Self-consistent mean field theory studies of the thermodynamics and quantum spin dynamics of magnetic Skyrmions

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Received 21 October 2016, revised 23 January 2017
Accepted for publication 8 February 2017
Published 27 March 2017

Abstract
A self-consistent mean field theory is introduced and used to investigate the thermodynamics and spin dynamics of an $S = 1$ quantum spin system with a magnetic Skyrmion. The temperature dependence of the Skyrmion profile as well as the phase diagram are calculated. In addition, the spin dynamics of a magnetic Skyrmion is described by solving the time dependent Schrödinger equation with additional damping term. The Skyrmion annihilation process driven by an electric field is used to compare the trajectories of the quantum mechanical simulation with a semi-classical description for the spin expectation values using a differential equation similar to the classical Landau–Lifshitz–Gilbert equation.

Keywords: Skyrmion, quantum spin dynamics, self-consistent mean field theory

Supplementary material for this article is available online
(Some figures may appear in colour only in the online journal)

1. Introduction
Magnetic Skyrmions have undergone an intensive attention during the last years caused by the ideas to use them for data storage and as part of logic devices [1–5]. The advantages of magnetic Skyrmions are their stability cause by the topology, the high mobility which allows to use very low current densities to change the position and the small sizes (from $\sim$1 nm in the case of Fe/Ir(111) [6] to $\sim$90 nm in the case of Fe$_{0.5}$Co$_{0.5}$Si [7]). Moreover, magnetic Skyrmions can be found in magnetic bulk materials like MnSi [8], FeGe [9] respectively Fe$_{1-x}$Co$_x$Si [10] and in thin film structures on the macroscopic (nano to micrometer length) [11] as well as on the atomic length scale as Fe/Ir(111) [12], Pd/Fe/Ir(111) [13] respectively (Pt$_{0.95}$Ir$_{0.05}$)/Fe/Pd(111) [14]. Therefore, several experimental techniques like neutron scattering [8], Lorentz transmission microscopy [9], magnetic transmission x-ray microscopy [15], magneto optical Kerr effect (MOKE) microscopy [11] or Spin polarized scanning tunneling microscopy [13] have been used to investigate magnetic Skyrmions. In addition to the experimental investigations combined analytical and numerical calculations [16, 17] as well as Monte Carlo [7, 18–20] and spin dynamics simulations [1, 14, 21–24] have been performed to get a deeper understanding of the topic and more informations about statics, thermodynamics and the dynamics of magnetic Skyrmions. Especially spin dynamics simulations can be used to describe the dynamics of magnetic Skyrmions. Depending on the length scale micromagnetic or atomistic spin dynamics simulations can be used to investigate the movement of magnetic Skyrmions in race track devices [1–3] or to find the best way to pin and depin magnetic Skyrmions [25]. Furthermore, due to spin dynamics simulations several ways to create and annihilate magnetic Skyrmions using electric current pulses [26], spin waves [27], Laser [28], and due to uniaxial stress [29] have been proposed. So far, nearly all descriptions are classical.
This is correct in most of the cases especially for bulk materials. However, with a further reduction of the system size quantum effects become important and can’t be longer ignored. Furthermore, Usov et al. [30] and Nieves et al. [31] have pointed out that a classical description is not always convenient or flexible enough to give an adequate description. A quantum mechanical description also offers new perspectives and leads to new opportunities [32, 33]. Within this publication a quantum mechanical self-consistent mean field theory is used to describe the thermodynamics and spin dynamics of magnetic Skyrmions. This description shall be seen as an alternative to the common classical spin dynamics and Monte Carlo simulations.

In general mean field theories offer the chance to investigate complex many-body systems by reducing them to local one-body problems. This fact together with the dispelling of the fluctuations make mean field theories successful. Several mean field theories and methods like the Ginzburg–Landau theory [34, 35], the Stoner model of itinerant magnets [36], the random phase approximation (RPA) in the description of many-body Green’s functions [36], the cluster mean field method [37], and the Hartree–Fock theory [38, 39] have been proposed and intensively used.

Within this study the used quantum mechanical self-consistent mean field theory helps to increase the system size which can be addressed. Actually it is possible to describe the dynamics and thermodynamics of 60 quantum spins $S = 1/2$ on a square lattice via exact diagonalization. With other methods like the Lanczos algorithm the addressable system size can be increased. However, also in these cases the calculations are restricted to small system sizes of a few hundred spins. With aid of the self-consistent mean field theory used in this paper the description becomes local and therefore entanglement among the spins plays no role. This means, the Hilbert space and therefore the corresponding matrices of the system are drastically reduced which allows us to address larger system sizes: within this publication a square lattice of $200 \times 200 = 40000$ quantum spins with spin quantum number $S = 1$ is described.

