Reviewers' comments:

Reviewer #1 (Remarks to the Author):

In the present manuscript, A.F. Schaffer and co-authors present the study on the thermally-driven stochastic dynamics of magnetic skyrmions in a confined geometry. In particular, the authors developed Monte Carlo model, and used the model to simulate time-dependent thermally-excited skyrmion behaviors within confined geometries. Using material parameters comparable to interface-DMI stabilized skyrmions within Pd/Fe/It or Co/Pt type very thin multilayers system, the authors reveal how skyrmion texture and also arrangement evolve over time when thermal energy is given.

I believe this presented investigation is particularly interesting and important, as this study could be used to better understand the experimental observation of magnetic skyrmions in such systems using spin-polarized STM & MFM techniques, which basically averages magnetic contrast over >ms of measurement time. Moreover, with increasing interest on the thermal diffusion-driven behaviours of magnetic skyrmions, the present study provides important insight on the geometry-driven skyrmion motion and arrangement, which will largely help to design skyrmion devices depending on the device purpose.

Thus, I believe this manuscript is overall important, well-written, and also appropriate credit is given to previous works. However, I still have a couple suggestions for the authors as below to further strengthen the present study. Withe these suggestions addressed, I believe that the present study by A.F. Schaffer and co-authors should be published in Communications Physics.

Minor concerns:

1.From the presented skyrmion size/texture/arrangement change over a time (Fig.2, 5, 6 and Movie), it seems to me that strong skyrmion boundary deformation happens. Thus, I am wondering if this transformation is also accompanies the skyrmion number deformation of a time, or it's just shape-wise changes while keeping skyrmion number to be always intergers. It will be helpful if the authors could plot the time-dependent skyrmion number (topological number) variance as well, to understand how strong topological characteristic changes over time in such systems.

2.From Fig. 6, it is interesting to me that a pinned skyrmion (which may be a achiral bubble that is not topologically protected) survives quite stably over a time, while other chiral skyrmions sometimes get generated/annihilated through boundary. It would be helpful if the authors could comment on this topology & stability issue.

Reviewer #2 (Remarks to the Author): ***see attached file***

Reviewer 2 attached file

Reviewer Comments: *Stochastic dynamics and pattern formation of geometrically confined skyrmions* Schaffer, et al.

The authors study the diffusive dynamics of skyrmions in confined geometries by means of micromagnetic and quasiparticle simulations. The manuscript claims to show that skyrmions undergo thermally driven diffusive motion on two different timescales, driven by local deformation of skyrmions and geometric confinement, respectively. The paper also examines the role of time averaging in observing skyrmion motion and presents a quasiparticle Monte Carlo approach for calculating the skyrmion probability density function. In principle this is an interesting idea and could be important to compare with experimental data. However, I found this paper quite lacking in several respects and at this time I cannot recommend publication.

My primary reason for rejection is that I find no evidence in this paper of the main claim that there are two different time scales for the skyrmion motion. The author present as evidence the three-paneled Figure 4a and Figure 5 for different spatial geometries. These figures simply show that the time-averaged signal of a diffusive particle is different than a single shot measurement. The authors do not present traces of individual skyrmions or calculate the mean squared displacement (as in Fig 2 of Ref. 25), which would show whether there were clearly different regimes of skyrmion motion or if the observed behavior is solely due to signal averaging. It would be quite interesting if the skyrmions to exhibit different dynamics at different times *and* if the authors show how to extract this information from the time averaged signal. However as presented the discussion is far from complete.

The authors present no mathematical expressions or fits to justify their hypothesis of two dynamical regimes. Additionally, if the dynamics at long timescales is truly governed by skyrmion-skyrmion interactions and interactions with the sample boundary, the crossover time should depend on the size of the sample and the density of skyrmions in the sample. At a minimum I would expect a numerical paper such as this one to comment on how the results scale with system size at fixed total skyrmion number. Furthermore, in the case of the 'phantom skyrmions', as in the case of two or five skyrmions, how would one extract the true skrymion number from this signal?

