

Quantum computing of magnetic-skyrmion-like patterns in Heisenberg ferromagnets

Matej Komelj^{1,2,*}, Vinko Sršan^{1,3}, Kristina Žužek^{1,3} and Sašo Šturm^{1,3}

¹*Jožef Stefan Institute, Jamova cesta 39, SI-1000 Ljubljana, Slovenia*

²*Faculty of Mathematics and Physics, University of Ljubljana, 1000 Ljubljana, Slovenia*

³*International Postgraduate School Jožef Stefan, Jamova cesta 39, SI-1000 Ljubljana, Slovenia*



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We diagonalize the quantum two-dimensional spin-1/2 Heisenberg model with Dzyaloshinsky-Moriya interaction (DMI) by applying the variational quantum eigensolver, running on a quantum-computer simulator, which turns out to be a more efficient approach than a classical direct diagonalization for systems with more than 17 sites. The calculated external-magnetic-field dependence of the total energy, of the magnetization, and of the topological charge exhibits a distinctive discontinuity which hints at the existence of zero-temperature magnetic-skyrmion-like structures at the quantum level, controlled by the combination of the exchange-coupling and the DMI parameters. The potentially measurable jump in the magnetization upon changing the field indicates the investigated objects are stable enough for eventual applications in spintronics or even as information carriers.

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The exciting field of quantum computing is interesting from the point of view of developing the required hardware and software, as well as by means of applying the respective algorithms for certain tasks, where they might at least outperform classical approaches or even make unsolved problems solvable [1]. Although the number of commercially available platforms for quantum computations constantly grows, the implementation of the basic components, for example, of the information carriers in terms of qubits and of the respective logical gates is not yet standardized [2]. Any attempts at simplifying the existing setups, particularly by avoiding the necessity for operating at extremely low temperatures, are highly desired. In this manner, magnetic skyrmions might represent a considerable alternative worth exploring [3,4].

Vortex-like magnetization $\vec{m}(x, y)$ patterns, here confined to the x - y plane, are characterized by the topological charge Q (sometimes referred as the topological number or index) [5]:

$$Q = \frac{1}{4\pi} \int \vec{m}(x, y) \cdot \left(\frac{\partial \vec{m}(x, y)}{\partial x} \times \frac{\partial \vec{m}(x, y)}{\partial y} \right) dx dy. \quad (1)$$

Strictly speaking, a proper skyrmion is distinguished by an integer $|Q| \geq 1$ and its stability arises from a topological protection. However, according to a less rigid definition, it is an energy barrier which stabilizes the corresponding magnetization textures, the creation and annihilation of which are triggered by external parameters, such as surrounding magnetic fields [6]. The stability, induced by either a topological protection or an energy barrier, and the ability to switch them

on and off give skyrmions the potential to be applied in future memory devices.

Whereas macroscopic skyrmions exist at certain finite-temperature ranges, a theory predicts them at quantum level for $T = 0$ [7,8]. However, even in that case, a direct diagonalization of lattice quantum models with magnetic interactions is demanding since the set of possible states grows exponentially with the number of sites, representing single magnetic moments [9]. The basic Hamiltonian, the solutions of which might include a skyrmionic phase in dependence of the parameters, is associated with the two-dimensional 1/2-spin anisotropic Heisenberg (XXZ) model in a perpendicular external magnetic field, B_z :

$$H = J_{\parallel} \sum_{\langle i, j \rangle} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) + J_{\perp} \sum_{\langle i, j \rangle} \sigma_i^z \sigma_j^z + \sum_{\langle i, j \rangle} \vec{D}_{ij} \cdot (\vec{\sigma}_i \times \vec{\sigma}_j) + B_z \sum_i \sigma_i^z, \quad (2)$$

where $\vec{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$ are Pauli matrices and $\langle i, j \rangle$ denotes a sum over the nearest neighbors. The exchange coupling constants $J_{\parallel} < 0$ and $J_{\perp} > 0$ imply a ferromagnetic ordering with the x - y easy-plane anisotropy. Note, the results and conclusions presented below are qualitatively the same if an isotropic exchange $J_{\parallel} = J_{\perp}$ is considered, but in that case the z contribution to the magnetization is the dominant contribution; hence, the in-plane vortex patterns are less pronounced. The third term, describing the antisymmetric exchange in the form of the Dzyaloshinsky-Moriya interaction (DMI) [10,11], is the key for the formation of skyrmion-like patterns. It favors neighboring magnetic moments at the sites where i and j are perpendicular to each other, either parallel or antiparallel to the coupling vector $\vec{D}_{ij}$. However, the presence of the DMI is not the only way to stabilize skyrmion-like structures on the quantum level. For example, frustrations in a Heisenberg model with the next-nearest-neighbor exchange interactions exhibit similar solutions [12] but these are not the subject of