The publication is organized as follows: in section 2 the Hamilton operator $\hat{H}$ of the quantum mechanical self-consistent mean field theory is introduced. Section 3 describes the temperature dependence of the local magnetization inside and outside the Skyrmion. The eigenvalues and the eigenfunction corresponding to the ground state of $\hat{H}$ are discussed in section 4, followed by the description of the switching dynamics of the magnetic Skyrmion driven by an electric field oriented perpendicular to the film plane (section 5). Finally, the publication ends with a summary (section 6).

2. Model

The investigated system is a quantum mechanical spin system with $200 \times 200$ spins $S = 1$ on a square lattice with periodic boundary conditions. The intention is not to investigate a particular material but to give a general description by using the following Hamilton operator:

$$\hat{H} = - J \sum_{n,m} \hat{S}_n \cdot (\hat{S}_m) - \sum_{n,m} D_{nm} \cdot (\hat{S}_n \times (\hat{S}_m)) - g \mu_B \sum_n B \cdot \hat{S}_n. \quad (1)$$

$\hat{H}$ describes the interaction of the spin operator $\hat{S}_n$ with the surrounding spins by their expectation values $\langle \hat{S}_n \rangle$. Therefore, the description is reduced to the description of local spins.

The first term of the Hamilton operator $\hat{H}$ describes the nearest neighbor ferromagnetic ($J > 0$) exchange interaction and the second term the Dzyaloshinshky–Moriya interaction. Together with the exchange interaction the Dzyaloshinshky–Moriya interaction lead to a non-collinear spin configuration (spin-spiral). The $D_{nm}$ are the characteristic vectors of the Dzyaloshinshky–Moriya interaction responsible for the direction and sense of rotation of the spin-spiral [40, 41]. Within this publication the $D_{nm}$ are assumed to be oriented inside the 2D film plane perpendicular to the connection between nearest neighbor lattice sites $r_{nm}$ i.e. $D_{nm} \perp r_{nm}$. The assumed strength of the Dzyaloshinshky–Moriya interaction $D_{nm} = |D_{nm}|$ in dimensionless units is $D_{nm}/J \approx 0.314$. The third term of the Hamilton operator $\hat{H}$ describes the coupling of the spins to an external magnetic field $B$ (Zeeman term), where $g$ is the Landé factor and $\mu_B$ the Bohr magneton. To stabilize the magnetic Skyrmion an external magnetic field in $+z$-direction, perpendicular to the film plane ($xy$-plane), is assumed. The resulting spin configuration (magnetic Skyrmion) can be seen in figure 1.

To show the announced local character of the Hamilton operator $\hat{H}$ it is convenient to define the effective field $B_{\text{eff}}_n = \frac{\partial \hat{H}}{\partial \hat{S}_n}$ with $B_{\text{eff}}_n = (B_{\text{eff}}^x_n, B_{\text{eff}}^y_n, B_{\text{eff}}^z_n)^T$ and the strength $B_{\text{eff}}^x_n = |B_{\text{eff}}^x_n|$. With the definition of $B_{\text{eff}}^x_n$ the Hamilton operator $\hat{H}$ can be written as:

$$\hat{H} = - \sum_n B_{\text{eff}}^x_n \cdot \hat{S}_n. \quad (2)$$

Then, with

$$\hat{h}_n = - B_{\text{eff}}^x_n \cdot \hat{S}_n, \quad (3)$$

$\hat{H}$ can be finally written as sum of local Hamilton operators $\hat{h}_n$:

$$\hat{H} = \sum_n \hat{h}_n, \quad (4)$$

which shows the local character of $\hat{H}$ and suppresses entanglement and therefore quantum fluctuations. On the other hand, the local character allows us to address the system size of $200 \times 200$ spins with spin quantum number $S = 1$.

3. Thermodynamical studies

To study the temperature dependence of the magnetic Skyrmion methods of the statistical physics can be used. From quantum statistics it is known that the spin expectation value for a single spin at lattice site $n$ is defined by:

$$\langle \hat{S}_n \rangle = \frac{\text{Tr}(\hat{S}_n \exp(-\beta \hat{H}))}{\text{Tr}(\exp(-\beta \hat{H}))}, \quad (5)$$
where \( \beta \) is the inverse temperature, i.e. \( \beta = \frac{1}{kT} \). In case of a quantum spin system the trace is the sum over all quantum numbers. Therefore, after some algebra one finds an equation which can be solved numerically:

\[
\langle S_n \rangle = g\mu_B B_0 (\beta B_n^\text{eff}) \mathbf{b}_n^\text{eff}.
\]  

Within this equation \( B_0 (\beta B_n^\text{eff}) \) is the Brillouin function:

\[
B_0 (\beta B_n^\text{eff}) = \frac{2S + 1}{2S} \coth \left( \frac{2S + 1}{2S} \beta B_n^\text{eff} \right) - \frac{1}{2S} \coth \left( \frac{1}{2S} \beta B_n^\text{eff} \right),
\]  

and \( \mathbf{b}_n^\text{eff} \) the unit vector in the direction of the effective field \( B_n^\text{eff} \), i.e. \( \mathbf{b}_n^\text{eff} = \mathbf{B}_n^\text{eff} / B_n^\text{eff} \).

