Geometrical torque on magnetic moments coupled to a correlated antiferromagnet

— Supplemental Material —

Nicolas Lenzing,¹ David Krüger,¹ and Michael Potthoff^{1,2}

¹ University of Hamburg, Department of Physics, Notkestraße 9-11, 22607 Hamburg, Germany ² The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

Section A: SO(2) symmetry analysis. The retarded spin susceptibility is defined as

$$\chi_{ii',\alpha\alpha'}(t) = -i\Theta(t)\langle [s_{i\alpha}(t), s_{i'\alpha'}(0)] \rangle, \qquad (7)$$

where Θ is the step function, $s_{i\alpha}(t) = e^{iH_{\rm el}t}s_{i\alpha}e^{-iH_{\rm el}t}$, and $\langle \cdots \rangle$ is the ground-state expectation value. Fourier transformation to frequency space yields the Lehmann representation in terms of an energy eigenbasis { $|\Psi_n\rangle$ }:

$$\chi_{ii',\alpha\alpha'}(\omega) = \sum_{n} \left(\frac{\langle \Psi_0 | s_{i\alpha} | \Psi_n \rangle \langle \Psi_n | s_{i'\alpha'} | \Psi_0 \rangle}{\omega + i\eta - (E_n - E_0)} - \frac{\langle \Psi_0 | s_{i'\alpha'} | \Psi_n \rangle \langle \Psi_n | s_{i\alpha} | \Psi_0 \rangle}{\omega + i\eta - (E_0 - E_n)} \right).$$
(8)

We have the relation $\chi_{ii',\alpha\alpha'}(\omega)^* = \chi_{ii',\alpha\alpha'}(-\omega)$. The spectral density $-(1/\pi) \text{Im} \chi_{ii',\alpha\alpha'}(\omega) = \chi_{ii',\alpha\alpha'}(\omega) - \chi_{ii',\alpha\alpha'}(-\omega)/2i$ is an antisymmetric function of ω .

In the AF phase with order parameter $\boldsymbol{m} = \boldsymbol{m}\boldsymbol{e}_{z}$, there is a remaining SO(2) symmetry of the nondegenerate energy eigenstates under spin rotations around \boldsymbol{e}_{z} , which is unitarily represented by $U_{\mathrm{R}} = e^{-is_{\mathrm{tot},z}\varphi}$ on the Fock space with the z-component of the total spin $\boldsymbol{s}_{\mathrm{tot}} = \sum_{i} \boldsymbol{s}_{i}$ as the unbroken generator and the rotation angle φ . We have $U_{\mathrm{R}}^{\dagger}|\Psi_{n}\rangle = e^{i\phi_{n}}|\Psi_{n}\rangle$ with phases ϕ_{n} . Since \boldsymbol{s}_{i} is a vector operator, we have $U_{\mathrm{R}}^{\dagger}s_{i\alpha}U_{\mathrm{R}} = \sum_{\beta}R_{\alpha\beta}s_{i\beta}$, where $\underline{R} = \underline{R}(\varphi)$ is the standard real 3×3 matrix representation of SO(2) rotations around \boldsymbol{e}_{z} . Hence, the first matrix element in Eq. (4) can be written as $\langle \Psi_{0}|U_{\mathrm{R}}U_{\mathrm{R}}^{\dagger}s_{i\alpha}U_{\mathrm{R}}U_{\mathrm{R}}^{\dagger}|\Psi_{n}\rangle =$ $\sum_{\beta}R_{\alpha\beta}(\varphi)e^{i\phi_{0}}\langle \Psi_{0}|s_{i\beta}|\Psi_{n}\rangle e^{-i\phi_{n}}$. The phase factors cancel with those from the second matrix element, and we thus find: $\chi_{ii',\alpha\alpha'}(\omega) = \sum_{\beta\beta'}R_{\alpha\beta}(\varphi)\chi_{ii',\beta\beta'}(\omega)R_{\beta'\alpha'}^{T}(\varphi)$, i.e., $[\underline{\chi}_{ii'}(\omega), \underline{R}(\varphi)] = 0$ for all i, i' and φ . It is easily verified directly that this implies

$$\underline{\chi}_{ii'}(\omega) = \begin{pmatrix} \chi_{ii',xx}(\omega) & \chi_{ii',xy}(\omega) & 0\\ -\chi_{ii',xy}(\omega) & \chi_{ii',xx}(\omega) & 0\\ 0 & 0 & \chi_{ii',zz}(\omega) \end{pmatrix}, \quad (9)$$

i.e., there are only 3 independent entries for each pair i, i' (note that R is reducible, and furthermore Schur's lemma does not apply to representations over \mathbb{R}).