*Contact author: matej.komelj@ijs.si

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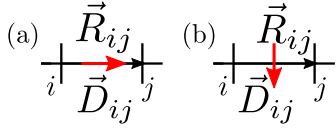


FIG. 1. The DMI vector $\vec{D}_{ij}$ pointing parallel (a) or perpendicular (b) to the vector $\vec{R}_{ij}$ between the i th and j th site yielding Bloch- or Néel-type skyrmion-like structures, respectively.

the present paper. An application of a Hamiltonian like Eq. (2) on a multiple-qubit state is straight forward since it is formulated by Pauli matrices, which are among the basic logical gates in quantum computing. Therefore, it makes sense to explore its properties by diagonalizing it using the variational quantum eigensolver (VQE) [13], which is a common tool for finding the ground state of a physical system in quantum chemistry and quantum magnetism [14]. A migration to an appropriate hardware should be feasible.

For the sake of simplicity we fix $|J_{\parallel}| = |\vec{D}_{ij}|$ as the unit and impose a ferromagnetic in-plane ordering by setting $J_{\parallel} < 0$. The DMI vectors $\vec{D}_{ij}$ with two different directions are considered: either parallel or perpendicular to the vector $\vec{R}_{ij}$, pointing from site i to site j , as sketched in Fig. 1. The magnitude $|\vec{D}_{ij}|$ is rather high for macroscopic systems containing skyrmions with diameters up to ~ 100 nm, but is in agreement with the choice from Ref. [8] for skyrmions on the quantum level. The evolution of the magnetization pattern is controlled by the out-of-plane component B_z of the external magnetic field expressed in units of $\mu_B |J_{\parallel}|$, where μ_B is the Bohr magneton. Open boundary conditions are taken into account.

Special consideration is given to the calculation of the topological charge Q defined by Eq. (1). The diagonalization of the Hamiltonian (2) yields the magnetization $\vec{m}(x_i, y_i)$ at the mesh nodes with the coordinates (x_i, y_i) , obtained as the Pauli matrices' expectation values $\vec{m}(x_i, y_i) \equiv (\langle \sigma_i^x \rangle, \langle \sigma_i^y \rangle, \langle \sigma_i^z \rangle)$. In order to calculate the partial derivatives and the surface integral in Eq. (2), the field $\vec{m}(x, y)$ needs to be interpolated between the mesh points. The easiest way is to divide the mesh into triangles t , defined by three neighboring nodes $t \equiv (i, j, k)$. In linear approximation the magnetization is a sum over all triangles, $\vec{m}(x, y) \approx \sum_t \vec{m}_t(x, y)$, where inside the triangle t , $\vec{m}_t(x, y) = \vec{a}_t x + \vec{b}_t y + \vec{c}_t$, and outside the triangle t , $\vec{m}_t(x, y) = 0$. The vectors $\vec{a}_t$, $\vec{b}_t$, and $\vec{c}_t$ are determined from the magnetization values at the i , j , and k nodes, obtained as the expectation values of the corresponding Pauli matrices for the associated qubits. It is easy to see that the topological charge (1) in this approximation is a sum over all triangles with the areas S_t : $q \approx (1/4\pi) \sum_t S_t (\vec{a}_t \times \vec{b}_t) \cdot \vec{c}_t$. This approach of applying the concept of the topological charge on discrete systems can be regarded as a simplified version of a more sophisticated winding number [12,15,16].