Figure 1 shows the Skyrmion configuration for \( T = 0 \) K and \( |B|/B_C = B/B_C \approx 0.41 \), where \( B_C \) is defined as the critical magnetic field value at \( T = 0 \) K at which the magnetic Skyrmion disappears. For \( B > B_C \) the ferromagnetic state is the ground state. Such a Skyrmion configuration or similar ones can be created by solving equation (6) self-consistently starting with a random configuration or with an initially given skyrmionic structure. The description itself is not restricted to \( S = 1 \), the same Skyrmion configuration can be found for any spin quantum number \( S \) and also in the case of a classical spin (\( S = \infty \)). Figure 1(a) shows the whole spin system (\( z \)-component of the spin expectation value \( \langle \hat{S}_z \rangle \)). Clearly visible is the magnetic Skyrmion located at \( x = 139 \ a, y = 86 \) a, where \( a \) is the lattice constant. Figure 1(b) provides the microscopic structure of the magnetic Skyrmion which due to the in plane Dzyaloshinsky–Moriya interaction shows a Hedgehog structure. Such a magnetic Skyrmion is called Néel type magnetic Skyrmion and can be also found using other numerical methods like Langevin spin dynamics [42] or Monte Carlo simulations [18]. Figures 1(c) and (d) give the profiles which appear for a cut through the middle of the magnetic Skyrmion (\( y = 86 \ a = \text{const.} \)). The temperature dependence of the magnetic Skyrmion is shown in figure 2. In detail, figures 2(a) and (b) show the same profiles as in figures 1(c) and (d) for \( T/T_C^{\text{Sk}} = 0 \) and \( T/T_C^{\text{Sk}} = 0.956 \), where the dimensionless temperature is scaled with respect to the critical temperature \( T_C^{\text{Sk}} \) at which the magnetic Skyrmion disappears (see figure 2(c)). As expected the magnetization decreases with increasing temperature. However, the general appearance of the magnetic Skyrmion does not change, i.e. only the size of the magnetic Skyrmion reduces with increasing temperature. This can be manifested with aid of the Skyrmion radius \( \Delta_S^{\text{Sk}} \). In the following, radius \( \Delta_S^{\text{Sk}} \) is defined as the distance between the two zero crossings of \( \langle \hat{S}_z \rangle \) (see figure 2(b)). The decrease of \( \Delta_S^{\text{Sk}} \) with increasing temperature is shown in figure 2(c), additionally the abrupt disappearance at \( T_C^{\text{Sk}} \). Above \( T_C^{\text{Sk}} \) the ferromagnetic state is the ground state corresponding to \( \Delta_S^{\text{Sk}} = 0 \). The abrupt change of the Skyrmion radius \( \Delta_S^{\text{Sk}} \) form \( \Delta_S^{\text{Sk}} \approx 4.8 \ a \) to \( \Delta_S^{\text{Sk}} = 0 \ a \) corresponds to the abrupt disappearance of the magnetic Skyrmion at \( T_C^{\text{Sk}} \). In the thermodynamic limes such a behavior indicates
Figure 2. Magnetic Skyrmion temperature dependence: (a) and (b) Skyrmion profiles at \( T/T_C = 0 \) K and \( T/T_C^{SB} \approx 0.956 \), (c) Skyrmion width as a function of temperature.

Figure 3. Temperature dependence: (a) and (b) spin expectation value \( \langle \hat{S}_z \rangle \) and \( \langle |\hat{S}_z| \rangle \) as a function of temperature for \( B/B_C \approx 0.41 \), where \( B_C \) is the critical magnetic field (transition magnetic Skyrmion \( \leftrightarrow \) Ferromagnet) at \( T = 0 \) K. The spin expectation values and the corresponding absolute values are calculated for the center of the Skyrmion and the surrounding domain. \( T_C^{SB} \) is the critical temperature where the magnetic Skyrmions disappear (transition magnetic Skyrmion \( \leftrightarrow \) Ferromagnet) and \( T_{C,FM}^{DM} \) corresponds to the transition transition Ferromagnet \( \leftrightarrow \) Paramagnet. (c) Corresponding phase diagram. The temperature scale is normalized with the Curie temperature \( T_C \) (transition Ferromagnet \( \leftrightarrow \) Paramagnet) at \( B = 0 \) T.