Additionally, the description of the quasiparticle Monte-Carlo approach for the probability distribution function is lacking. What are the assumptions in this method? Why is it fitting for this problem? On page 6 of the manuscript the authors briefly discuss the construction of the quasiparticle model based on a dilute skyrmion limit where strong deformation of the skyrmions does not occur. However, in the figures it seems that some of the skyrmions are quite deformed from their original shape at 20ns. What is the 'dilute limit' and is it appropriate for a confined geometry? I would recommend a widely expanded discussion of the validity of the quasiparticle approach for the probability distribution function (as opposed to one based on the Thiele equation), because to my knowledge this has not been developed previously and without a longer explanation the reader is left wondering why it's necessary. For example, a figure showing direct comparison of the quasiparticle Monte-Carlo with the integrated LLG result would help show whether the Monte-Carlo method truly captures the salient features.

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I believe this presented investigation is particularly interesting and important, as this study could be used to better understand the experimental observation of magnetic skyrmions in such systems using spin-polarized STM & MFM techniques, which basically averages magnetic contrast over >ms of measurement time. Moreover, with increasing interest on the thermal diffusion-driven behaviours of magnetic skyrmions, the present study provides important insight on the geometry-driven skyrmion motion and arrangement, which will largely help to design skyrmion devices depending on the device purpose.

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[Reply 1-0]

We thank the Reviewer for the careful reading of our manuscript and the useful suggestions. Following the recommendations, we significantly revised the discussion, and are convinced that the present version is suitable for publication in Communications Physics.

Minor concerns:

[Comment 1-1]

From the presented skyrmion size/texture/arrangement change over a time (Fig.2, 5, 6 and Movie), it seems to me that strong skyrmion boundary deformation happens. Thus, I am wondering if this transformation is also accompanies the skyrmion number deformation of a time, or it's just shape-wise changes while keeping skyrmion number to be always intergers. It will be helpful if the authors could plot the time-dependent skyrmion number (topological number) variance as well, to understand how strong topological characteristic changes over time in such systems.

[Reply 1-1]

In the case of periodic boundary conditions, the topological number remains an integer despite the deformation of its shape due to thermal fluctuations. The time dependence of the topological number for that case is illustrated in, e.g., Fig. 7 of Ref. (21). In the present study free boundary conditions are used, where the topological number is no longer an integer and indeed fluctuates over time; however, this can be attributed to the thermal excitation of the spins at the boundary, not to the deformation of the skyrmions. We clarified this point during the discussion of Fig. 3 on page 2, and the standard deviation of the topological number for fixed temperatures is shown in the Figure with error bars. Below the temperature T1, no skyrmion collapse or creation takes place, and the fluctuations in the skyrmion number are caused solely by edge effects.

[Comment 1-2]

From Fig. 6, it is interesting to me that a pinned skyrmion (which may be a achiral bubble that is not topologically protected) survives quite stably over a time, while other chiral skyrmions sometimes get generated/annihilated through boundary. It would be helpful if the authors could comment on this topology & stability issue.

[Reply 1-2]

In the considered system skyrmions are stabilized by the Dzyaloshinsky-Moriya interaction, and they all possess the same finite topological charge. The pinned feature in Fig. 8 (previously Fig. 6) is also a magnetic skyrmion. Strictly speaking, the topological stability, that is, the impossibility to erase a skyrmion by applying external fields, does exist in continuous systems only. On a discrete lattice skyrmions have a finite lifetime due to the possibility of collapse and escape or creation through the boundary; this is investigated in more detail in, e.g., Refs. (20)-(24). Therefore, in the manuscript we avoided referring to topological stability or topological protection. As we work with the discrete lattice, the skyrmions are stable if their lifetime is much larger than the observation time. At the time scale of the simulations shown in Fig. 8, all five skyrmions are stable and they do not escape the island due to thermal fluctuations. Similarly, also the darker spots appearing at the boundary (e.g. in the 10 ns snapshot) do not lead to the nucleation of additional skyrmions.

Reviewer #2

Reviewer Comments: Stochastic dynamics and pattern formation of geometrically confined

skyrmions Schaffer, et al.