The diagonalization of the Hamiltonian (2) is performed by applying the VQE method, implemented in the open-source PYTHON package TANGELO [17]. We emulate the N -qubit quantum circuit on the noiseless simulator backend, which is incorporated in the package. The eigenstate $|\Phi\rangle$ is expressed by the hardware-efficient ansatz [18], composed of the entangler U_{ENT} , inserted between two sets $i = 1$ and 2 of the Euler rotations: $|\Phi\rangle = \prod_{q=1}^N [U(\vec{\theta}^{q,1})] \times U_{\text{ENT}} \times$

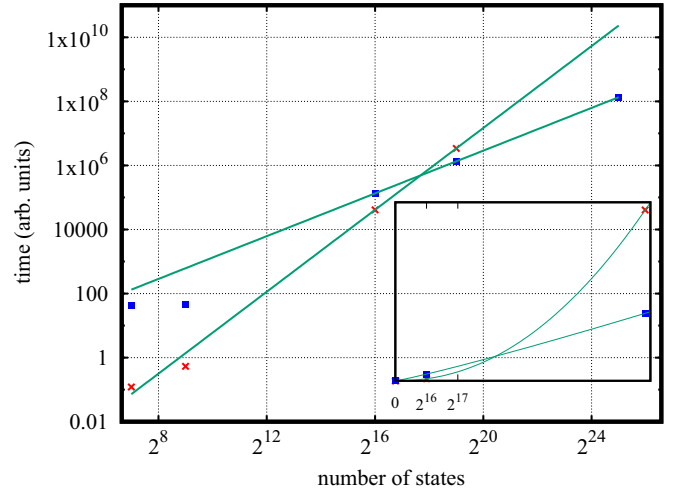


FIG. 2. A comparison between the performance of the VQE (■) and the Lanczos (×) algorithms using a logarithmic scale. The scalabilities are $\mathcal{O}(n^{1.1})$ and $\mathcal{O}(n^{2.1})$, with n being the number of sites. The linear-scale inset indicates the VQE is more efficient for $N > 17$.

$\prod_{q=1}^N [U(\vec{\theta}^{q,2})] |00 \dots 0\rangle$, where $U(\vec{\theta}^{q,i})$ is expressed by the $R_x(\theta)$ and $R_z(\theta)$ gates as $U(\vec{\theta}^{q,i}) = R_z(\theta_1^{q,i}) R_x(\theta_2^{q,i}) R_z(\theta_3^{q,i})$. The angles $\vec{\theta}^{q,i} = (\theta_1^{q,i}, \theta_2^{q,i}, \theta_3^{q,i})$ represent $6 \times N$ variational parameters that need to be optimized in order to find the N -qubit ground state associated with the energy E .

The power of the VQE algorithm is demonstrated by means of a comparison with the performance of the implicitly restarted Lanczos method [19,20] run serially on the same platform (Fig. 2). The tests are carried out on square lattices with $N = 9, 16$, and 25 (only the VQE) sites, as well as, for a better statistics, on triangular lattices with $N = 7$ and 19. The corresponding fits reveal that the VQE scales nearly linearly $\mathcal{O}(N^{1.1})$ and the Lanczos algorithm scales slightly worse than quadratically $\mathcal{O}(N^{2.1})$ for finding the ground state of the Hamiltonian (2). This comparison clearly indicates the VQE is faster for $N > 17$, which makes solving the problem with the classical algorithm considerably more time-consuming already for a 5×5 square lattice characterized by 2^{25} states. Furthermore, a symmetry breaking is known to slow the VQE convergence, which can be improved by applying a specially prepared ansatz [21,22]. This issue is not considered in the present work, where the only criterion is an agreement with the Lanczos-method results within the numerical accuracy. Hence, a further optimization might result in an even better VQE performance.

The subsequent calculations are performed by applying the VQE algorithm on a square lattice with $N = 16$. We stick to the lattice size at which the classical approach is still slightly faster, because collecting all the data points, presented in Figs. 3 and 5 for $N > 17$ would be time-consuming by means of quantum computing too, but not necessary for a proof of concept. However, in the following we justify that it is completely achievable. The results for $\vec{D}_{ij} \parallel \vec{R}_{ij}$ and $J_{\perp} = 0.5|J_{\parallel}|$ are presented in Fig. 3. The energy E linearly drops with the field B_z as expected from the Zeeman interaction, described by the third term in Eq. (2), except for a transparent jump at $B_z = 1.884$, which clearly hints at a transition in magnetic ordering.