a phase transition of first order while a continuous decrease of the order parameter indicates a phase transition of second order. In this case the order parameter is the Skyrmion radius \( \Delta_{Sk} \), alternative the Skyrmion number \( Q \), which characterizes the topology of the system [43], can be used [20] or the local magnetization (spin expectation value \( \langle \hat{S}_z \rangle \)). The local magnetization shows the same abrupt decrease at the critical temperature \( T_{C,Sk} \) if \( \langle \hat{S}_z \rangle \) corresponds to a lattice site \( n \) inside the magnetic Skyrmion. In the case of the surrounding ferromagnetic environment \( \langle \hat{S}_z \rangle \) shows a continuous decrease with increasing temperature furthermore a higher critical temperature \( T_{C,FM}^{DM} > T_{C,Sk}^{DM} \). Figure 3(a) shows the absolute values of the spin expectation values \( \langle |\hat{S}_z| \rangle \) corresponding to the center of the Skyrmion, i.e. \( x = 139 \) a, \( y = 86 \) a (red curve) and the surrounding ferromagnetic domain, i.e. \( x = 80 \) a, \( y = 80 \) a (black curve). Both curves show a perfect agreement at low temperatures although the magnetizations (spin expectation values) corresponding to the Skyrmion and the Ferromagnet have opposite orientations (see figure 3(a)). At \( T \approx 0.7 T_C \) the curves start to deviate: the magnetization inside the Skyrmion disappears faster than the magnetization of the surrounding Ferromagnet. The jump back in figure 3(a) respectively the jump from negative to positive spin expectation values \( \langle |\hat{S}_z| \rangle \) in figure 3(b) correspond to the disappearance of the magnetic Skyrmion at \( T_{C,Sk}^{SB} \approx 0.86 T_C \). At temperatures above \( T_{C,Sk}^{SB} \) the curves for \( \langle |\hat{S}_z| \rangle \) respectively \( \langle \hat{S}_z \rangle \) show again a perfect agreement caused by the disappeared difference in the local magnetization due to the fact that the magnetic Skyrmion is gone and the system is now completely ferromagnetic. Then, after a further temperature increase the Ferromagnet becomes paramagnetic at \( T_{C,FM}^{DM} \approx 1.03 T_C \). The fact that \( T_{C,FM}^{DM} > T_C \) is caused by the appearance of the external magnetic field \( B \) which is needed to stabilize the magnetic Skyrmion and which increases the critical temperature \( T_{C,FM}^{DM} \). At this point it has to be mentioned that both critical temperatures \( T_{C,Sk}^{DM} \) and \( T_{C,FM}^{DM} \) depend on the strength of the applied magnetic field, e.g. \( T_{C,FM}^{DM} = T_C \) if \( B = 0 \).

The magnetic field dependence of the critical temperatures and therefore the phase diagram is shown in figure 3(b): the transition from the Skyrmion phase to the ferromagnetic phase is marked by the black line and the black dots and the transition from the ferromagnetic, Skyrmion and spin-spiral phase to the paramagnetic phase is indicated by the red line and squares. In addition, there is a further transition from the spin-spiral phase to the Skyrmion phase with increasing external field marked by the green line and diamonds.

The phase diagram is similar to phase diagrams calculated with classical Monte Carlo calculations in [7, 19]. However, there is one significant difference. In [7, 19] the Skyrmion phase is divided into a Skyrmion lattice (SKX) and a Skyrmion gas phase marked as SKX + FM. To see the transition between the Skyrmion lattice and Skyrmion gas phase thermal fluctuations are necessary. Without thermal fluctuations all magnetic Skyrmions behave identical when changing temperature or the external field. This means the used mean field method does not allow a transition between the Skyrmion lattice and a Skyrmion gas phase. Thermal
fluctuations are needed to allow that locally Skyrmions disappear or get created at different times. In the case of the used quantum mechanical self-consistent mean field theory a Skyrmion lattice will disappear only when changing to one of the other phases: Spin–Spiral, Ferromagnet or Paramagnet. This is also true for a single magnetic Skyrmion as shown in figure 1 or a set of separated magnetic Skyrmion (Skyrmion gas). In other words both Skyrmion phases: Skyrmion lattice and Skyrmion gas phase are coexisting in the whole region marked as Skyrmion phase in the phase diagram (figure 3(b)). Furthermore, it can be assumed that the missing thermal fluctuations in the used self-consistent mean field theory description lead to increased critical temperatures / magnetic field values in comparison to e.g. Monte Carlo or Langevin spin dynamics simulations where thermal fluctuations are taken into account [42, 44, 45]. On the other hand the advantage of the self-consistent mean field theory lays in the fact that the resulting Skyrmion configuration is without overlaying noise and therefore a time average as in the cases of Monte Carlo or Langevin spin dynamics simulations is not needed which reduces the simulation time.

