Interaction of excitons with magnetic topological defects in 2D magnetic monolayers: localization and anomalous Hall effect

M Kazemi¹, V A Shahnazaryan²*⁴, Y V Zhumagulov²³, P F Bessarab¹²⁴* and I A Shelykh¹²

¹ Science Institute, University of Iceland, Dunhagi 3, IS-107 Reykjavik, Iceland
² ITMO University, School of Physics and Engineering, St. Petersburg 197101, Russia
³ University of Regensburg, Regensburg 93040, Germany
⁴ Department of Physics and Electrical Engineering, Linnaeus University, SE-39231 Kalmar, Sweden
* Author to whom any correspondence should be addressed.
E-mail: vshahnazaryan@gmail.com

Keywords: exciton, skyrmion, magnetic monolayer, CrI3 monolayer, asymmetric scattering, exciton localization, topological defect

Supplementary material for this article is available online

Abstract

Novel 2D material CrI3 reveals unique combination of 2D ferromagnetism and robust excitonic response. We demonstrate that the possibility of the formation of magnetic topological defects, such as Néel skyrmions, together with large excitonic Zeeman splitting, leads to giant scattering asymmetry, which is the necessary prerequisite for the excitonic anomalous Hall effect. In addition, the diamagnetic effect breaks the inversion symmetry, and in certain cases can result in exciton localization on the skyrmion. This enables the formation of magnetoexcitonic quantum dots with tunable parameters.

1. Introduction

Dimensionality has a dramatic impact on the physical properties of a system. Although we live in a three-dimensional (3D) world, the recent progress of technology allowed experimental realization of structures of lower dimensionality. In these systems the motion of a particle is restricted to one or two dimensions, which results in certain peculiarities of their physical behavior coming from dramatic enhancement of the role of quantum fluctuations.

Two-dimensional (2D) systems are of particular interest, as they lie between 3D systems where formation of Off Diagonal Long Range Order is possible at finite temperatures and 1D systems where fluctuations completely destroy long range order and lead to the exponential decay of quantum correlations in real space at any finite temperature. In 2D systems, the situation is more tricky: although long range correlations are destroyed, their decay at low temperature is much slower than in the 1D case. This is a characteristics of the Berezinskii–Kosterlitz–Thouless phase which is intimately connected with spontaneous creation of topological excitations. Their type depends on the nature of the system in question. In 2D magnets, they are skyrmions [1–3]. For 2D superfluid systems, characteristic for geometries with excitons [4–8] or exciton polaritons [9–11], such defects are vortex-antivortex pairs [12–15].

Systems where several order parameters interact via particle-like entities exhibit particularly interesting, hybrid behavior. In multiferroics, magnetic skyrmions induce nontrivial dielectric order, which enables a mechanism for an electric-field control of skyrmions [16]. In heterostructures combining chiral magnet and superconductor, co-existing magnetic skyrmions and superconducting vortices create a platform for nucleation and control of Majorana fermions, a prerequisite for topological quantum computing [17].

Recently, materials combining magnetic properties with robust excitonic response have been discovered [18]. These are 2D antiferromagnets MPS3 (M = Ni, Fe, Mn) [19–22], and ferromagnets CrX3 (X = I, Br) [23–26]. In seeming contradiction to the Mermin-Wagner theorem [27], the finite-temperature long-range magnetic order is enabled in these systems thanks to the magnetic anisotropy [28]. Even more intriguingly, application of electric field or stress breaks the structural inversion symmetry leading to the emergence of uncompensated anti-symmetric exchange between the magnetic atoms [29–31]—the Dzyaloshinskii–Moriya (DM) interaction—that favors noncollinear
alignment of magnetic moments. Interplay between magnetic anisotropy, Heisenberg exchange and DM interaction opens a possibility for complex magnetic order in 2D magnets, including the emergence of localized states with nontrivial topology such as skyrmions [32, 33].

The combination of huge optical oscillator strengths with giant Zeeman splitting in CrI₃ leads to various magneto-optical phenomena including giant Kerr response [23], giant magneto band-structure effect [34], magnetic circular dichroism [35], onset of 2D magnetoplasmons [36] and resonant inverse Faraday effect [37]. Moreover, potential emergence of magnetic skyrmions in 2D excitonic materials opens up new exciting physics and interesting applications.

Here, we demonstrate the effects of scattering and localization of excitons on magnetic skyrmions in 2D ferromagnets, as illustrated in figure 1(a). We focus on the CrI₃ monolayer system, but also study the effect of the parameter variation to demonstrate the relevance of our results to 2D ferromagnets with excitonic response in general. The scattering on a skyrmion is characterized by strong asymmetry, implying the possibility of anomalous Hall transport of excitons. The anomalous Hall effect of excitons is a subject of recent intense research. This includes the experimental demonstration of intrinsic anomalous Hall effect [38], and the theoretical studies of the side jump and skew scattering mechanisms [39, 40]. The exciton spin Hall effect was intensively studied in the context of strong light-matter coupling [41, 42]. Our proposal thus represents a novel mechanism for exciton anomalous Hall effect. Finally, the possibility to localize excitons leads to the formation of analogs of quantum dots with tunable properties, which can be used as polarization selective single photon emitters.