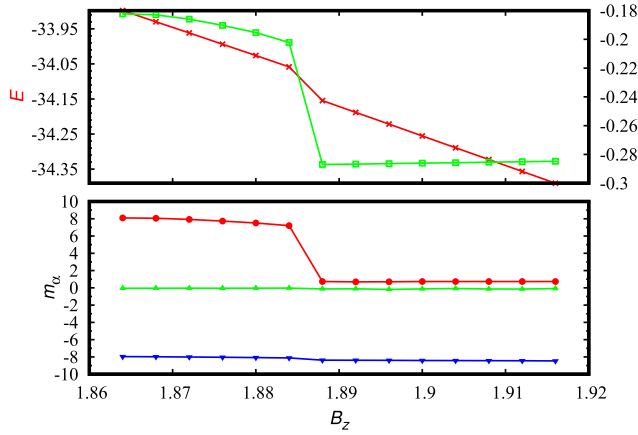


FIG. 3. The external field B_z dependence of the energy E ($\times$), the topological charge Q ($\square$), and the magnetization components m_α with $\alpha = x$ ($\bullet$), y ($\blacktriangle$), and z ($\blacktriangledown$) for $\vec{D}_{ij} \parallel \vec{R}_{ij}$. B_z and E are given in dimensionless units relative to $|J_\parallel|$.

This is confirmed by a change in the dependencies of the topological charge Q (1) and of the magnetization x component m_x from a finite value to a nearly zero value. The magnetization components m_α , $\alpha = x, y$, and z , are calculated as the sums of the expectation values of the corresponding Pauli matrices at particular mesh nodes as $m_\alpha = \sum_i \langle \sigma_i^\alpha \rangle$. There is apparently no transition of the m_y and m_z components, which remain nearly zero and finite, respectively. The assumption about the magnetization-pattern transition is further demonstrated in Fig. 4. Whereas there is a certain ordering at $B_z < 1.884$, reflected in a finite magnetization along the x axis (m_x in Fig. 3), a vortex-like spiral structure, resembling a Bloch-type skyrmion-like structure with helicity $\gamma = \pi/2$, is formed for $B_z > 1.884$, accompanied by a jump in $|Q|$ by more than 50% and a simultaneous drop in the m_x , creating a certain x - y -plane symmetry in the magnetization pattern.

The situation is very similar in the case of $\vec{D}_{ij} \perp \vec{R}_{ij}$ and $J_\perp = 0.25|J_\parallel|$ (Figs. 5 and 6). In this case, $J_\perp = 0.5|J_\parallel|$, used for $\vec{D}_{ij} \parallel \vec{R}_{ij}$, does not yield any transition to skyrmion-like ordering. The choice of the exchange and the DMI coupling parameters is quite arbitrary and it does not qualitatively influence the results. Contrary to the previous case, the topological charge Q is positive; hence, up to the transition point at $B_z = 1.222$, it parabolically increases, whereas the magnetization component m_x drops. In this case, a small transition is observable in the m_y and m_z components too.

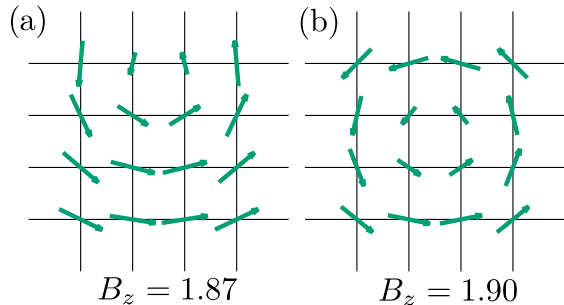


FIG. 4. The magnetization pattern for $\vec{D}_{ij} \parallel \vec{R}_{ij}$ and $J_\perp = 0.5|J_\parallel|$ at $B_z = 1.87$ (a) and $B_z = 1.90$ (b).