4. Eigenfunctions of $\hat{H}$

Due to the fact that $\hat{H}$ (equations (1)–(4)) is a quantum mechanical operator respectively, in the sense of mathematics, a matrix it is possible to calculate the corresponding eigenvalues and eigenvectors. In section 2 it has been shown that the Hamiltonian $\hat{H}$ can be written as sum of the local Hamilton operators $\hat{h}_{ni}$. Therefore, the problem reduces to calculate the eigenvalues $E_n$ and eigenvectors $\phi_n$ of $\hat{h}_n$:

$$\hat{h}_n \phi_n = E_n \phi_n.$$  \hfill (8)

Finally, the eigenvalues and eigenfunctions (eigenvectors) of $\hat{H}$ are the product states of $\phi_n$ respectively the sum over all $E_n$.

Mathematically, equation (8) is a matrix equation with Hamilton operator $\hat{h}_n$:

$$\hat{h}_n = \begin{pmatrix} -B_n^0 & \frac{-B_n^0 + iB_n^y}{\sqrt{2}} & 0 \\ \frac{-B_n^0 - iB_n^y}{\sqrt{2}} & 0 & \frac{-B_n^0 + iB_n^y}{\sqrt{2}} \\ 0 & \frac{-B_n^0 - iB_n^y}{\sqrt{2}} & B_n^x \end{pmatrix}$$ \hfill (9)

and eigenvectors:

$$\phi_n = \begin{pmatrix} \phi_{n1} \\ \phi_{n0} \\ \phi_{n1} \end{pmatrix}$$ \hfill (10)

Using a standard diagonalization method the eigenenergies $E_n$ of $\hat{h}_n$ can be easily calculated. The results are:

$$E_n^\pm = \pm B_n^{\text{eff}},$$ \hfill (11)

$$E_n^0 = 0.$$ \hfill (12)

Here, the ground state energy is $E_n^0 = -B_n^{\text{eff}}$, where

$$B_n^{\text{eff}} = \sqrt{(B_n^0)^2 + (B_n^y)^2 + (B_n^z)^2},$$ \hfill (13)

are the effective fields which reduce the simulation time. Figures 4(b)–(f) provide detailed pictures zoomed into the area of the Skyrmion showing the real part of $\phi_n^-$ (figure 4(b)), the real respectively imaginary part of $\phi_n^0$ [figure 4(c) respectively (d)], and the real and imaginary part of $\phi_n^+$ (figures 4(e) and (f)). Not shown in figure 4 is the imaginary part of $\phi_n^+$ which has been set equal to zero during the calculation.

5. Quantum spin dynamics

So far, the Hamilton operator $\hat{H}$ has been used to describe the thermodynamics of the magnetic Skyrmion. However, the Hamilton operator $\hat{H}$ can also be used to describe the spin dynamics of the magnetic Skyrmion where the underlying equation of motion is the time dependent Schrödinger equation with an additional damping term [46]:

$$i\hbar(1 - \lambda^2) \frac{d}{dt} |\Psi\rangle = \hat{H}|\Psi\rangle - i\lambda(\hat{H} - (\hat{H}^\dagger)|\Psi\rangle.$$ \hfill (15)

Within this differential equation $\lambda$ is a constant describing the strength of the energy dissipation ($\lambda \geq 0$), furthermore, $\langle \hat{H} \rangle = \langle \Psi | \hat{H} |\Psi\rangle$, with $\hat{H}$ given by equation (4).

As said before, due to the fact that the Hamilton operator $\hat{H}$ can be written as sum of the Hamilton operators $\hat{h}_n$ the wave function $|\Psi\rangle$ is a product state (Hartree ansatz) of the local wave functions $|\psi_n\rangle$:

$$|\Psi\rangle = \bigotimes_{n=1}^{N} |\psi_n\rangle.$$ \hfill (16)

Therefore, we can expect a spin dynamics which is similar to the dynamics provided by a description using classical spins [23, 25, 47] caused by omitting of the entanglement as result of the product state and the mean field Hamilton operator $\hat{H}$. Then, due to equations (4) and (16) the time dependent
The Schrödinger equation (15) can be written as a set of coupled differential equations:

\[ \text{i}\hbar(1 - \lambda^2) \frac{d}{dt} |\psi_n\rangle = \hat{h}_0 |\psi_n\rangle - \text{i}\lambda(\hat{h}_\sigma - \langle \hat{h}_\sigma \rangle)(|\psi_n\rangle), \]

where \( \langle \hat{h}_\sigma \rangle = \langle \psi_n | \hat{h}_\sigma | \psi_n \rangle \). The wave functions \(|\psi_n\rangle\) itself can be constructed with aid of the Zeeman basis [48] with basis vectors \(|j\rangle \in \{\uparrow, \downarrow\}\):

\[ |\psi_n\rangle = \sum_j a_n |j\rangle. \]

In case the system is in the ground state the coefficients \(a_n\) are equal to \(\phi^{-n}\) and the wave functions \(|\psi_n\rangle\) are equal to the eigenvectors \(\phi_n\) given in section 4.

