Commensurability governing skyrmion diffusion in confined geometries

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ABSTRACT

Magnetic skyrmions are topological magnetic structures, which exhibit quasi-particle properties and can show enhanced stability with respect to thermal noise. Recently, thermal Brownian diffusion of these quasi-particles has been found in continuous films and applications to unconventional computing have received significant attention, which however require structured elements. Thus as the next necessary step, we study skyrmion diffusion in confined geometries and find that the diffusion is governed by the interplay between the total number of skyrmions and the structure geometry. In particular, we ascertain the effect of circular and triangular geometries and find that for triangular geometries the behavior is drastically different for skyrmion numbers that are commensurate or incommensurate with a symmetric filling of the element. This commensurability effect is corroborated by molecular dynamics simulation.
INTRODUCTION

Magnetic skyrmions are particle-like magnetization whirls with topologically enhanced stability, which have been discovered in a large range of systems without certain symmetries, including bulk materials and magnetic films [1–5]. They are found to exist over a wide range of temperatures, with critical temperatures ranging from a few K to far above room temperature in different systems [6–11]. Owing to their potential small size, dynamics at low driving current, and topological properties, magnetic skyrmions have attracted intense interest in fundamental research and a wide variety of applications have been proposed. Current induced skyrmion motion could be used, amongst others, in racetrack memory, logic devices, and spin-transfer nano-oscillators [12–16]. An important issue is current induced Joule heating and in general the temperature of the environment. In some materials and for applications such as a skyrmion-based racetrack memory device [12] that relies on deterministic dynamics [17], thermal noise generates issues and can even dominate skyrmion nucleation, stability and addressability [18–20]. In contrast, thermal dynamics has actually been exploited recently for devices that aim at non-conventional logic, such as reservoir computing [21], and in particular skyrmion-based probabilistic computing [22] and token-based Brownian computing [23].

Similar to Brownian motion at finite temperature for conventional particles [24], which has been observed in many branches of science, skyrmion thermal diffusion also exhibits Brownian motion characteristics as recently observed experimentally in low-pinning multilayers [22]. The skyrmion diffusion behavior depends amongst other aspects on the skyrmion spin structure, the system temperature, and applied fields [22]. In particular, an in-plane field induces skyrmion deformations leading to anisotropic diffusion [25]. Finally, the diffusion constant was found to increase as a function of temperature and can be controlled by electric fields tuning the magnetic properties [23]. The influence of the skyrmion winding number on the diffusion has also been studied [26]. While these studies have been carried out on “infinite” systems realized by samples such as continuous films, where the skyrmion motion on the timescale of the observation is much smaller than the sample, one would expect that for devices, geometrical confinement effects can drastically alter the dynamics. In particular, the symmetry of the geometry is expected to change the dynamics and is key to the operation of devices where diffusion is employed. Theoretically Schäffer et al. predict two different time scales of thermal driven motion of ensembles of magnetic skyrmions in a confined geometry [27]. Here, the fluctuating dynamics depends on the interaction between skyrmions and edges, as well as the interaction between the skyrmions themselves. Furthermore, the skyrmion arrangements in a confined geometry are crucial for the addressability when using skyrmions as information carriers in data storage, and dependence of the thermal dynamics on arrangements and geometry is not clear. In particular, the influence of the number of skyrmions compared to the geometries size is key to understanding how to control and eventually use thermal skyrmion dynamics, but also to understand the underlying interactions that govern dynamics. The study of diffusion in extreme confinement conditions is also a necessary requirement for the experimental realization of basic computational components, such as C-joints, ratchets, hubs and wires, and the eventual realization of elementary circuits for token-based Brownian computing [23,25].

In this work, we experimentally study the skyrmions diffusion in confined geometries varying both the symmetry of the geometry as well as the number of skyrmions from a sparse population to a fully lattice-like situation. By tuning skyrmion numbers in a confined geometry with isotropic (circle) and non-isotropic (triangle) structures in a low pinning Ta/CoFeB/Ta/MgO/Ta multilayer system, we analyze skyrmion stability and confinement effects leading to a strong
dependence of the dynamics on geometry and skyrmion population. In the triangle, we find that the dynamics varies drastically for skyrmion numbers that can form a regular order, thus being commensurate with the geometry compared to skyrmion numbers that are incommensurate with respect to the geometries size. Corresponding thermal dynamics and mean square displacements (MSD) are quantitatively identified and corroborated by molecular dynamics simulation of a soft disc model.