Section B: Spatial symmetries. With Eq. (8), we immediately see that the spin-Berry curvature is related to the spin susceptibility via

$$\Omega_{mm',\alpha\alpha'} = -iJ^2 \frac{\partial}{\partial\omega} \chi_{i_m i_{m'},\alpha\alpha'}(\omega) \Big|_{\omega=0}$$
(10)

up to correction terms of order J^3 , see Eq. (5). Therefore, the same reasoning as above can be applied to the spin-Berry curvature tensor and yields the same result for its structure:

$$\underline{\Omega}_{mm'} = \begin{pmatrix} \Omega_{mm',xx} & \Omega_{mm',xy} & 0\\ -\Omega_{mm',xy} & \Omega_{mm',xx} & 0\\ 0 & 0 & \Omega_{mm',zz} \end{pmatrix} .$$
(11)

In addition, for a given pair of sites i_m and $i_{m'}$, we may consider a combined transformation $T \circ I$, composed of the space inversion $\mathbf{R}_i \mapsto \mathbf{R}_{i_m} - \mathbf{R}_i$ with respect to i_m followed by the translation $\mathbf{R}_i \mapsto \mathbf{R}_i + (\mathbf{R}_{i_m} - \mathbf{R}_{i_{m'}})$ with the translation vector $\mathbf{R}_{i_m} - \mathbf{R}_{i_{m'}}$. $T \circ I$ is a discrete symmetry of the hypercubic lattice and interchanges i_m with $i_{m'}$. This implies that the Hamiltonian commutes with the standard unitary (and also Hermitian) representation U_{TI} of $T \circ I$.

For i_m and $i_{m'}$ in the same sublattice, the symmetrybroken ground state is an eigenstate of $U_{\rm TI}$ as well. Analogously to the SO(2) spin-rotation symmetry discussed above, we can thus immediately see from the analysis of the matrix elements in Eq. (4) that $\Omega_{mm',\alpha\alpha'}$ = $\Omega_{m'm,\alpha\alpha'}$. For the spin-Berry curvature we have the additional antisymmetry, $\Omega_{mm',\alpha\alpha'} = -\Omega_{m'm,\alpha'\alpha}$, which follows from Eq. (3). With this we get $\Omega_{mm',\alpha\alpha'}$ = $-\Omega_{mm',\alpha'\alpha}$, i.e., for each pair m, m', the spin-Berry curvature tensor is antisymmetric in the indices α, α' separately. Hence, with Eq. (11), we see that only the elements $\Omega_{mm',xy} = -\Omega_{mm',yx}$ can be nonzero. Analogously, for the spin susceptibility, the $T \circ I$ symmetry of the Hamiltonian implies $\chi_{ii',\alpha\alpha'}(\omega) = \chi_{i'i,\alpha\alpha'}(\omega)$. With the additional symmetry, $\chi_{ii',\alpha\alpha'}(0) = \chi_{i'i,\alpha'\alpha}(0)$, which follows from Eq. (8), this implies that the susceptibility matrix Eq. (9) is diagonal for $\omega = 0$.

For i_m and $i_{m'}$ in different sublattices, we concatenate the transformation $T \circ I$ with a flip F of the z-component of all spins. This is unitarily represented by $U_{\rm F}$, which is defined via $U_{\rm F}^{\dagger}c_{i\uparrow}U_{\rm F} = c_{i\downarrow}$ and $U_{\rm F}^{\dagger}c_{i\downarrow}U_{\rm F} = c_{i\uparrow}$. We have $[U_{\rm F}, U_{\rm TI}] = 0$ and $[U_{\rm F}, H_{\rm el}] = 0$. The symmetry-broken ground state and the corresponding excited states are eigenstates of $U \equiv U_{\rm TI}U_{\rm F}$. Hence, we find for the $\alpha = \alpha'$ matrix elements

$$\langle \Psi_0 | s_{i_m \alpha} | \Psi_n \rangle \langle \Psi_n | s_{i_{m'} \alpha} | \Psi_0 \rangle$$

$$= \langle \Psi_0 | U^{\dagger} s_{i_m \alpha} U | \Psi_n \rangle \langle \Psi_n | U^{\dagger} s_{i_{m'} \alpha} U | \Psi_0 \rangle$$