In general, the interest in the wave functions \(|\psi_n\rangle\) is restricted apart from the fact that the wave functions can provide additional information about the quantum system and therefore shouldn’t be ignored. Important and also necessary for the dynamics are the spin expectation values:

\[ \langle \hat{S}_n \rangle = \langle \psi | \hat{S}_n | \psi \rangle = |\psi_n | \hat{S}_n | \psi_n \rangle. \]

In the previous publications [46, 47] it has been shown that without entanglement the dynamics of the spin expectation values are well described by the following differential equation:

\[ (1 - \lambda^2) \frac{d}{dt} \langle \hat{S}_n \rangle = \gamma \langle \hat{S}_n \rangle \times \text{B}_n^{\text{eff}} - \gamma \lambda \langle \hat{S}_n \rangle \times (\langle \hat{S}_n \rangle \times \text{B}_n^{\text{eff}}), \]

where \( \gamma = g\mu_B / \hbar \) is the gyromagnetic ratio. In the case of the quantum mechanical self-consistent mean field theory the product state equation (16) lead to the absence of entanglement which justifies the use of this differential equation to describe the spin dynamics.

The important point here is that due to the absence of entanglement the absolute values \(|\phi_n|\) are fixed and don’t change, i.e. during the dynamics the spin expectation values \(\langle \hat{S}_n \rangle\) only change their orientations. This is the same for the dynamics of classical spins \(\text{S}_n\) described by the Landau–Lifshitz–Gilbert (LLG) equation. Indeed, equation (20) is similar to the LLG equation which means that we can expect a similar dynamics as for classical spin systems [23, 25, 49, 50].

**Figure 4.** Eigenfunction of the ground state of a magnetic Skyrmion with \(S = 1\).
The only difference is the reversed sense of rotation \( \gamma \rightarrow -\gamma \) of the precessional term [first term on the right hand side of equation (20)].

To prove the correctness of the quantum mechanical self-consistent mean field theory and to show the equivalence between equations (17) and (20) the annihilation process forced by an electric field has been simulated. Recently, Hsu et al [51] have demonstrated that it is possible to use a local electric field generated by a scanning tunneling microscope (STM) to create or annihilate magnetic Skyrmions. The theoretical explanation for this phenomenon is the tuning of the Dzyaloshinsky–Moriya interaction caused by the electric field:

\[
\mathbf{D}_{nm} = \mathbf{D}_{nm}^0 + \omega_{mn} (\mathbf{E} \times \mathbf{r}_{nm}).
\]  

(21)

Within this formula \( \mathbf{D}_{nm} \) is the vector of the Dzyaloshinsky–Moriya interaction after modification due to the electric field \( \mathbf{E} \). The original Dzyaloshinsky–Moriya vector is \( \mathbf{D}_{nm}^0 \) while \( \mathbf{r}_{nm} \) is the vector pointing from lattice site \( m \) to lattice site \( n \). The prefactor \( \omega_{mn} \) describes the strength of the modification due to the electric field. During the experiment by Hsu et al modification of the Dzyaloshinsky–Moriya vectors is local and only appears underneath the STM tip. The electric field vector \( \mathbf{E} \) is perpendicular to the film plane and therefore to the in-plane vectors \( \mathbf{r}_{nm} \) and \( \mathbf{D}_{nm}^0 \), i.e. \( \mathbf{E} \perp \mathbf{r}_{nm} \) respectively \( \mathbf{E} \perp \mathbf{D}_{nm}^0 \). Depending on the orientation and strength of \( \mathbf{E} \) the Dzyaloshinsky–Moriya interaction increases or gets reduced. An electric field pointing away from the tip toward the film plane decreases the Dzyaloshinsky–Moriya interaction and therefore the magnetic Skyrmion gets annihilated. The opposite orientation leads to increase of Dzyaloshinsky–Moriya interaction. For the simulations a constant modification \( \omega_{mn} = \text{const.} \) within a radius of 20 lattice sites has been assumed. Inside this circle the Dzyaloshinsky–Moriya interaction has been set zero, i.e. \( \mathbf{D}_{nm} = 0 \), while outside the circle the strength of the Dzyaloshinsky–Moriya interaction has not been modified. This modification simulates in a simplified way the influence of the electric field provided by the scanning tunneling microscope tip. The center of the circle is the position of the STM tip which causes the modification.

