures 4 (a) and (b). In such complicated network structures, we calculate the NN distance
 15 between merons,⁵¹ which is analogous to the distance between meron and anti-meron in a simple
 16 pair as discussed in the bimeron case. By examining the hyperbolic secant shape of the soliton
 17 profiles, their vortex or anti-vortex in-plane swirling, and integrated half integer topological charge,
 18 we can identify the meron type and its center location on the lattice with the help of a k-means
 19 clustering algorithm, hence obtaining the NN distance.⁵² In this algorithm, we set the center of the
 20 corresponding meron on the hexagonal lattice site. This choice does not affect the result because
 21 our simulation shows that the energy variation of different center position is negligible ($\sim$
 22 $10^{-4} \mu\text{eV}$) with a cell.

23
 24 After collecting the ensemble of 1,360 distinct MC simulations, we generate the corresponding
 25 statistical distribution of the NN distance shown as the histogram in Figures 5 (a)–(d) with different
 26 exchange interactions J . In the rest part of this article, we will show that, using the bimeron
 27 interaction obtained above, we can develop a phenomenological model to capture the statistical
 28 NN distance distribution in Figures 5 (a)–(d).

29
 30 By imitating the NN model in 2D free gas, we start from a probability integration equation for
 31 multi-meron systems with the rigid core approximation.⁵³

$$f(r) = \left(1 - \int_{2r_0}^r f(r') dr'\right) \rho(r), \quad (7)$$

where $f(r)$ represents the probability of finding an antithesis of a meron at the distance r , $\rho(r)$ represents the probability of the bimeron having a distance of r with one soliton fixed at the origin.

We further assume that $\rho(r)$ obeys the exponential relation with energy $E(r)$, which can be obtained from the discrete meron pair profile in Figure 3 (d). Thus $\rho(r)$ can be written as $\frac{N}{Z} 2\pi r e^{-\frac{E(r)}{E(2r_0)}}$, in which $E(2r_0)$ is the reference energy, and the normalization factor $Z_0 = \int_{2r_0}^L 2\pi r e^{-\frac{E(r)}{E(2r_0)}} dr$. N is the total number of merons achieved from MC simulations. By introducing the energy $E(r)$ which can be obtained from the discrete meron pair profile in Figure 3 (d), we get the model describing the NN meron/anti-meron distance from Eq (7)

$$f(r) = Z_1 r \frac{N}{z_0} \exp\left(-\frac{E(r)}{E(2r_0)}\right) \exp\left(-2\pi \frac{N}{Z} \int_{r_0}^r r' e^{-\frac{E(r')}{E(2r_0)}} dr'\right), \quad (8)$$

where Z_1 is the normalization factor. As shown in Figures 5 (a-d), this model is in good agreement with statistical results from MC simulation, especially under the long-distance condition. On the other hand, limited by the rigid core assumption and neglecting possible merging process of merons and anti-merons, there are slight discrepancies at the small (short-range) distance. Nevertheless, the general agreement of our model with MC simulations in Figures 5 confirms that the discrete profile model not only works for single meron but also is suitable for studying multi-meron states in materials, which expands the scope of the model.

Follow the same part with single and bimeron studies, we have also studied the impact of the exchange interaction J on the NN distance of merons. An observed trend from Figures 5 (a) - (d) is that the large exchange strength J gives a shorter averaged NN distance and tighter distribution. Figure 5 (e) plots the highest probability distance and the averaged distance vs J . When J increases, the most probable distance exhibits a decreasing trend. This is because a larger J results in stronger attractive interactions between meron and anti-meron as we discussed above. This will intrinsically lead to a smaller NN distance.

Finally, we must emphasize that, although the interaction energy between merons is relatively weak (Figure 3 (d)), this attractive interaction is significant in deciding the statistics of merons. In figures 5 (a)-(d), we plot the result of the non-interacting free 2D gas in a dashed curve. Without the weak attracting interaction, the most probable distance is substantially overestimated. For example, for monolayer CrCl_3 (Figure 5 (b)), the ideal gas model gives the most probable NN distance at $210\text{\AA}$ while that from the discrete model is $116\text{\AA}$. Moreover, the width of the distribution of ideal-gas model is broader, resulting in a larger averaged NN distance of $267\text{\AA}$. The number is larger than the discrete model ($169\text{\AA}$) because of the neglect of attractive interactions. The similar discrepancies are also observed at different exchange interaction J , as summarized in Figure 5 (e).