$$= \langle \Psi_0 | s_{i_{m'} \alpha} | \Psi_n \rangle \langle \Psi_n | s_{i_m \alpha} | \Psi_0 \rangle ,$$
(12)

and thus $\Omega_{mm',\alpha\alpha} = \Omega_{m'm,\alpha\alpha}$. With the antisymmetry of the full tensor, $\Omega_{mm',\alpha\alpha'} = -\Omega_{m'm,\alpha'\alpha}$, we thus find $\Omega_{mm',\alpha\alpha} = 0$. On the other hand,

$$\begin{split} \langle \Psi_0 | s_{i_m x} | \Psi_n \rangle \langle \Psi_n | s_{i_{m'} y} | \Psi_0 \rangle \\ &= \langle \Psi_0 | U^{\dagger} s_{i_m x} U | \Psi_n \rangle \langle \Psi_n | U^{\dagger} s_{i_{m'} y} U | \Psi_0 \rangle \\ &= - \langle \Psi_0 | s_{i_{m'} x} | \Psi_n \rangle \langle \Psi_n | s_{i_m y} | \Psi_0 \rangle , \end{split}$$
(13)

since $U_{\rm F}^{\dagger} s_{ix} U_{\rm F} = s_{ix}$ but $U_{\rm F}^{\dagger} s_{iy} U_{\rm F} = -s_{iy}$. This implies $\Omega_{mm',xy} = -\Omega_{m'm,xy}$, and with the antisymmetry of the full tensor we find $\Omega_{mm',xy} = \Omega_{mm',yx}$. Together with Eq. (11), we see that $\Omega_{mm',xy} = 0$, and hence the matrix $\Omega_{mm'} = 0$ in Eq. (11).

Summing up, for arbitrary sites i_m and i_{m^\prime} we have

$$\underline{\Omega}_{mm'} = \begin{pmatrix} 0 & \Omega & 0\\ -\Omega & 0 & 0\\ 0 & 0 & 0 \end{pmatrix} , \qquad (14)$$

and hence the spin-Berry curvature is fixed by a single real number $\Omega \equiv \Omega_{mm',xy} = \Omega_{m'm,xy}$. Furthermore, $\Omega = 0$ if $i_m, i_{m'}$ belong to different sublattices.

Section C: Random phase approximation. The random phase approximation (RPA) represents a standard weak-coupling approach to the magnetic susceptibility, see, e.g., Refs. 41, 42. It can be motivated in various ways, for example, via a partial diagrammatic summation. In general, the RPA Luttinger-Ward functional $\Phi[G]$ [43, 44] is given as the sum of the two closed and self-consistently renormalized first-order diagrams, i.e., by the Hartree and the Fock diagram. For the Hubbard model the Fock diagram vanishes such that we are left with

$$\Phi[\mathbf{G}] = U \sum_{i} \frac{1}{\beta^2} \sum_{n,n'} G_{ii,\uparrow}(i\omega_n) G_{ii,\downarrow}(i\omega_{n'}) .$$
(15)

Here, *i* runs over the sites of the hypercubic lattice, $\sigma = \uparrow, \downarrow$ refers to the spin projection relative to the *z* axis, *n* labels the fermionic Matsubara frequencies $i\omega_n$, and β is the inverse temperature. Computations are done in the zero-temperature limit $1/\beta \to 0$, which is taken at the end. Furthermore, $G_{ii,\sigma}$ denotes the local one-particle Green's function at site *i* in the symmetrybroken AF state, as obtained within the self-consistent Hartree-Fock approximation. The Hartree-Fock selfenergy is generated by the Luttinger-Ward functional: $\Sigma_{ii,\sigma}(i\omega_n) = \beta \delta \Phi / \delta G_{ii\sigma}(i\omega_n) = U \beta^{-1} \sum_n G_{ii,-\sigma}(i\omega_n) = U \langle c_{i-\sigma}^{\dagger} c_{i-\sigma} \rangle.$

On the two-particle level, the RPA yields a local and frequency-independent irreducible vertex

$$\Gamma^{(\text{loc})}_{\sigma,-\sigma}(i\omega_n,i\omega_{n'}) = \beta^2 \frac{\delta^2 \Phi}{\delta G_{ii,-\sigma}(i\omega_n)\delta G_{ii,\sigma}(i\omega_{n'})} = U.$$
(16)