Figure 5. (a)–(c) Profiles of the magnetic Skyrmion calculated with the aid of the time dependent Schrödinger equation (17). (d)–(f) Trajectories of three spins S1–S3, marked as dots within the Skyrmion profiles, during the annihilation process forced by an electric field. The curves are calculated by solving the time dependent Schrödinger equation (17) (qm) as well as the semi-classical equation (20) (scl). The dynamics is divided into three phases (i): shrinking, (ii): collapse, and (iii): shock wave.
of the Dzyaloshinsky–Moriya interaction. The STM tip and therefore the circle has been positioned in such a way that the magnetic Skyrmion is inside. This leads due to $D_0 = 0$ (ferromagnetic ground state) to the annihilation of the magnetic Skyrmion. The exact position of the tip is 0.5 lattice constants in both directions $x$ and $y$ away from the center of the magnetic Skyrmion. The reason for the small misalignment is to break the symmetry of the central spin which otherwise has no distinguished spin torque during the annihilation process. In the real experiment by Hsu et al the symmetry is broken either by thermal fluctuations, by misalignment of the STM tip or due to an asymmetry of the electric field due to a non-symmetric tip.

The results of the performed simulations are shown in figures 5–8. Figure 5 provides the trajectories of the three spins. In detail, figure 5(a) provides the profile (cut through the middle of the Skyrmion) corresponding to the $x$-component, figure 5(b) the $y$-component, and figure 5(c) the $z$-component of the spin expectation value $\langle S_n^z \rangle$. The colored dots correspond to the three spins mentioned before. The trajectories in figures 5(d)–(f) are calculated by two independent methods: 1. solving the time dependent Schrödinger equation (17) and 2. solving the semi-classical differential equation (20). The trajectories calculated by solving the time dependent Schrödinger have the same colors as the dots in figures 5(a)–(c): the black dots in figures 5(a)–(c) correspond to the black trajectories in figures 5(d)–(f), the red dots to the red trajectories and the green dots to the green trajectories. To highlight the trajectories of the semi-classical differential equation (20) these curves have been plotted with different colors. Now, the remarkable fact is that the trajectories of both methods show a perfect agreement.

![Figure 6](image6.png)

**Figure 6.** Skyrmion profiles during the electric field forced annihilation process: (a) phase (i): shrinking, (b) phase (ii): collapse, and (c) phase (iii): shock wave.

![Figure 7](image7.png)

**Figure 7.** In-plane components of the magnetic Skyrmion during the annihilation process. The small arrows indicate the in-plane direction of the magnetization.

![Figure 8](image8.png)

**Figure 8.** Real parts of the coefficients $a_{n0}$ and $a_{n1}$ of the wave functions $|\psi_n\rangle$ during the electric field forced Skyrmion annihilation. (a) $\text{Re}(a_{n0})$ at $t = 10$ ps, (b) $\text{Re}(a_{n1})$ at $t = 50$ ps.
mention once again that this agreement is a consequence of the absent entanglement.

The question which arrives at this point is what are the advantages and disadvantages of using the semi-classical differential equation (20) instead of solving the time dependent Schrödinger equation? The advantage of the semi-classical differential equation is the fact that we have to calculate only three (one for \( \langle S_n^x \rangle \), \( \langle S_n^y \rangle \), and \( \langle S_n^z \rangle \)) instead of six (real and imaginary part of \( a_{x\eta}, a_{y\eta}, a_{z\eta} \)) differential equations per lattice site. Furthermore, the spin expectation values \( \langle S_n^\eta \rangle \) are directly given, while for the time dependent Schrödinger equation first the wave functions \( \psi_n^\eta \) have to be calculated and in a second step the expectation values \( \langle S_n^\eta \rangle \), \( \eta \in \{x, y, z\} \).

Therefore, it can be said that the effort and therefore the possibility and strength of numerical errors are reduced by using the semi-classical differential equation (20) instead of the time dependent Schrödinger equation (17). On the other hand equation (20) does not provide informations coming from the wave functions \( \psi_n^\eta \). In general changes to other descriptions, in this case from the (semi-)classical to the quantum mechanical spin dynamics, lead to an alternated view which can lead to new perceptions. Additionally, in the case of entanglement it is necessary to solve the time dependent Schrödinger equation, which when using the self-consistent mean field theory lead to identical results as for the semi-classical description using equation (20), however paid with a higher numerical costs.