In summary, we built a discrete model in light of the sequential discussion of planar 2D magnets¹ to explore the merons' general properties covering the single merons, meron pairs, and their low-temperature equilibrium properties. By comparing with the continuum approach and cross-validating with MC simulation results, we demonstrate that such a discrete model accurately captures the important characters of meron solitons in 2D magnetic systems. The results confirm the discrete approach as a concrete way to explore topological meron properties and reproduce their interactions accurately that are crucial for understanding experimental measurements, such as the distance (correlation) distribution of dense nanoscale networks of merons and anti-merons in 2D magnets and 3D magnetic surfaces.⁵¹ Furthermore, with the improved explicit interaction from our discrete model, more interesting models can be constructed to study the dynamic properties of merons in real materials. This model would be useful for exploring the meron profile of pinning, dragging, and zoning in presence of moderate magnetic defects or external dynamic perturbations, which are directly connected with experimental realizations and further promising applications.

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Supporting Information:

Schematic illustration of meron energy and meron anti-meron asymptotical interaction under continuum approach (.docx)

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Author Contributions

L.Y. supervised the project. X.L performed the calculations and drafted the paper. All authors discussed the results and edited the paper.

Notes

The authors declare no competing financial interest.

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Figures:

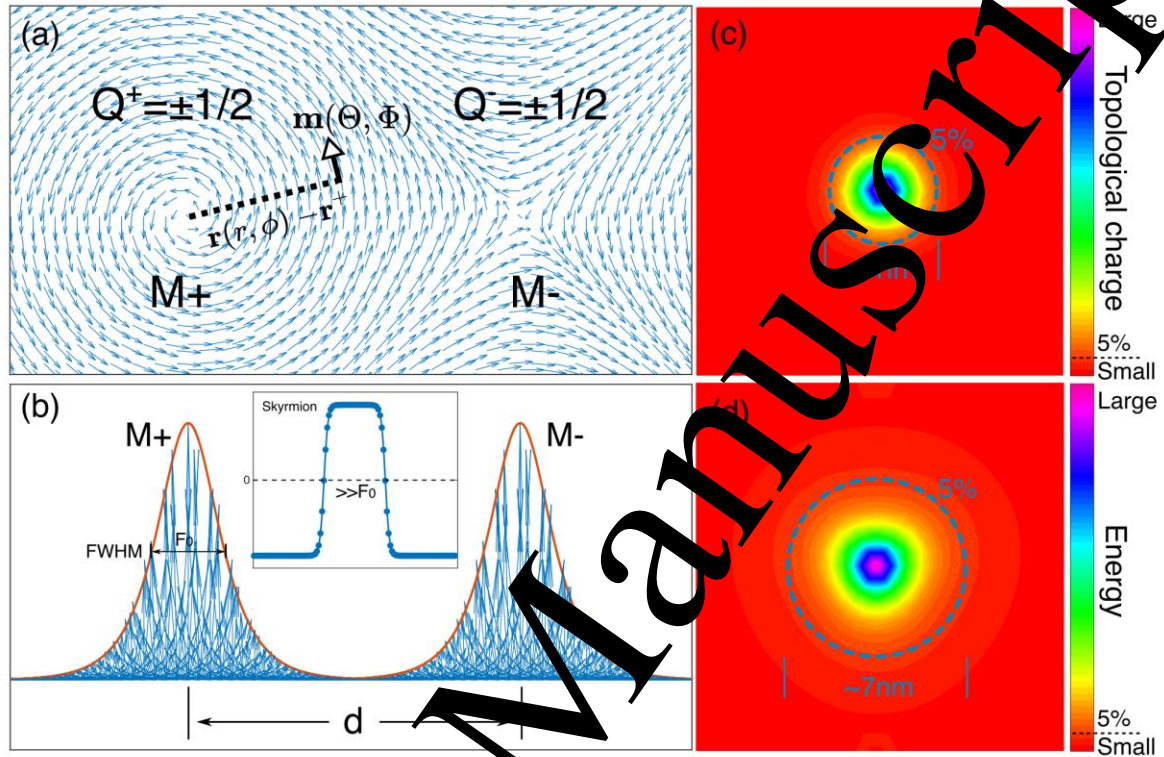


Figure1 (a) Top view (in-plane chirality) of merons on 2D magnetic lattices. For the articulating purpose, meron and anti-meron are labeled by in-plane swirling types (M^+ for the vortex type and M^- for the anti-vortex type). The polar coordinate $\vec{r}(r, \phi)$ and $\vec{m}$ are illustrated in the dashed line and arrow, respectively (b) Side view of merons. The inset is the structure of a skyrmion. (c) and (d) Schematic figures of the topological charge and energy distribution of a single meron. The dashed circle indicates an isoline with 5% of the maximal value and the estimated diameters are listed in figures.