This means that there is no feedback of two-particle correlations on the single-particle Green's function. The structureless vertex allows us to easily get the transversal magnetic susceptibility $\chi_{rs,+-}(\mathbf{k},\omega) = \langle \langle s_{r,\mathbf{k}}^+; s_{s,\mathbf{k}}^- \rangle \rangle_{\omega}$ as the solution of a strongly simplified Bethe-Salpether equation in the particle-hole channel:

$$\underline{\chi}_{+-}(\boldsymbol{k}, i\nu_n) = \underline{\chi}_{+-}^{(0)}(\boldsymbol{k}, i\nu_n) + \underline{\chi}_{+-}^{(0)}(\boldsymbol{k}, i\nu_n)U\underline{\chi}_{+-}(\boldsymbol{k}, i\nu_n).$$
(17)

Here, $\underline{\chi}_{+-}$ is a 2 × 2 matrix in the sublattice degrees of freedom, and $\underline{\chi}_{+-}^{(0)}$ the bare susceptibility matrix, which is computed with the Hartree-Fock one-particle propagators. The equation is diagonal in the wave vectors \boldsymbol{k} of the first magnetic Brillouin zone and in the bosonic Matsubara frequencies $i\nu_n$. The transversal susceptibility χ_{+-} is related to the susceptibility tensor $\chi_{\alpha\alpha'}$ introduced in Eqs. (7) and (8), via $\chi_{+-} = 2(\chi_{xx} - i\chi_{xy})$. From the renormalized zeroth-order diagram, we get the Hartree-Fock susceptibility in Eq. (17) as

$$\chi_{rs,+-}^{(0)}(\boldsymbol{k},i\nu_{n}) = \frac{-1}{L}\frac{1}{\beta}\sum_{\boldsymbol{q},n'}G_{sr,\uparrow}(\boldsymbol{q},i\omega_{n'})$$
$$\times G_{rs,\downarrow}(\boldsymbol{q}+\boldsymbol{k},i\nu_{n}+i\omega_{n'}). \quad (18)$$

After performing the summation over the fermionic frequencies $i\omega_n$ analytically, we can replace $i\nu_n \mapsto \nu + i\eta$ to find the retarded susceptibility on the real-frequency axis. The frequency derivative in Eq. (10) is done numerically. In the thermodynamical limit, the q sum over the magnetic Brillouin zone in Eq. (18) can be converted into a q-space integration. The latter is computed in two or three dimensions via a standard adaptive q-space integration technique for arbitrary $\nu \in \mathbb{R}$ and for each allowed wave vector \boldsymbol{k} in the magnetic Brillouin zone of a finite lattice with L sites and periodic boundary conditions. Practical computations are performed at a finite Lorentzian broadening parameter $\eta > 0$ replacing the infinitesimal η , and convergence with respect to L is controlled by runs for different system sizes L. The main numerical error is due to extrapolation of the data for $\eta \to 0.$

Section D: Magnon spectrum of an antiferromagnet. In the strong-U limit of the Hubbard model, the lowenergy physics is captured by the s = 1/2 antiferromagnetic Heisenberg model

$$H = J_{\rm H} \sum_{\langle ij \rangle} \left(\frac{1}{2} (s_i^+ s_j^- + s_i^- s_j^+) + \Delta s_i^z s_j^z \right)$$
(19)

with $J_{\rm H} = 4t^2/U$ and $\Delta = 1$. An anisotropy parameter $\Delta > 1$ can be used to discuss the effect of opening a gap in the dispersion. The sum runs over all nearest-neighbor pairs $\langle ij \rangle$.

We apply the standard Holstein-Primakoff transfomation for the model on the bipartite hypercubic lattice with dimension D. For sites i in sublattice A, the spin operators are expressed in terms of bosonic annihilators and creators, i.e.,

$$s_{i}^{z} = s - a_{i}^{\dagger} a_{i} ,$$

$$s_{i}^{+} = \sqrt{2s} \sqrt{1 - \frac{\hat{n}_{i}}{2s}} a_{i} ,$$

$$s_{i}^{-} = \sqrt{2s} a_{i}^{\dagger} \sqrt{1 - \frac{\hat{n}_{i}}{2s}} ,$$
(20)

while for sites $j \in B$

$$s_{j}^{z} = -s + b_{j}^{\dagger} b_{j} ,$$

$$s_{j}^{+} = \sqrt{2s} b_{j}^{\dagger} \sqrt{1 - \frac{\hat{n}_{j}}{2s}} ,$$

$$s_{j}^{-} = \sqrt{2s} \sqrt{1 - \frac{\hat{n}_{j}}{2s}} b_{j} .$$
(21)

The transformed Hamiltonian reads

$$H = J_{\rm H}s \sum_{\langle ij\rangle} [(a_i b_j + a_i^{\dagger} b_j^{\dagger}) + \Delta(a_i^{\dagger} a_i + b_j^{\dagger} b_j)] - \frac{L}{2} z J_{\rm H} \Delta s^2 , \qquad (22)$$

where z = 2D is the coordination number, and L is the number of lattice sites. Quartic and higher-order magnon interaction terms resulting for the expansion of the square root have been disregarded.