The authors study the diffusive dynamics of skyrmions in confined geometries by means of micromagnetic and quasiparticle simulations. The manuscript claims to show that skyrmions undergo thermally driven diffusive motion on two different timescales, driven by local deformation of skyrmions and geometric confinement, respectively. The paper also examines the role of time averaging in observing skyrmion motion and presents a quasiparticle Monte Carlo approach for calculating the skyrmion probability density function. In principle this is an interesting idea and could be important to compare with experimental data. However, I found this paper quite lacking in several respects and at this time I cannot recommend publication.

[Reply 2-0]

We thank the Reviewer for the careful reading of our manuscript and the useful suggestions. Following the recommendations, we significantly revised the discussion, and are convinced that the present version is suitable for publication in Communications Physics.

[Comment 2-1]

My primary reason for rejection is that I find no evidence in this paper of the main claim that there are two different time scales for the skyrmion motion. The author present as evidence the three-paneled Figure 4a and Figure 5 for different spatial geometries. These figures simply show that the time-averaged signal of a diffusive particle is different than a single shot measurement. The authors do not present traces of individual skyrmions or calculate the mean squared displacement (as in Fig 2 of Ref. 25), which would show whether there were clearly different regimes of skyrmion motion or if the observed behavior is solely due to signal averaging. It would be quite interesting if the skyrmions to exhibit different dynamics at different times and if the authors show how to extract this information from the time averaged signal. However as presented the discussion is far from complete.

[Reply 2-1]

The main claim of the manuscript is not that there are two different time scales characterizing the displacement or diffusive motion of the skyrmion, but rather that the interplay of two types of dynamics has to be taken into account: deformation and displacement at different time scales. The magnetization dynamics on the short time scale foremost results in deformations of the skyrmions, whereas the long time scale accounts for the spatial movement of an entire skyrmion. To clarify this point, the manuscript has been modified accordingly, supported by new calculations, which especially focus on the dynamics on the short time scale. While the deformation is described in Fig. 7, the spatial movement is shown below and in Fig. 6 of the revised manuscript.
Firstly, we investigate how fast the time-averaged magnetization configurations converge over 20 ns long simulations, showing an asymptotic decay to the equilibrium probability distribution (cf. Fig. 6). Secondly, we study the deformations of skyrmions on the time scale of (>0.5 ps), by extracting the average skyrmion radius for 50 different initializations of the pseudo random number generator but identical initial magnetic states. The results are shown in Fig. 7. On the one hand, the fluctuations lead to an increased size of the skyrmions compared to the relaxed states at zero temperature. We can also see an oscillating pattern corresponding to internal modes of the skyrmion such as breathing modes.

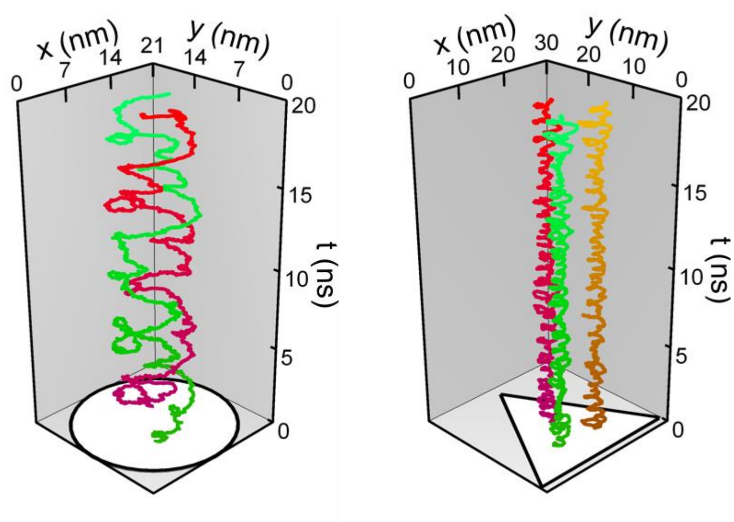

Fig. R 1 Traces of two skyrmions inside the disk system and of three skyrmions in the triangular shaped island illustrating the delocalized or localized behavior of the skyrmion ensembles.