RESULTS

Multilayer stacks of Ta(5)/Co$_{20}$Fe$_{18}$B$_{20}$(0.9)/Ta(0.08)/MgO(2)/Ta(5) were deposited by DC magnetron sputtering as previously used (Ref. [22]) and with the thickness of individual layers given in nanometers in parentheses. Our sample exhibits perpendicular magnetic anisotropy (PMA). To observe skyrmions and image their Brownian motion, the temporally and spatially resolved polar magneto-optic Kerr effect (MOKE) microscope with a time resolution of 62.5 ms was performed. The sample temperature is set to 341.5 K using a Peltier element so that we can obtain an appropriate skyrmion diffusion and stabilize multiple skyrmions in confined geometries. To study confinement effects, we patterned magnetic circular and triangular structures using electron beam lithography (EBL) and Ar ion etching, where the circular structure exhibits isotropic cylindrical symmetry and the triangular structure shows a lower symmetry. The diameter of the circle is 16.8 μm and the side length of the equilateral triangle is 26.8 μm, respectively.

To explore the thermal diffusion of skyrmion in confinement, we need to develop necessary tools to study skyrmions in different arrangements with different skyrmion numbers and individually study the behavior resulting from the interplay of the number of skyrmions and the size of the element. Then we can explore the arrangements of skyrmions finally depending on the element geometry, where we choose a highly symmetric circular geometry and less symmetric triangular geometry. As a first step, we therefore need to nucleate different numbers of skyrmions in our elements. Figure 1 shows the stabilization of multiple skyrmions in the circular geometry as a function of out-of-plane (OOP) field. By appropriately tuning the OOP field strength and fixing it to certain values, and subsequently applying an in-plane field pulse with 80 mT to saturate the sample and switching if off, a different number of skyrmions (from 1 to 8) can be nucleated and stabilized in the circle, as shown in Fig. 1 (a). Since the skyrmion diffusion depends on the skyrmion size [22], we control the size by an OOP magnetic field to keep a constant size for the different configurations with different numbers of skyrmions as used in the following. We show in Fig. 1 (b) and (c) for which field values we can stabilize which numbers of skyrmions and what the resulting skyrmion diameters are. At lower fields, skyrmions deform into stripe domains while at high fields they annihilate. For example, in the case of the configuration with one skyrmion, the skyrmion is annihilated to form a single domain state when the field is above 0.132 mT, and it is deformed to form stripe domains when the field is below 0.115 mT. For the configurations with large skyrmion numbers, note that the upper and lower range of field decreases at the same time. The interaction between skyrmions and the confinement suppresses skyrmion deformation under the lower critical field, and this limitation becomes more and more obvious for larger skyrmion numbers. The decrease of the upper critical field is because the skyrmion cannot keep a certain number due to increasing skyrmion-skyrmion interactions.

The modulation range of $d$, for the configurations with one skyrmion is much larger than that with multiple skyrmions. As for multiple skyrmions, the skyrmion-skyrmion interaction becomes dominant for the determination of the size
compared to the external field effect. Note that the error bar presented here includes the statistical error from averaging over all frames and skyrmions, and the error due to the spatial resolution of 0.13 μm of the 50x magnification lens (half of the spatial resolution). Due to the competition between skyrmions, the upper critical values of $d_s$ decrease as a function of skyrmion numbers, whereas the lower values show a small variation for all configurations. To study the Brownian motion under nominally identical conditions, we adjust the OOP field to keep the skyrmion diameter $d_s \sim 1.9 \text{ μm}$ for all configurations in a circle in the following measurements, as represented by the black dashed line in Fig. 1 (c).

With the results above, we can now firstly compare the behavior of different numbers of skyrmions with identical diameters in the geometry with the highest symmetry, the circular geometry. In Fig. 2, results for initial numbers of skyrmions of 2, 5 and 8 presented in Fig. 1 (a) are depicted. Figure 2 (a) shows a time-averaged OOP magnetization component, calculated over 9600 snapshots. Corresponding skyrmion trajectories are shown in Fig. 2 (b), where we see that the diffusive motion leading to complex trajectories with circular outer contours is caused by repulsive interactions between skyrmions and between skyrmions and boundaries. In particular as the circular geometry exhibits cylindrical symmetry, the resulting probability distributions for the skyrmion positions are cylindrically symmetric, and the bright skyrmions form a bright ring-like area. The contrast along the angular direction is a result of the finite measurement time and possible preferred positions due to a non-flat energy landscape. For an increasing number of skyrmions, the repulsive interactions lead to an increase of the radius of the resulting brightness ring, until one of the skyrmions is localized in the center (see example of 8 skyrmions). Finally, we analyze in Fig. 2 (c), the OOP magnetization component $m_{z}(r)$ as a function of the distance from center to edge which is calculated from the integration of the MOKE signals along the angular direction. For 8 skyrmions, in addition to the increase of the radius of the ring, a signal peak appears at $r = 0 \text{ μm}$. From this we can find that the arrangements of higher number skyrmions fit the circular geometry with an angular order, which shows a degree of freedom in angular direction, thus the diffusion shows collective rotation for the outer shell of skyrmions.