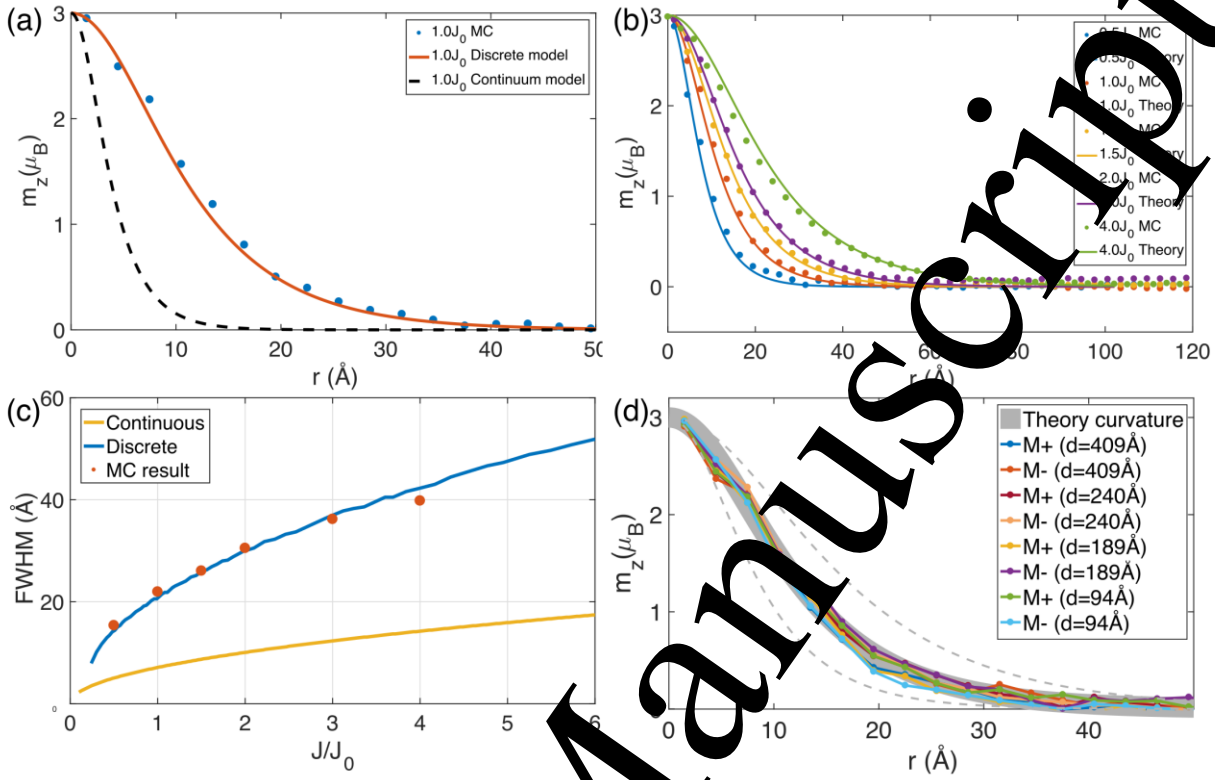


Figure 2 Out of plane spin component ($\hat{z}$) of single meron profile. (a) Dots and lines are the MC simulated results and fitted profile theory results. (b) Comparison of the out of plane spin component ($\hat{z}$) from continuum model, discrete model and MC simulation under fixed $J = J_0$. (c) FWHM of single meron with different J from continuum model, discrete model, and MC simulation. (d) Out-of-plane spin component ($\hat{z}$) of single meron extracted from MC simulation with the meron pair distance under a fixed $J = J_0$. The dashed line indicates the curves of $J = 0.5J_0$ and $J = 2J_0$ from (b) to guide readers' eyes.