Figure R1 shows an example for the suggested trajectories, where we extracted the traces of the centers of the skyrmions for two different cases, corresponding to Fig. 4a (2) and Fig. 5 (3), respectively. As discussed in the manuscript, in case of the disk system the two skyrmions experience a flat energy surface, leading to a rather delocalized behavior of the skyrmions. In contrast to that the random movement for the three skyrmions in the triangular system is constrained.

[Comment 2-2]

The authors present no mathematical expressions or fits to justify their hypothesis of two dynamical regimes. Additionally, if the dynamics at long timescales is truly governed by skyrmion-skyrmion interactions and interactions with the sample boundary, the crossover time should depend on the size of the sample and the density of skyrmions in the sample. At a minimum I would expect a numerical paper such as this one to comment on how the results scale with system size at fixed total skyrmion number. Furthermore, in the case of the 'phantom skyrmions', as in the case of two or five skyrmions, how would one extract the true skrymion number from this signal?

[Reply 2-2]

As mentioned in the reply to the previous question, under the short time scale we understand the deformations of a skyrmion, while the long time scale is connected to the translational motion. Therefore, if the two regimes can be distinguished in the system as demonstrated by Figs. 6 and 7, the short time scale does not depend on the size of the sample or the density of skyrmions, i.e. it is expected that the oscillation frequency of 60 GHz shown in Fig. 7 would be similar for other geometries. The long time scale may be characterized by different characteristic times which are indeed dependent on the sample size and the skyrmion density, but each of these characteristic times are on the order of a few nanoseconds. The dependence of these characteristic times on the number of skyrmions in the system is shown in the newly added Figs. 6a and b: if the skyrmions form a close-packed configuration which is compatible with the shape of the island (3 or 7 skyrmions for the disk, 3 or 6 skyrmions for the triangle), the time-averaged magnetic signal will converge faster to its asymptotic form since the skyrmions have less place to move.

Concerning the scaling issue, new results are added to the Monte Carlo simulations for larger islands in Fig. 10. Indeed, for larger islands, the pattern formation does not occur anymore, as the dynamics is mainly dominated by the stochastic motion and not by the competing skyrmion-skyrmion and skyrmion-boundary interaction. The energy barriers between the local minima of the energy surface are diminished for larger islands. Similarly to low skyrmion densities, higher temperatures also lead to a broad skyrmion distribution, as the time required to overcome the energy barriers is reduced, assuming an Arrhenius-like behavior.

Regarding the question of how to extract the true skyrmion number from such measurements, the measured time-averaged signal, such as in Fig. 8b, can still be useful. One could imagine a reference measurement of a completely magnetized sample. Every additional skyrmion hosted on the island will lead to a diminished out-of-plane component of the net magnetization. Comparing the experimental data to time-averaged micromagnetic simulations or to the results of the Monte Carlo method developed in the manuscript could lead to a quantitative determination of the number of skyrmions in the system.

[Comment 2-3]

Additionally, the description of the quasiparticle Monte-Carlo approach for the probability distribution function is lacking. What are the assumptions in this method? Why is it fitting for this problem?

[Reply 2-3]

The main assumption for the Monte Carlo approach is that the thermal deformations of the skyrmions do not lead to creation or collapse processes, including such events at the boundaries. The appropriate temperature regime for the chosen material combination is determined in the first subsection of the results during the discussion of Fig. 3, and in the Methods where the calculated skyrmion-boundary and skyrmion-skyrmion interaction potentials are presented. The discussion about the applicability of the Monte Carlo method, now moved to the Methods, was extended following these questions.

[Comment 2-4]

On page 6 of the manuscript the authors briefly discuss the construction of the quasiparticle model based on a dilute skyrmion limit where strong deformation of the skyrmions does not occur. However, in the figures it seems that some of the skyrmions are quite deformed from their original shape at 20ns. What is the 'dilute limit' and is it appropriate for a confined geometry?

[Reply 2-4]

Strong deformations in this context mean deformations strong enough to destroy the skyrmions. Deformations below this critical strength only provoke an excitation of the magnetic texture. To clarify this point, we removed the unclear term "dilute limit" from the manuscript.