Having established that the filling of a geometry with a certain number of skyrmions impacts the skyrmion arrangements even in a high symmetry structure, we next study a more complex geometry. For the triangular geometry, Fig. 3 (a) depicts the configurations with an ascending number of skyrmions from 1 to 10 (Top row). As for the circular geometry we set the skyrmion size $d_s \sim 1.9 \text{ μm}$ for all configurations by adjusting the OOP field. The time-averaged frames are shown in the bottom row of Fig. 3 (a). The lower symmetry of the triangle results in a distinct distribution of skyrmion positions different from the high symmetry discs. For configurations with 1, 3, 6 and 10 skyrmions, the symmetry of time-averaged frames is in agreement with the initial configurations, which already represent a state that is commensurate with the geometry. Except for the “one skyrmion” configuration, skyrmions assemble into a triangular order with strong brightness contrast due to the confinement resulting from the boundary and skyrmion-skyrmion interactions, and the symmetry coincides with the triangular geometry. For the other configurations, where the combination of skyrmions and triangles results in an incommensurate state, skyrmions can diffuse over a comparatively larger area. The corresponding time-averaged pictures show that in the limited measurement time not all positions have been equally populated allowing us to ascertain from the dwell times a non-flat energy landscape.

To corroborate the intricate dependence of commensurability on skyrmion motion in triangular confinement, we have undertaken Molecular dynamics simulations with a Langevin thermostat ($dt = 0.001, \gamma = 1$). Skyrmions are represented
by soft discs interacting with each other via the following potential:

\[ V(r) = (\frac{r}{\sigma})^n. \]

\( \sigma = 1 \) and \( n = 10 \) were chosen in agreement with our previous work on skyrmion lattices in continuous films [28]. For simplicity, the skyrmion-wall potential which models the triangular constraint is also described by the same equation. The side length of the triangle is set to \( 5\sigma \) (corresponding to five skyrmion diameters) so that up to four skyrmions can align in one line in agreement with the experimental setup. Note that our equation of motion does not contain a gyrotropic coupling term. It is expected that the static behavior is unaffected by the Magnus force [29], even though the latter may influence dynamical properties like the mean squared displacement. The non-flat energy landscape, which can be observed in the experiments, has also been neglected in our idealized simulations.

As shown in Fig. 3 (b), structures with triangular symmetry arise for all investigated skyrmion numbers. In agreement with the experiments, simulations also show a commensurate state with a stable triangular geometry for 1, 3, 6 and 10 skyrmions. For other skyrmion numbers, as in the experiment, no stable triangle can be formed leading to a stronger diffusion of individual skyrmions. In these simulations, skyrmions at the corner of a triangle are mostly stable, while the remaining skyrmions fluctuate between the remaining positions of the triangular lattice. In the experiments, non-commensurate structures are less symmetric, which can likely be attributed to the non-flat energy landscape neglected in the simulations combined with the finite measurement time.

So while qualitatively the commensurability clearly plays a role, finally, we explore the diffusion and the impact of the commensurability quantitatively. The diffusion dynamics of Brownian motion under thermal noise can be expressed as [30,31]

\[ < [r_{x,y}(t') - r_{x,y}(t)]^2 > = < (\Delta r_{x,y})^2 > = 4D\Delta t, \]

where the left side expresses the MSD at the positions of the skyrmion center \( r_{x,y} \) at \( t' \) and \( t, \Delta t = t' - t \) is the time between two positions and \( D \) is the diffusion coefficient. Based on the recorded videos, the experimental results of MSDs as a function of time are calculated, as shown in Fig. 4 (a). We see that there are two qualitatively different behaviors occurring: (i) we see that the MSDs of configurations corresponding to commensurate states (1, 3, 6, 10) reach a saturation, and the saturation value of the MSD decreases with ascending skyrmion numbers. This is in agreement with the idea that a larger number of skyrmions in a commensurate state decreases the space accessible to each skyrmion; (ii) for incommensurate structures, skyrmions cover larger distances and the MSD does not reach a plateau value and thus does not saturate over the observed time scale. Just like for the commensurate states, the MSD is lower for higher skyrmion numbers.