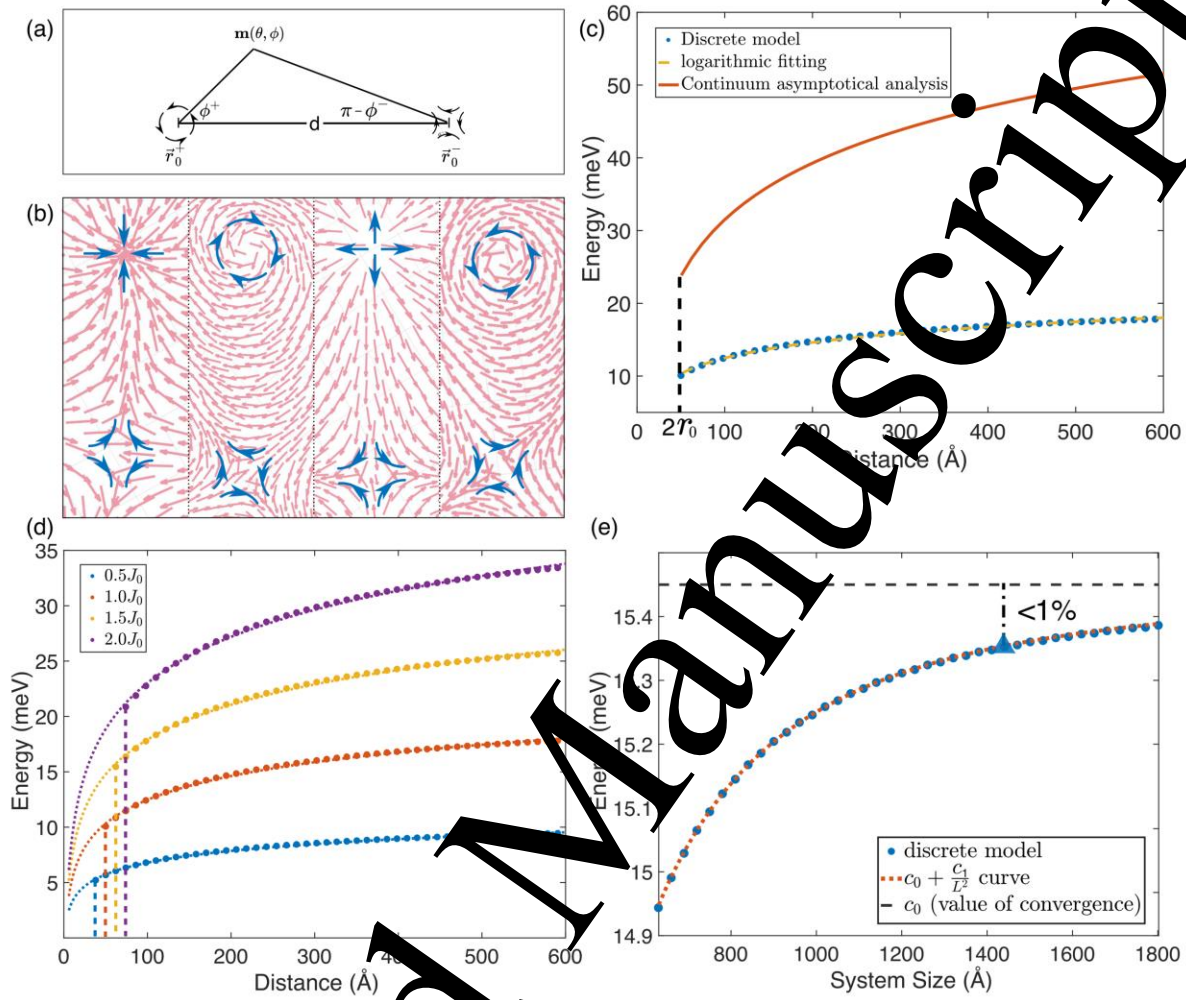


Figure 3 (a) Schematic of a meron pair and definitions of coordinates (b) Typical meron pairs observed in MC simulations with a phase factor δ close to $0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$. The in-plane swirling is marked in a 3x3 supercell. (c) Meron pair energy vs the distance between meron and anti-meron with a truncation at $2r_0$. (d) Comparison of pair energies with different exchange interaction J . The dot lines are the fitting logarithmic scale. (e) Convergence of meron pair energy against the system size at $J = J_0$ and fixed distance of 240 Å.