2. Results

2.1. Band structure and excitons

Figure 1 (b) shows the band structure of ferromagnetic CrI₃ monolayer calculated using the density functional theory (DFT) with bandgap correction by scissor operator (see section 4). The direct bandgap is \( E_g = 2.59 \text{ eV} \), in agreement with previous calculations [43, 44]. We found the transition energy of the brightest low-lying exciton is \( E_X = 1.65 \text{ eV} \), which is observed in the experimental differential reflection spectrum as the T2 state [35], as well as in theoretical studies [43–45]. The corresponding exciton state is formed near direct bandgap at the crystallographic point G by the electrons mainly located in the \( m_s = 5.09 m_0 \), and the holes in the upper valence band with effective mass \( m_v = -0.59 m_0 \), with \( m_0 \) being the free electron mass. The exciton has a clearly defined spin structure since it is completely localised in the upper valence band and the three lower conduction bands, which have strictly determined spin direction. The most straightforward possible estimation of exciton Zeeman splitting is the difference between the energies of the lower conduction band and the fourth conduction band, which correspond to different spin directions, plus the energy difference between the upper conduction band and the second upper conduction band at the crystallographic point G. The resulting value of the Zeeman splitting is equivalent to 0.37 eV.

2.2. Magnetic skyrmions

Magnetic structure of a CrI₃ monolayer can be described as a 2D honeycomb lattice of classical spins localized on Cr atoms. It is assumed that the system is subject to the external electric field breaking the structural inversion symmetry. As a result, in addition to the contributions due to the Heisenberg exchange, out-of-plane magnetic anisotropy and external magnetic field, the magnetic Hamiltonian of CrI₃ also includes the DM interaction energy [33]. Each contribution is characterized by an effective interaction parameter: \( J, K \), and \( D \) (see section 4 for the detailed description of the Hamiltonian). Magnitude of the interaction parameters is mostly taken from [33], but some variation of the parameter values is also considered.

Isolated skyrmion states are obtained via the energy minimization of the magnetic structure [46] starting from a rough initial guess for the skyrmion profile. Minimum-energy skyrmion state for \( J = 1.26 \text{ meV}, D = 0.59 \text{ meV}, K = 0.50 \text{ meV}, \) and zero magnetic field is shown in figure 2(a). How the skyrmion state changes with the DM interaction and external magnetic field is illustrated in figures 2(b) and (c), respectively. Continuous representation of the skyrmion profiles is obtained by fitting the following ansatz to the simulation data [47]:

\[
\Theta(\rho, c, w) = 2 \arctan \left( \frac{\cosh \left( \frac{\rho}{a} \right)}{\sinh \left( \frac{\rho}{a} \right)} \right),
\]

where \( \Theta(\rho, c, w) \) is the polar angle of the magnetization at the distance \( \rho \) from the skyrmion center and \( c, w \) are the fit parameters. The normal and the radial components of the unit magnetization vector \( \vec{M} \) are defined as:

\[
\vec{M}_z = \cos \Theta, \quad \vec{M}_\rho = \sin \Theta.
\]

The skyrmion profiles corresponding to figures 2(a)–(c) are shown in figure 2(d). The skyrmion size can be obtained from the profiles as a radius \( R \) of the \( \vec{M}_z = 0 \) contours. The radius of skyrmions in CrI₃ demonstrates monotonic decrease (increase) with \( B (D) \), see figure 3, which is consistent with the general theory of the skyrmion states [48, 49]. The non-coplanar magnetic texture of a skyrmion creates an electromagnetic field [50] leading to the asymmetrical scattering and localization of excitons, as explained in what follows.
Let us first consider the scattering of individual excitons on skyrmions. We consider the center-of-mass dynamics of spinor exciton interacting with the magnetization field due to the skyrmion state. The corresponding Schrödinger equation has the form

$$\left[ -\frac{\hbar^2}{2\mu_X} \nabla^2 + U \right] |\Psi\rangle = E_{\text{CM}} |\Psi\rangle,$$  \hspace{2cm} (3)