Figure 4 (b) displays the initial stages of the MSD in corresponding simulations. Similar to the experiments, the plateau value decreases with ascending skyrmion number for commensurate states. For the incommensurate states, the skyrmions are able to move between different positions, and therefore the MSDs reach a saturation value much slower. While simulation results agree with experiments qualitatively, there are small differences, which can likely be attributed to non-flat energy landscape and/or our coarse-grained model and our assumed (potentially somewhat too strong) wall interactions, particularly for systems with 2 or 9 skyrmions. In the case of 2 skyrmions, simulations reach a plateau similar to the commensurate states, but at a higher value and after a longer period of time. This is a consequence of the skyrmions


only moving between positions in a fairly small triangle in the inner part of the full triangle. In the case of 9 skyrmions, the simulated MSD is much smaller than for all other simulations, because only two skyrmions switch positions most of the time while the others are mostly stable. Again, this may be an indication of a somewhat softer interaction in the real system, additional disorder induced resulting in a non-flat energy landscape and our somewhat simplified equation of motion. However, the qualitative behavior is fully reproduced showing that commensurability effects govern the dynamics in confined geometries.

CONCLUSION

In conclusion, our investigations of the skyrmion arrangement and diffusion behavior in magnetic multilayer system Ta(5)/Co$_{20}$Fe$_{60}$B$_{20}$(0.9)/Ta(0.08)/MgO(2)/Ta(5), in confined geometries demonstrate that the intricate interplay between the skyrmion number and the geometry governs, both the arrangement as well as the diffusion of the skyrmions. In highly symmetric discs we find that multiple skyrmions with higher numbers are arranged in an angular order, as well as the diffusion of skyrmions, where the skyrmions show rotation in angular direction. In particular, we discover a commensurability effect in triangular confinement, where the arrangement and in particular the diffusion qualitatively depend on the commensurability of the skyrmion number and the geometry: by tuning skyrmion numbers to 1, 3, 6 and 10 in the triangle, we find that states commensurate with the geometry are formed and lead to saturation of the MSDs as a function of time. The saturation value for the MSD decreases for higher skyrmion numbers as less space is accessible to individual skyrmions. In contrast, for the incommensurate states, the MSDs exhibit a non-monotonic relation and do not reach a saturation value over the observed timescale. Our molecular dynamics simulations show qualitative agreement with the experimental results corroborating the basic dependence of skyrmion numbers on motion in triangular confinement. Our findings reveal a new commensurability effect of thermal dynamics of skyrmions in confinement geometries, and provide a potential method to control diffusive dynamics by tuning skyrmion numbers and geometry shape. In particular our work shows that one needs to consider not only the number of skyrmions when engineering the thermal dynamics but also the commensurability leading to behavior that varies strongly between commensurate and incommensurate fillings of an element. Our study of these extreme confinement conditions will also be useful as a first necessary step towards the construction of basic computational components in Brownian computing, and may eventually pave the way for the experimental realization by clearly demonstrating the challenges for controlled thermal dynamics given by a filling of a geometry with a commensurate or incommensurate numbers of skyrmions.
Fig. 1 (a) Kerr images of multiple skyrmions in circle, the skyrmion numbers varies from 1 to 8. (b) Phase diagram of the OOP field dependence of the magnetic skyrmions stabilization as a function of skyrmion numbers. (c) The corresponding skyrmion diameter $d_s$ with increasing skyrmion numbers at each field in (b), dashed line represents skyrmion diameter around $1.9 \, \mu \text{m}$.

Fig. 2 (a) Time-averaged out-of-plane magnetization component over 9600 snapshots for the configurations with 2, 5 and 8 skyrmions in the circular geometry. The bright and dark areas represent the skyrmion diffusion and unfavorable positions, respectively. (b) Corresponding skyrmions trajectories visualized in different colors and (c) time-averaged and normalized signal along angular direction as a function of distance from center to edge.
Fig. 3 (a) Experiment results of skyrmions in triangular geometry. The top row is the configurations with different skyrmion numbers, and the bottom row is the time-averaged configurations over 9600 Kerr images. (b) Simulations of the histograms of skyrmion center positions for configurations of 1 to 10 skyrmions inside the triangle containing positions from 1 million independent frames.

Fig. 4 (a) Experiments and (b) simulations of MSDs for different skyrmion configurations (represented by different colors) in the triangular geometry as a function of step time $\Delta t$. 
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AUTHOR CONTRIBUTION

M.K., P.V. Q. L. and J. W. proposed and supervised the study. N.K. and B.S. patterned the different sample geometries. C.S., N.K and K.R. prepared the measurement set-up and conducted the experiments using the Kerr microscope. C.S. evaluated the experimental data with the help of Y.G. J.R., Y.G., M.B. and J. R. performed the molecular dynamics simulations with the help of F.D.. C.S. drafted the manuscript with the help of N.K., J.R., M.K. and P.V. All the authors commented on the manuscript.

COMPETING INTERESTS

The authors declare no competing interests.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

CODE AVAILABILITY STATEMENT

The code that support the findings of this study is available from the corresponding author upon reasonable request.
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