So far we have got a rough idea about the annihilation process provided by figure 5. The process itself can be divided into three phases marked by the roman numbers: the first phase (phase i) is characterized by the shrinking of the Skyrmion. During the second phase (phase ii) the Skyrmion collapses. And the third phase (phase iii) is a shock wave running trough the system. Corresponding to this dynamics figure 6 shows the profile of the Skyrmion during these three phases: figure 6(a) corresponds to phase (i), figure 6(b) to phase (ii) and figure 6(c) to phase (iii). Figure 7 shows the in-plane components of the magnetization. Clearly visible the twist of the Skyrmion during the annihilation process. This twist can be also seen in the wave functions \( |\psi_n^\eta\rangle \). Figure 8 shows the real parts of \( a_{x\eta} \) and \( a_{z\eta} \) during the first (i) and third (iii) phase. There, the twist is clearly visible. For comparison figures 4(c) and (d) show the not twisted initial configurations.

6. Summary

The paper is divided in three parts where a quantum mechanical self-consistent mean field theory has been used to describe the thermodynamics, the ground state wave function and spin dynamics of a magnetic Skyrmion. The first part describes the thermodynamics. The main results of this part are the temperature dependent profile of the Skyrmion and the phase diagram. The later is a result of the analysis of the transitions between the different phases which can be found by changing the temperature respectively external magnetic field. The second part of the paper provides the eigenvalues and eigenvectors of the local Hamilton operators \( \hat{H}_n \) which can be used as the starting point for the spin dynamics of the magnetic Skyrmion which is described in the third part of the paper. It is shown that the trajectories of the spin expectation values \( \langle \hat{S}_n^\eta \rangle \) can be described either quantum mechanically by solving the time dependent Schrödinger equation (15) or semi-classically by dealing with the semi-classical differential equation (20). The description using the time-dependent Schrödinger equation is similar to the one of the time-dependent Hartree method [52]. This method provides the full information about the spin system via the wave functions. The disadvantage of this method is the numerical effort which becomes drastically reduced when using the semi-classical differential equation (20) instead of the time-dependent Schrödinger equation (15). Concerning the physics: the investigated scenario to prove the used methods is the annihilation process of the Skyrmion using an external electric field. The process of annihilation itself is caused by the local reduction respectively annihilation of the Dzyaloshinsky–Moriya interaction and can be divided into three phases: size reduction of the magnetic Skyrmion, collapse and resulting shock wave due to an energy win during the collapse.

References

[1] Zhang X, Zhao G P, Fangohr H, Liu J P, Xia W X, Xia J and Morvan F J 2015 Sci. Rep. 5 7643
[2] Zhou Y and Ezawa M 2014 Nat. Commun. 5 4652
[3] Fert A, Crox V and Sampaio J 2013 Nat. Nanotechnol. 8 152
[4] Zhang X, Ezawa M and Zhou Y 2015 Sci. Rep. 5 9400
[5] Zhang X, Zhou Y, Ezawa M, Zhao G P and Zhao W 2015 Sci. Rep. 5 11369
[6] Heinze S, von Bergmann K, Menzel M, Brede J, Kubetzka A, Wiesendanger R, Bihlmayer G and Blügel S 2011 Nat. Phys. 7 713
[7] Yu X Z, Onose Y, Kanazawa N, Park J H, Han J H, Matsu i Y, Nagao sa N and Tokura Y 2010 Nature 465 901
[8] Mühlbauer S, Binz B, Jonietz F, Pfleiderer C, Rosch A, Neubauer A, Georgii R and Böni P 2009 Science 323 915
[9] Yu X. Z, Kanazawa N, Onose Y, Kimoto K, Zhang W. Z, Ishiwata S, Matsui Y and Tokura Y 2011 Nat. Mater. 10 106
[10] Münzner W et al 2010 Phys. Rev. B 81 041203
[11] Jiang W et al 2015 Science 349 283
[12] Hagemeister J, Iaia D, Vedmedenko E Y, von Bergmann K, Kubetzka A and Wiesendanger R 2016 Phys. Rev. Lett. 117 207202
[13] Romming N, Hanneken C, Menzel M, Bickel J E, Wolter B, Bergmann K V, Kubetzka A and Wiesendanger R 2013 Science 341 636
[14] Rózsa L, Deak A, Simon E, Yanes R, Udvardi L, Szunyogh L and Nowak U 2016 Phys. Rev. Lett. 117 157205
[15] Woo S et al 2016 Nat. Mater. 15 501
[16] Leonov A O, Monchesky T L, Romming N, Kubetzka A, Bogdanov A N and Wiesendanger R 2016 New J. Phys. 18 065003
[17] Bogdanov A N and Rößler U K 2001 Phys. Rev. Lett. 87 0372031
[18] Hagemeister J, Romming N, von Bergmann K, Vedmedenko E Y and Wiesendanger R 2015 Nat. Comm. 6 9455
[19] Li Y-Q, Liu Y-H and Zhou Y 2011 Phys. Rev. B 84 205123