where $\mu_X$ is the exciton total mass, $\mathbb{I}_2$ is the $2 \times 2$ identity matrix, $U = \lambda \hat{\sigma}$, where $\lambda$ is the interaction energy, and $E_{\text{CM}}$ is the exciton center of mass energy. We restrict the treatment with the spin conserving exciton elastic scattering off the skyrmion. The general scattering of massive spinor particle on magnetic skyrmion is discussed in [51, 52]. In order to exclude the spin degree of freedom, we apply the adiabatic elimination approach [53], expanding the exciton state in the basis $|\Psi\rangle = |\psi_1\rangle |\chi_1\rangle + |\psi_2\rangle |\chi_2\rangle$. Here $\chi_{1,2}$ are the eigenstates of skyrmion potential $U$, corresponding to eigenvalues $\mu_{1,2} = \mp \lambda$. Assuming $\psi_2 = 0$, we project the Schrödinger equation to the state $|\chi_1\rangle$. It is of crucial importance, that in the effective spinless model, synthetic U(1) gauge field appears. It plays the role of an effective magnetic field and is responsible for giant asymmetry of the scattering. Physically, the presence of a skyrmion means, that the symmetry
of the system in z-direction is broken, i.e. the unity vectors \( \hat{e}_z \) and \(-\hat{e}_z \) are not equivalent. Therefore, if an exciton possesses a finite value of wave vector \( \vec{k} \), directions \([\vec{k} \times \hat{e}_z] \) and \([-\vec{k} \times \hat{e}_z]\), corresponding to the scattering to the right and to the left are not equivalent as well. Moreover, non-equivalence of these two directions can be understood if one considers a scattering of an exciton on a skyrmion in adiabatic approximation using the Berry phase argument. Indeed, consider the contribution of the trajectories with exciton making a round trip around the skyrmion in clockwise (scattering to the right) and anticlockwise (scattering to the left) directions. The spin of the exciton in this approximation follows the magnetization pattern of the skyrmion, and it can be seen from figure 1(a) that it will cover a non-zero solid angle, which means that a wavefunction of the exciton will acquire a geometric phase whose sign depends on the direction of the circumvention around the skyrmion. Therefore, the trajectories with round trips contribute differently to the total scattering amplitude for scattering angles \( \theta \) and \(-\theta \) due to the opposite signs of the phase in the interference terms.

The resulting equation reads (see the supplemental material (SM) for details):

\[
\left[ \frac{1}{2\mu_X}(\vec{p} - e\vec{A})^2 + W - \lambda \right] \psi_1 = E_{CM}\psi_1, \tag{4}
\]

where

\[
\vec{A} = -\frac{h}{e} \left[ 1 + \frac{\mathcal{L}_z}{2 \rho} \phi \right], \tag{5}
\]

\[
W = \frac{h^2}{8\mu_X} \left[ (\mathcal{L}_z \mathcal{L}_z' - \mathcal{L}_x \mathcal{L}_x')^2 + \mathcal{L}_x^2 / \rho^2 \right] \tag{6}
\]

are vector and scalar gauge potentials, respectively. Here \( e \) denotes the unit charge, \( \phi \) is the unit vector in the azimuthal direction, and the prime denotes the derivative with respect to \( \rho \). Interestingly, the gauge potentials do not depend on the interaction energy \( \lambda \). Consequently, the scattering cross-section in the adiabatic elimination approach is independent of \( \lambda \), as it only leads to rigid energy shift in equation (4).

The presence of the vector potential \( \vec{A} \) gives rise to an effective magnetic field \( \vec{B}_{\text{eff}} = \nabla \times \vec{A} \). Due to the symmetry of the vector potential, the magnetic field is normal to the plane and reads

\[
E_{\text{eff}} = \frac{A_{\phi}}{\rho} + \frac{\partial A_{\phi}}{\partial \rho}. \tag{7}
\]

The radial dependence of the vector potential is presented in figure 4(a). Notably, the maximal absolute value of the vector potential decreases versus the skyrmion size. Conversely, the maxima appears at larger distance from the skyrmion center. Outside the skyrmion region, the vector potential demonstrates a \( 1/\rho \) scaling. Figure 4(b) shows the emergent effective magnetic field due to skyrmion. The giant values of the field are explained by the rapid variation of vector potential at sub-nm scale, driven by the nature of the skyrmion magnetization texture. We mention that for a skyrmion having the size of \( \sim 16 \text{ nm} \) due to topological winding of the texture an effective magnetic field of \( B_{\text{eff}} \approx 13 \text{ T} \) was reported earlier [54].

The radial dependence of scalar potential is shown in figure 4(c), demonstrating a good localization within the skyrmion. Notably, it has a local minima at \( \rho = 0 \), which can lead to the formation of the excitonic quasibound states and scattering resonances. However, characteristic energies of these resonances correspond to the wave vectors of the excitons lying far outside the light cone, which can not be directly created optically, and are thus not analyzed in this work.

The differential cross-section can be expanded up to third order in skyrmion potential strength [55]:

\[
\omega(k, \vec{k}') \approx \omega^{(2)}(k, \vec{k}') + \omega^{(3)}(k, \vec{k}') + \omega^{(3)}(\vec{k}, \vec{k}'), \tag{8}
\]

where the lowest order term \( \omega^{(2)}(k, \vec{k}') \) is symmetric. The third order term contains an irrelevant
symmetric correction $\omega^{(3)}(\vec{k}, \vec{k}')$ and an asymmetric contribution $\omega^{(3)}_a(\vec{k}, \vec{k}')$ (see section 4). The cross-section of exciton scattering is presented in figure 5. The exciton wave vector has upper limit defined by optical excitation range $k_{\text{max}} = nE_x/(\hbar c)$. Here $n \approx 2$ is the refractive index of surrounding media [43], $c$ is the speed of light. Together with excitonic resonance $E_x = 1.65$ eV, this yields $k_{\text{max}} \approx 16.5 \mu m^{-1}$, and the exciton total mass is $\mu_X = m_e + |m_h| \approx 5.6m_e$. Figure 5(a) illustrates the scattering amplitude versus the scattering angle for several values of the wave vector. At the $\theta \to 0$ limit the scattering cross-section diverges as $\omega^{(2)}(\theta \to 0) \sim 4/(k^2\theta^2)$ due to the $A \sim 1/r$ tale of the vector potential, similar to the scattering off the Coulomb potential [56]. Therefore, the region of divergence depends weakly on the skyrmion and exciton parameters. The universal shape of the scattering cross-section at small angles could be modified only if the skyrmion radius $R \sim 1/k$, which corresponds to the $\mu m$ scale. This is in contrast to rather small skyrmions in the CrI$_3$ system, see figure 2.