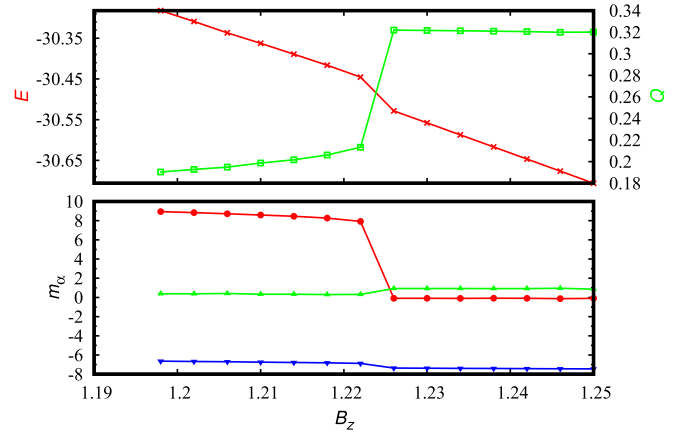


FIG. 5. The external field B_z dependence of the energy E ($\times$), the topological charge Q ($\square$), and the magnetization components m_α with $\alpha = x$ ($\bullet$), y ($\blacktriangle$), and z ($\blacktriangledown$) for $\vec{D}_{ij} \perp \vec{R}_{ij}$. B_z and E are given in dimensionless units relative to $|J_\parallel|$.

However, it is obvious that an in-plane-symmetric state, similar to a Néel-type skyrmion-like structure with helicity $\gamma = 0$, is transformed from an x -direction preferential ordering in Fig. 6(a).

Neither the pattern in Fig. 4(b) nor the pattern in Fig. 6(b) can be regarded as proper skyrmions since they are not characterized by integer topological charges. The reason is probably a restricted geometry due to a limited number of applied mesh nodes (qubits), which does not make the creation of a complete structure possible, although a VQE calculation on a 5×5 square lattice for $\vec{D}_{ij} \parallel \vec{R}_{ij}$ reveals the existence of a Bloch-type skyrmion-like pattern at $B_z = 1.5$ (Fig. 7).

Hence, it is very likely that the external-field B_z driven transitions, from partially disordered to magnetically ordered states, demonstrated in Figs. 3 and 5, clearly indicate a formation of new, skyrmion-like phases in agreement with the assumption about the existence of quantum skyrmions at $T = 0$ [8,23,24]. Although the energy difference of about $0.1|J_\parallel|$ between two phases at the transition point is of the same order of magnitude as, for example, the magnetocrystalline-anisotropy energy, preventing a demagnetization of a ferromagnet, it does not itself guarantee the stability of a skyrmion as an information carrier. Nevertheless, it has been argued that a similar energy landscape yielded sufficiently long lifetimes for stable single skyrmionic bits [25]. The present work demonstrates quantum computing by means

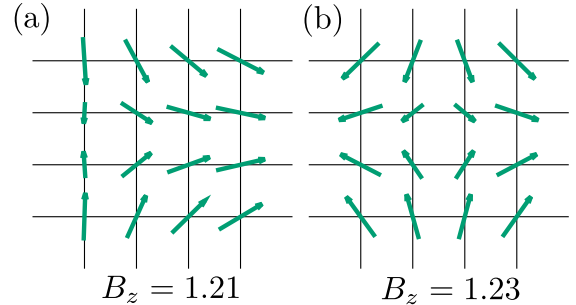


FIG. 6. The magnetization pattern for $\vec{D}_{ij} \perp \vec{R}_{ij}$ and $J_\perp = 0.25|J_\parallel|$ at $B_z = 1.21$ (a) and $B_z = 1.23$ (b).

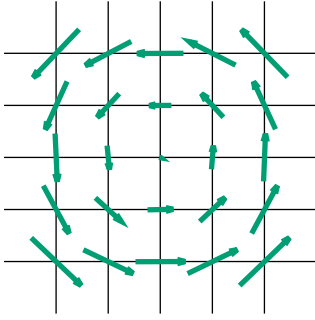


FIG. 7. The magnetization pattern for $\vec{D}_{ij} \parallel \vec{R}_{ij}$, $J_{\perp} = 0.5|J_{\parallel}|$, and $B_z = 1.5$ on a 5×5 square lattice.

of the VQE as a suitable and promising tool for investigations of quantum magnetism. The results predict the existence of magnetic skyrmion-like structures due to an antisymmetric DMI at the quantum level and call for eventual experiments on new materials in order to detect and characterize such objects, to apply them as potential carriers of information, and to implement the respective gates [26].

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The data that support the findings of this article are openly available [8].

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