We drop the additive energy constant and blockdiagonalize H via Fourier transformation:

$$a_i = \frac{1}{\sqrt{L/2}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\boldsymbol{R}_i} a_{\boldsymbol{k}} , \quad b_j = \frac{1}{\sqrt{L/2}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{R}_j} b_{\boldsymbol{k}} .$$
(23)

Here, \mathbf{R}_i are the translation vectors of the magnetic A sublattice (the same for \mathbf{R}_j and the B sublattice), consisting of L/2 unit cells, and \mathbf{k} is an allowed wave vector of the first magnetic Brillouin zone (mBz). Defining $\gamma_{\mathbf{k}} \equiv \sum_{\boldsymbol{\delta}} \cos(\mathbf{k}\boldsymbol{\delta})$ with nearest-neighbor vectors $\boldsymbol{\delta}$, the Fourier-transformed model reads as

$$H = J_{\rm H}s \sum_{\boldsymbol{k}} [\gamma_{\boldsymbol{k}}(a_{\boldsymbol{k}}b_{\boldsymbol{k}} + b_{\boldsymbol{k}}^{\dagger}a_{\boldsymbol{k}}^{\dagger}) + z\Delta(a_{\boldsymbol{k}}a_{\boldsymbol{k}}^{\dagger} + b_{\boldsymbol{k}}^{\dagger}b_{\boldsymbol{k}})] \quad (24)$$

and can be diagonalized by Bogoliubov transformation

$$a_{\mathbf{k}} = u_{\mathbf{k}}\alpha_{\mathbf{k}} + v_{\mathbf{k}}\beta_{\mathbf{k}}^{\dagger}, \quad b_{\mathbf{k}} = u_{\mathbf{k}}\beta_{\mathbf{k}} + v_{\mathbf{k}}\alpha_{\mathbf{k}}^{\dagger}$$
(25)

with real coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. We require

$$u_{k}^{2} - v_{k}^{2} = 1 , \qquad (26)$$

to ensure that α_k and β_k satisfy bosonic commutation relations, as well as

$$2z\Delta u_{\boldsymbol{k}}v_{\boldsymbol{k}} + \gamma_{\boldsymbol{k}}(u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2) \stackrel{!}{=} 0, \qquad (27)$$

as usual, to get the Hamiltonian to the form

$$H = J_{\rm H} s \sum_{\boldsymbol{k}} \omega(\boldsymbol{k}) (\alpha_{\boldsymbol{k}}^{\dagger} \alpha_{\boldsymbol{k}} + \beta_{\boldsymbol{k}}^{\dagger} \beta_{\boldsymbol{k}}) , \qquad (28)$$

where we again dropped an unimportant constant energy term. The magnon spectrum consists of two degenerate branches with dispersion $J_{\rm H} s \,\omega(\mathbf{k})$ given by

$$\omega(\mathbf{k}) = \sqrt{(z\Delta)^2 - \gamma_{\mathbf{k}}^2} = \sqrt{z^2 \Delta^2 - \left(\sum_{\boldsymbol{\delta}} \cos(\mathbf{k}\boldsymbol{\delta})\right)^2}.$$
(29)

Close to $\mathbf{k} = 0$ and in the isotropic case $\Delta = 1$, the dispersion $J_{\rm H} s \,\omega(\mathbf{k})$ is linear,

$$\omega(\mathbf{k}) = 2\sqrt{D}k + \mathcal{O}(k^3) , \qquad (30)$$

while for $\Delta > 1$ the spectrum is gapped, and $\omega(\mathbf{k}) = 2S\sqrt{\Delta^2 - 1} + \mathcal{O}(k^2)$.