For the characterization of scattering asymmetry we introduce the asymmetry degree

$$\gamma = \frac{|\omega(k, \theta) - \omega(k, -\theta)|}{\omega(k, \theta) + \omega(k, -\theta)}. \quad (9)$$

This quantity is illustrated in figure 5(b). One clearly sees that scattering is highly asymmetric ($\gamma$ can reach values of 0.5), and the asymmetry rate has a moderate dependence on scattering wave vector. At $\theta = 0$ we get $\gamma = 0$, as expected from the symmetry considerations. On the other hand, the scattering asymmetry increases as scattering trajectories with closed loops around the skyrmion become more prominent in the region where the total cross-section starts growing. As a result, the asymmetry peaks at intermediate angles, and the position of the peak varies slowly with the exciton wave vector (see figure 5(b)).

The presence of asymmetric scattering results in the anomalous Hall effect for excitons, which is characterized by the Hall angle defined as the ratio between transverse and longitudinal currents. Assuming the initial excitation of excitons with wave
Figure 6. (a) The center-of-mass wave function of exciton localized on skyrmion. The colors correspond to different profiles of skyrmion shown in figure 2. The solid and dashed curves correspond to spin-up and spin-down components of the wave function. Here the diamagnetic ratio is $\xi/\lambda = 2.5$, and the inset illustrates the case of a large skyrmion, with moderate diamagnetic ratio $\xi/\lambda = 0.7$. (b) The binding energy, and (c) the radius of exciton localization on skyrmion versus the diamagnetic ratio. For smaller skyrmions, the localized states emerge only at very large values of diamagnetic shift. The thin line in panel (b) shows the interaction energy $\lambda$.

vector $\vec{k}$ directed to the center of skyrmion, one finds the following Hall angle $\alpha$ in the regime of the elastic scattering:

$$|\alpha(k)| \approx \left| \frac{j_+}{j_-} \right| = \left| \frac{\int_0^{\pi} k \tan \theta \omega(k, \theta) d\theta}{\int_0^{\pi} k \omega(k, \theta) d\theta} \right|. \quad (10)$$

The calculated value of the Hall angle is $\alpha \sim 0.025 - 0.035$, in line with previous theoretical [40], and experimental [38] reports. The wave vector dependence of the Hall angle is shown in figure 1 of the SM.

2.4. Exciton localization
In the regime of large magnetic fields the diamagnetic term has a strong impact on the excitonic spectrum. Given by ferromagnetic nature of considered material, in equation (3) we account for quadratic terms in magnetic field, which can be phenomenologically included in our model:

$$\hat{H}_{\text{dia}} = \xi \mathbf{d}_z^2 \mathbb{1}_z, \quad (11)$$

where $\xi$ is the diamagnetic shift energy, which is taken as a phenomenological parameter. At sufficiently large values of $\xi$ the presence of diamagnetic term can result in exciton localization at skyrmion. We seek for the $s-$state solution in the form $\Psi = (\psi_+, \psi_- e^{\phi})$. The radial profiles of the components of exciton wave function are plotted in figure 6(a). Quite naturally, for smaller skyrmion the area of exciton localization is more compact. Further, with the enhancement of diamagnetic term the binding energy increases, as shown in figure 6(b). For the skyrmion of smaller radius the localized state appears at larger values of diamagnetic shift. Figure 6(c) illustrates the effective radius of localization $l = \langle \Psi|\rho|\Psi \rangle$.

The saturation of localization radius at elevated values of diamagnetic shift is explained by the repulsion of exciton wave function components toward the skyrmion edge, cf the black curves in figure 6(a) and the inset therein.

3. Conclusions and discussion
In conclusion, we developed a theory addressing the co-existence of excitons and magnetic skyrmions in a 2D material. Within the theory, the band structure and exciton states are calculated using DFT, and the magnetic properties including the properties of skyrmion states are obtained via atomistic spin simulations. We applied the theory to the celebrated CrI$_3$ monolayer system, yet the phenomena we predicted should be relevant for a class of 2D magnetic semiconductors with the possibility of broken structural inversion symmetry necessary for the emergence of uncompensated DM interaction.