[Comment 2-5]

I would recommend a widely expanded discussion of the validity of the quasiparticle approach for the probability distribution function (as opposed to one based on the Thiele equation), because to my knowledge this has not been developed previously and without a longer explanation the reader is left wondering why it's necessary. For example, a figure showing direct comparison of the quasiparticle Monte-Carlo with the integrated LLG result would help show whether the Monte-Carlo method truly captures the salient features.

[Reply 2-5]

We added a direct comparison of the time integrated micromagnetic results with the Monte Carlo method and compared the resulting maxima of the probability distributions in Fig. 9 of the revised manuscript. By extracting the positions of the skyrmions and calculating their distribution, the advantage of the quasiparticle approach is that it is computationally less intensive, meaning that using this method a much smoother distribution function can be obtained significantly faster than with the micromagnetic method, enabling a more reliable comparison with the experimental results.

Similarly to the Thiele equation, the Monte Carlo approach assumes point particles, the interaction between which has to be determined from an atomistic model. We do not claim that a similar procedure would not be possible based on the Thiele equation. Indeed, atomistic simulations of skyrmion diffusion were used to parametrize a generalized stochastic Thiele equation in Ref. (25), similarly to the parametrization of the quasiparticle method in the present manuscript. The difference between the present quasiparticle approach and the Thiele equation is restricted to the dynamics, and the quantitative comparison of the two methods is beyond the scope of the present study. This is analogous to the difference between spin lattice simulations based on Monte Carlo methods and on the Landau-

Lifshitz-Gilbert equation, both of which are used widely in the literature. To clarify these points, the last sentence of the Introduction was reformulated to compare the speed of the quasiparticle simulations to the micromagnetic model instead of that of the Thiele equation.

REVIEWERS' COMMENTS:

Reviewer #1 (Remarks to the Author):

I believe the authors sufficiently responded to all my initial comments, and now I support the publication of this work in Communications Physics.

Reviewer #2 (Remarks to the Author):

The authors have responded to the comments raised in my report, adding new results contrasting the short and long time dynamics of the skyrmions and additional direct comparison with the micro-magnetic simulations. In particular I found the additional Figure 6 very helpful for understanding how an experiment might extract the true number of skyrmions. Likewise the additional discussion clarified the advantages of this numerical approach compared to other approaches. I am satisfied with the responses and I think the paper is now suitable for publication.

I have some minor, optional suggestions:

Fig 6: the legend labels could be smaller, also it is missing an x-axis label.
Fig 7 caption: I think that this is showing two different simulations with one skyrmion each, correct? The language is a little bit ambiguous, as it could also be interpreted as 'two skyrmions on a single disk-shaped island'. I would suggest amending the caption to make the situation more clear. Also in that vein, why not show one skyrmion in the disk geometry and one in the triangle geometry? This would parallel the rest of the discussion nicely.

POINT BY POINT RESPONSE

Reviewer #2 (Remarks to the Author):

The authors have responded to the comments raised in my report, adding new results contrasting the short and long time dynamics of the skyrmions and additional direct comparison with the micro-magnetic simulations. In particular I found the additional Figure 6 very helpful for understanding how an experiment might extract the true number of skyrmions. Likewise the additional discussion clarified the advantages of this numerical approach compared to other approaches. I am satisfied with the responses and I think the paper is now suitable for publication.

I have some minor, optional suggestions:

Fig 6: the legend labels could be smaller, also it is missing an x-axis label.

We decreased the legend label size and added the missing x-axis label.

Fig 7 caption: I think that this is showing two different simulations with one skyrmion each, correct? The language is a little bit ambiguous, as it could also be interpreted as 'two skyrmions on a single disk-shaped island'. I would suggest amending the caption to make the situation more clear. Also in that vein, why not show one skyrmion in the disk geometry and one in the triangle geometry? This would parallel the rest of the discussion nicely.

The Figure shows the radial oscillations of two skyrmions placed on a single disk-shaped island simultaneously, the fast skyrmion deformation does not qualitatively depend on the interaction between the skyrmions or on the shape of the boundary. To show the complete information on the dynamics of all included skyrmions, we plot the resulting oscillations for both skyrmions. We made the caption less ambiguous by writing “Two skyrmions on a single disk […]”. Additionally we referred to both panels individually in the main text.