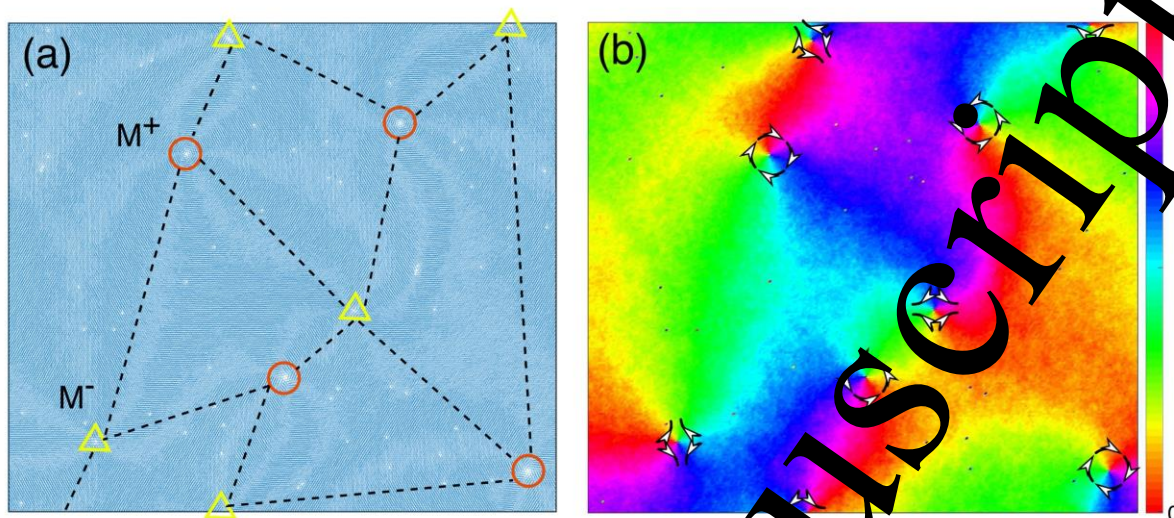


Figure 4 (a) Schematic plot of meron networks from MC simulations of monolayer CrCl₃. The merons and anti-merons are labeled by red circle (M⁺) and yellow triangle (M⁻) (b) In-plane phase map of (a). The swirling directions of meron and anti-meron are illustrated by arrowheads.

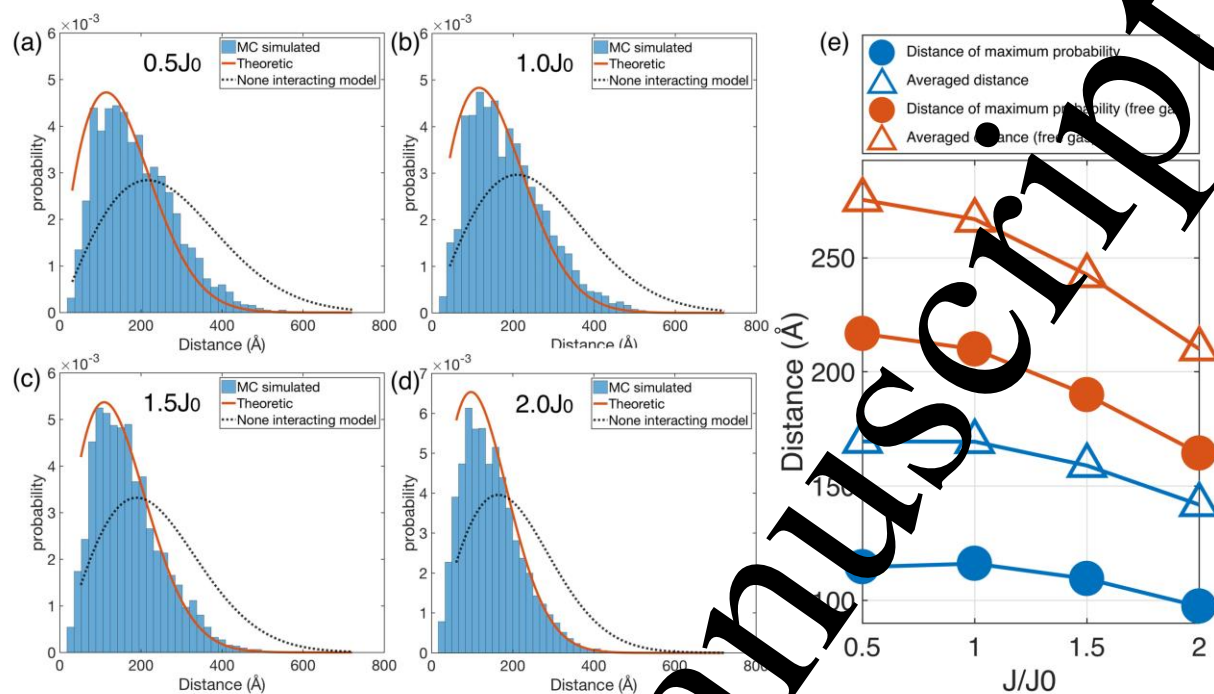


Figure 5 (a-d) Distribution of the NN distance between trions from MC simulations (the blue histogram), the discrete model (the red curve), and none-interacting model (the black dashed curve) under different exchange interaction J . (e) Summary of the most probable distance and averaged distance vs the exchange interaction J .

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