We revealed two scenarios of exciton-skyrmion interaction. The first scenario implies a spin-conserving exciton elastic scattering off the skyrmion. Here we apply an adiabatic elimination approach to discard the spin degree of freedom. Similar to the scattering of massive spinor paricle [51], the exciton scattering in spinless domain is characterized by giant asymmetry, provided by emerging synthetic U(1) gauge field. Such asymmetric scattering is a necessary prerequisite of the excitonic anomalous Hall effect [40]. The second scenario accounts for the impact of diamagnetic effect on the exciton-skyrmion interaction. The diamagnetic term breaks the inversion symmetry, which for sufficiently large values of diamagnetic energy shift leads to an efficient localization of spinful exciton on the skyrmion. This opens a way for creation of tunable analogs of magnetic
excitonic quantum dots, which can find their applications in the domain of quantum optics, for example as single photon emitters with tailored properties. Additionally, the exciton localization enables optical detection of skyrmions, which is particularly important for antiferromagnetic systems. We indeed foresee interesting phenomena resulting from the interaction of excitons with topological magnetic textures in antiferromagnets. For example, based on the analogy with the electron transport [57–60], we conjecture that skyrmions on two antiferromagnetically coupled sublattices deflect equal amount of excitons with opposite spins to opposite directions, leading to zero net exciton Hall transport, but finite exciton spin Hall transport. Such spin exciton Hall effect induced by topological magnetic textures as well as other phenomena remain to be explored.

In our work, we focus on excitonic response to the presence of magnetic skyrmions, but the opposite effect is also feasible thus enabling resonant optical control of skyrmions. Generalization of the theory to describe the dynamical response of magnetic skyrmions should be straightforward [37]. This will make it possible to simulate various phenomena associated with coupled exciton-skyrmion dynamics.

4. Methods

4.1. Calculation of band structure and exciton transitions

The band structure of a ferromagnetic single-layered CrI3 is calculated using the DFT approach implemented in the GPAW [61–63] code with LDA exchange-correlation functional. The lattice constant is taken as \( a_0 = 6.69 \) Å and the vacuum distance is 16 Å. The spin-orbit interaction is taken into account using the first-order perturbation theory [64]. The ground states calculation is done using the planewave basis with the \( 6 \times 6 \times 1 \) k-space grid with the plane wave cutoff equal to 600 eV. Exciton states are calculated using \textit{ab initio} Bethe-Salpeter equation method implemented in GPAW code [44, 65] on the \( 6 \times 6 \times 1 \) k-space grid with 16 valence and 14 conduction bands with 50 eV plane wave cutoff. In previous CrI3 GW bandstructure calculations [43, 45], the GW correction did not affect the effective masses of the conduction and valence bands, leading only to the band gap renormalization. Hence, the band gap correction can be added on top of the DFT-calculated result using the scissors operator [66, 67]. We applied the scissors-operator approach to obtain the well-established value of 2.59 eV for the band gap [43, 44].

4.2. Simulated magnetic subsystem

Magnetic subsystem of CrI3 is modeled as a single monolayer of classical vectors localized on vertices of a honeycomb lattice. The magnetic energy of the system reads:

\[
E = \frac{J}{2} \sum_{i,j} \vec{m}_i \cdot \vec{m}_j - \frac{D}{2} \sum_{i,j} \vec{d}_{ij} \cdot [\vec{m}_i \times \vec{m}_j] - k \sum_i (\vec{m}_i \cdot \vec{e}_z)^2 - \mu \sum_i \vec{B} \cdot \vec{m}_i. \tag{12}
\]

Here, \( \vec{m}_i \) is a unit vector in the direction of \( i \)th magnetic moment with magnitude \( \mu = 3 \) Bohr magnetons, \( \vec{B} \) is the external magnetic field, and \( \vec{d}_{ij} = \vec{r}_{ij} \times \vec{e}_z/|\vec{r}_{ij}| \) is the DM unit vector with \( \vec{e}_z \) and \( \vec{r}_{ij} \) being the unit vector along the monolayer normal and the vector pointing from site \( i \) to site \( j \), respectively [68]. The pairwise interactions are between the nearest neighbors only. Both the magnetic field and the anisotropy axis are along \( \vec{e}_z \). The size of the computational domain is chosen to be \( 50 \times 50 \) unit cells. Periodic boundary conditions are applied so as to model the extended 2D systems.

4.3. Exciton scattering

The differential cross-section of elastic scattering reads [51, 69]:

\[
\omega(\vec{k}, \vec{k}') = \frac{\mu^2}{2\pi \hbar^4} \left| \frac{T(\vec{k}, \vec{k}')}{k} \right|^2. \tag{13}
\]

Here \( \vec{k}, \vec{k}' \) correspond to the center of mass wave vectors of incident and scattered excitons, respectively, with \( k = |\vec{k}| = |\vec{k}'| \). The scattering \( T \)-matrix can be expanded as

\[
T(\vec{k}, \vec{k}') \approx V(\vec{k}, \vec{k}') + \sum_{\vec{k}''} \frac{V(\vec{k}', \vec{k}'')V(\vec{k}'', \vec{k})}{\varepsilon_k - \varepsilon_{k''} + i\eta}, \tag{14}
\]

where \( \varepsilon_k = \hbar^2 k^2/(2\mu_X) \). The matrix element \( V(\vec{k}, \vec{k}') \) within the first Born approximation has the form (see the SM for the derivation):

\[
V(\vec{k}', \vec{k}) = \frac{1}{2\pi} \int_0^\infty J_0(|\Delta \vec{k}|\rho) \left( \frac{e^2 A^2}{2\mu_X} + W \right) \rho d\rho
- \frac{i e \hbar}{\pi} \frac{|\vec{k}' \times \vec{k}|^2}{|\Delta \vec{k}|} \int_0^\infty J_1(|\Delta \vec{k}|A(\rho))\rho d\rho, \tag{15}
\]

where \( \Delta \vec{k} = \vec{k}' - \vec{k} \). Thus, the differential cross-section can be expanded up to third order in skyrmion potential strength [55]:

\[
\omega(\vec{k}, \vec{k}') \approx \omega^{(2)}(\vec{k}, \vec{k}') + \omega^{(3)}(\vec{k}, \vec{k}') + \omega^{(3)}(\vec{k}, \vec{k}'), \tag{16}
\]

where the lowest order term

\[
\omega^{(2)}(\vec{k}, \vec{k}') = \frac{\mu^2}{2\pi \hbar^4} \left| \frac{V(\vec{k}, \vec{k}')}{k} \right|^2 \tag{17}
\]
is symmetric. The third order terms read:

\[
\omega^{(3)}(\vec{k}, \vec{k}') = \frac{\hbar^2}{2m} 2^{\frac{1}{3}} \left\{ \text{Re} \left[ \sum_{\vec{k}''} V(\vec{k}, \vec{k}') V(\vec{k}'', \vec{k}) \delta(\epsilon_k - \epsilon_{k''}) \right] \right\},
\]

(18)

\[
\omega^{(3)}(\vec{k}, \vec{k}') = -\frac{\hbar^2}{2\hbar k} \text{Im} \left[ \sum_{\vec{k}''} V(\vec{k}, \vec{k}') V(\vec{k}'', \vec{k}) \delta(\epsilon_k - \epsilon_{k''}) \right],
\]

(19)

where \( \text{Re} \) denotes the principal value integration. The details of evaluation of equation (19) are presented in SM.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Acknowledgments

We thank Prof. I V Iorsh for valuable discussions. The work was supported by the Icelandic Research Fund Grants 163082-051 and 217750, the University of Iceland Research Fund (Grant No. 15673), and the Swedish Research Council (Grant No. 2020-05110). V S acknowledges the University of Iceland for the hospitality. Y V Z is grateful to Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) SPP 2244 (Project No. 443416183) for the financial support. This work was supported by the Ministry of Science and Higher Education of the Russian Federation (Project No. 075-15-2021-589). This work was partially funded by Priority 2030 Federal Academic Leadership Program. V S acknowledges the support of ‘Basis’ Foundation (Project No. 22-1-3-43-1).

Author contributions statement

Y V Z performed the DFT calculations of band structure and exciton states. M K and P F B calculated the magnetic skyrmion states. M K and V A S calculated the exciton scattering and localization on skyrmion. I A S formulated the original idea and supervised the work. All authors extensively discussed the results and participated in editing of the manuscript.

Conflict of interest

The authors declare no competing interests.

ORCID iDs

V A Shahnazaryan https://orcid.org/0000-0001-7892-0550
P F Bessarab https://orcid.org/0000-0003-3351-7172

References

[1] Roßler U K, Bogdanov A N and Pfleiderer C 2006 Spontaneous skyrmion ground states in magnetic metals Nature 442 797
[2] Kiselev N S, Bogdanov A N, Schäfer R and Rößler U K 2011 Chiral skyrmions in thin magnetic films: new objects for magnetic storage technologies? J. Phys. D: Appl. Phys. 44 392001
[3] Romming N, Kubetzka A, Hanneken C, von Bergmann K and Wiesendanger R 2015 Field-dependent size and shape of single magnetic skyrmions Phys. Rev. Lett. 114 177205
[4] Butov I V, Gossard A C and Chemla D S 2002 Macroscopically ordered state in an exciton system Nature 418 751
[5] Astrakharchik G E, Boronat J, Kurbakov I L and Lozovik Y E 2007 Quantum phase transition in a two-dimensional system of dipoles Phys. Rev. Lett. 98 060405
[6] High A A, Leonard J R, Hammad A T, Fogler M M, Butov I V, Kavokin A V, Campman K L and Gossard A C 2012 Spontaneous coherence in a cold exciton gas Nature 483 384
[7] Lozovik Y E, Ogarkov S L and Sokolik A A 2012 Condensation of electron-hole pairs in a two-layer graphene system: correlation effects Phys. Rev. B 86 045429
[8] Fogler M M, Butov L V and Novoselov K S 2014 High-temperature superfluidity with indirect excitons in van der Waals heterostructures Nat. Commun. 5 4555
[9] Kasprzak J et al 2006 Bose-Einstein condensation of exciton polaritons Nature 443 409
[10] Balili R, Hartwell V, Snoke D and West K 2007 Bose-Einstein condensation of microcavity polaritons in a trap Science 316 1007
[11] Amo A et al 2009 Collective fluid dynamics of a polariton condensate in a semiconductor microcavity Nature 457 291
[12] Lagoudakis K G, Wouters M, Richard M, Baas A, Carusotto I, Andre R, Dang L S and Deveaud-Pledran B 2008 Quantized vortices in an exciton-polariton condensate Nat. Phys. 4 706
[13] Tosi G, Christmann G, Berloff N G, Tsotgis P, Gao T, Hatzopoulos Z, Savvidis P G and Baumberg J J 2012 Geometrically locked vortex lattices in semiconductor quantum fluids Nat. Commun. 3 1243
[14] Gao T, Egorov O A, Estrecho E, Winkler K, Kamp M, Schneider C, Hofling S, Truscott A G and Ostrovskaya E A 2018 Controlled ordering of topological charges in an exciton-polariton chain Phys. Rev. Lett. 121 225302
[15] Kwon M-S, Oh B Y, Gong S-H, Kim J-H, Kang H K, Sang S, Song J D, Choi H and Cho Y-H 2019 Direct transfer of light’s orbital angular momentum onto a nonresonantly excited polariton superfluid Phys. Rev. Lett. 122 045302
[16] Seki S, Yu X Z, Ishiwata S and Tokura Y 2012 Observation of skyrmions in a multiferroic material Science 336 198
[17] Petrović A P et al 2021 Skyrmion-(anti)vortex coupling in a chiral magnet-superconductor heterostructure Phys. Rev. Lett. 126 117205
[18] Burch K S, Mandrus D and Park J-G 2018 Magnetism in two-dimensional van der Waals materials Nature 563 47
[19] Wildes A R et al 2015 Magnetic structure of the quasi-two-dimensional antiferromagnet NiPS₃ Phys. Rev. B 92 224408
[20] Kang S et al 2020 Coherent many-body exciton in van der Waals antiferromagnet NiPS₃ Nature 583 785
[21] Ho C-H, Hsu T-Y and Muhimmah L C 2021 The band-edge excitons observed in few-layer NiPS₃ npj 2D Mater. Appl. 5 8
[22] Birowska M, Faria Junior P F, Fabian J and Kunstmann J 2021 Large exciton binding energies in MnPs₃ as a case study of a van der Waals layered magnet Phys. Rev. B 103 L121108
[23] Huang B et al 2017 Layer-dependent ferromagnetism in a van der Waals crystal down to the monolayer limit Nature 546 270
[24] Zheng F, Zhao J, Liu Z, Li M, Zhou M, Zhang S and Zhang P 2018 Tunable spin states in the two-dimensional magnet CrI₃ Nanoscale 10 14298
[25] Kashin I V, Mazurenko V V, Katsnelson M I and Rudenko A N 2020 Orbital-resolved ferromagnetism of monolayer CrI₃ 2D Mater. 7 025036
[26] Kim M et al 2019 Micromagnetometry of two-dimensional ferromagnets Nat. Electron. 2 457
[27] Mermin N D and Wagner H 1966 Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic Heisenberg models Phys. Rev. Lett. 17 1133
[28] Lado J L and Fernández-Rossier J 2017 On the origin of magnetic anisotropy in two dimensional CrI3 2D Mater. 4 035002
[29] Liu J, Shi M, Lu J and Anantram M P 2018 Analysis of electrical-field-dependent Dzyaloshinskii-Moriya interaction and magneto-crystalline anisotropy in a two-dimensional ferromagnetic monolayer Phys. Rev. B 97 054416
[30] Ghosh S, Stojic N and Binggeli N 2019 Structural and magnetic response of CrI3 monolayer to electric field Physica B 570 166
[31] Vishkayi S I, Torbatian Z, Qaimzadeh A and Asgari R 2020 Strain and electric-field control of spin-spin interactions in monolayer CrI3 Phys. Rev. Mater. 4 094004
[32] Liu J, Shi M, Mo P and Lu J 2018 Electrical-field-induced magnetic Skyrmion ground state in a two-dimensional chromium tri-iodide ferromagnetic monolayer JPhys. Av. 8 055316
[33] Behera A K, Chowdhury S and Das S R 2019 Magnetic skyrmions in atomic thin CrI3 monolayer Appl. Phys. Lett. 114 232502
[34] Jiang P, Li L, Liao Z, Zhao Y and Zhong Z 2018 Spin direction-controlled electronic band structure in two-dimensional ferromagnetic CrI3 Nano Lett. 18 3844–9
[35] Seyler K L et al 2018 Ligand-field helical luminescence in a 2D ferromagnetic insulator Nat. Phys. 14 277
[36] Pervishko A A, Yudin D, Kumar Gudelli V, Delin A, Eriksson O and Guo G-Y 2020 Localized surface electromagnetic waves in CrI3-based magnetophotonic structures Opt. Express 28 20
[37] Kudlis A, Iorsh I and Shelykh I A 2021 All-optical resonant magnetization switching in CrI3 monolayers Phys. Rev. B 104 L020412
[38] Ong A, Zhang Y, Ideue T and Iwasa Y 2017 Exciton Hall effect in monolayer MoS2 Nat. Mater. 16 1193
[39] Glazov M M and Golub L E 2020 Skew scattering and side jump drive exciton valley Hall effect in two-dimensional crystals Phys. Rev. Lett. 123 157403
[40] Kozin V K, Shabashov V A, Kavokin A V and Shelykh I A 2021 Anomalous exciton Hall effect Phys. Rev. Lett. 126 036801
[41] Leyder C, Romanelli M, Karr J Ph, Giacobino E, Liew T C H, Glazov M M, Kavokin A V, Malpuech G and Bramati A 2007 Observation of the optical spin Hall effect Nat. Phys. 3 628
[42] Li Y-M, Li J, Shi I-L K, Zhang D, Yang W and Chang K 2015 Light-induced exciton spin Hall effect in van der Waals heterostructures Phys. Rev. Lett. 115 166804
[43] Wu, Li Z, Cao T and Louie S G 2019 Physical origin of giant excitonic and magnetooptical responses in two-dimensional ferromagnetic insulators Nat. Commun. 10 2371
[44] Olsen T 2021 Unifed treatment of magnons and excitons in monolayer CrI3 from many-body perturbation theory Phys. Rev. Lett. 127 166402
[45] Acharya S, Pashov D, Rudenko A N, Rösser M, van Schilfgaarde M and Katsnelson M I 2022 Real- and momentum-space description of the excitons in bulk and monolayer chromium tri-halides npj 2D Mater. Appl. 6 33
[46] Ivanov A V, Udzim V M and Jónsson H 2021 Fast and robust algorithm for energy minimization of spin systems applied in an analysis of high temperature spin configurations in terms of skyrmion density Comput. Phys. Commun. 260 107749
[47] Braun H-B 1994 Fluctuations and instabilities of ferromagnetic domain-wall pairs in an external magnetic field Phys. Rev. B 50 16485
[48] Bogdanov A and Hubert A 1994 Thermodynamically stable magnetic vortex states in magnetic crystals J. Magn. Magn. Mater. 138 255–69
[49] Bogdanov A and Hubert A 1994 The properties of isolated magnetic vortices Phys. Status Solidi b 186 527–43
[50] Nagaosa N and Tokura Y 2013 Topological properties and dynamics of magnetic skyrmions Nat. Nanotechnol. 8 699–711
[51] Denisov K S, Rozhansky I V, Averkiev N S and Läbleranta E 2016 Electron scattering on a magnetic skyrmion in the nonadiabatic approximation Phys. Rev. Lett. 117 027202
[52] Denisov K S 2020 Theory of an electron asymmetric scattering on skyrmion textures in two-dimensional systems J. Phys.: Condens. Matter 32 415302
[53] Dalibard J, Gerbier F, Juzeliunās G and Öhberg P 2011 Colloquium: artificial gauge potentials for neutral atoms Rev. Mod. Phys. 83 1523
[54] Ritz R, Halder M, Franz C, Bauer A, Wagner M, Bamler R, Rosch A and Pfleiderer C 2013 Giant generic topological Hall resistivity of Mn3Sn under pressure Phys. Rev. B 87 134424
[55] Sinitsyn N A, MacDonald A H, Jungwirth T, Dugaev V K and Sinova J 2007 Anomalous Hall effect in a two-dimensional dirac band: the link between the Kubo-Streda formula and the semiclassical Boltzmann equation approach Phys. Rev. B 75 045315
[56] Aharonov Y and Bohm D 1959 Significance of electromagnetic potentials in the quantum theory Phys. Rev. 115 485
[57] Bühl P M, Freimuth F, Blügel S and Mokrousov Y 2017 Topological spin Hall effect in antiferromagnetic skyrmions Phys. Status Solidi I 11700007
[58] Akosa C A, Tretiakov O A, Tatara G and Manchon A 2018 Theory of the topological spin Hall effect in antiferromagnetic skyrmions: impact on current-induced motion Phys. Rev. Lett. 121 097204
[59] Göbel B, Mook A, Henk J and Mertig I 2017 Antiferromagnetic skyrmion crystals: generation, topological Hall and topological spin Hall effect Phys. Rev. B 96 060406(R)
[60] Göbel B, Mook A, Henk J and Mertig I 2018 The family of topological Hall effects for electrons in skyrmion crystals Eur. Phys. J. B 91 179
[61] Mortensen J J, Hansen L B and Jacobsen K W 2005 Real-space grid implementation of the projector augmented wave method Phys. Rev. B 71 035109
[62] Enkovaara J et al 2010 Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method J. Phys.: Condens. Matter 22 253202
[63] Jan Y, Mortensen J J, Jacobsen K W and Thygesen K S 2011 Linear density response function in the projector augmented wave method: applications to solids, surfaces and interfaces Phys. Rev. B 83 245122
[64] Olsen T 2016 Designing in-plane heterostructures of quantum spin Hall insulators from first principles: 1T’-MoS2 with adsorbates Phys. Rev. B 94 235309
[65] Huser F, Olsen T and Thygesen K S 2013 How dielectric screening in two-dimensional crystals affects the convergence of excited-state calculations: monolayer MoS2 Phys. Rev. B 88 245309
[66] Levine Z and Allan D 1989 Linear optical response in silicon and germanium including self-energy effects Phys. Rev. Lett. 63 1719
[67] Gonze X and Lee C 1997 Dynamical matrices, Born effective charges, dielectric permitivity tensors and interatomic force constants from density-functional perturbation theory Phys. Rev. B 55 10555
[68] Yang H, Thiaville A, Rohart S, Fert A and Chshiev M 2015 Anatomy of Dzyaloshinskii-Moriya interaction at Co/Pt interfaces Phys. Rev. Lett. 115 267202
[69] Adhikari S K 1986 Quantum scattering in two dimensions Am. J. Phys. 54 362