From the conditions Eq. (26) and Eq. (27), we can deduce the well-known results

$$u_{\boldsymbol{k}}^{2} = \frac{1}{2} \left(\frac{z\Delta}{\sqrt{(z\Delta)^{2} - \gamma_{\boldsymbol{k}}^{2}}} + 1 \right) = \frac{1}{2} \left(\frac{z\Delta}{\omega(\boldsymbol{k})} + 1 \right) ,$$

$$v_{\boldsymbol{k}}^{2} = \frac{1}{2} \left(\frac{z\Delta}{\sqrt{(z\Delta)^{2} - \gamma_{\boldsymbol{k}}^{2}}} - 1 \right) = \frac{1}{2} \left(\frac{z\Delta}{\omega(\boldsymbol{k})} - 1 \right) (31)$$

and

$$u_{\boldsymbol{k}}v_{\boldsymbol{k}} = -\frac{\gamma_{\boldsymbol{k}}}{2\sqrt{(z\Delta)^2 - \gamma_{\boldsymbol{k}}^2}} = -\frac{\gamma_{\boldsymbol{k}}}{2\omega(\boldsymbol{k})}, \qquad (32)$$

see Refs. 47, 48.

Section E: Computing the spin-Berry curvature from the magnon Hamiltonian. The contribution of the magnon excitations to the spin-Berry curvature is obtained from

$$\Omega_{mm',\alpha\alpha'} = -2J^2 \operatorname{Im} \sum_{\boldsymbol{k},\eta=1,2} \frac{\langle 0|s_{i_m}^{\alpha}|\boldsymbol{k},\eta\rangle\langle\boldsymbol{k},\eta|s_{i_{m'}}^{\alpha'}|0\rangle}{(E_0 - E_{\boldsymbol{k}})^2},$$
(33)

where $|\mathbf{k}, 1\rangle \equiv \alpha_{\mathbf{k}}^{\dagger}|0\rangle$ and $|\mathbf{k}, 2\rangle \equiv \beta_{\mathbf{k}}^{\dagger}|0\rangle$ are the singlemagnon states. Following Eq. (14), it is sufficient to compute $\Omega_{mm'} = \Omega_{mm',xy} = -\Omega_{mm',yx}$. Furthermore, $\Omega_{mm'} \neq 0$ only for i_m and $i_{m'}$ in the same sublattice, as also argued in section B. Expressing the spin components in terms of the Bogoliubov operators,

$$s_{i}^{+} = \sqrt{2s} \frac{1}{\sqrt{L/2}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{R}_{i}} (u_{\mathbf{k}}\alpha_{\mathbf{k}} + v_{\mathbf{k}}\beta_{\mathbf{k}}^{\dagger})$$

$$s_{i}^{-} = \sqrt{2s} \frac{1}{\sqrt{L/2}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}_{i}} (u_{\mathbf{k}}\alpha_{\mathbf{k}}^{\dagger} + v_{\mathbf{k}}\beta_{\mathbf{k}})$$

$$s_{j}^{+} = \sqrt{2s} \frac{1}{\sqrt{L/2}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{R}_{j}} (u_{\mathbf{k}}\beta_{\mathbf{k}}^{\dagger} + v_{\mathbf{k}}\alpha_{\mathbf{k}})$$

$$s_{j}^{-} = \sqrt{2s} \frac{1}{\sqrt{L/2}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}_{j}} (u_{\mathbf{k}}\beta_{\mathbf{k}} + v_{\mathbf{k}}\alpha_{\mathbf{k}}^{\dagger}), \quad (34)$$

we find

$$\langle 0|s_i^x|\boldsymbol{k},1\rangle\langle\boldsymbol{k},1|s_{i'}^y|0\rangle = i\frac{s}{L}u_{\boldsymbol{k}}^2e^{-i\boldsymbol{k}(\boldsymbol{R}_i-\boldsymbol{R}_{i'})}, \langle 0|s_i^x|\boldsymbol{k},2\rangle\langle\boldsymbol{k},2|s_{i'}^y|0\rangle = -i\frac{s}{L}v_{\boldsymbol{k}}^2e^{i\boldsymbol{k}(\boldsymbol{R}_i-\boldsymbol{R}_{i'})}$$
(35)

for i, i' in sublattice A, and

$$\langle 0|s_j^x|\boldsymbol{k},1\rangle\langle \boldsymbol{k},1|s_{j'}^y|0\rangle = i\frac{s}{L}v_{\boldsymbol{k}}^2e^{-i\boldsymbol{k}(\boldsymbol{R}_j-\boldsymbol{R}_{j'})}, \langle 0|s_j^x|\boldsymbol{k},2\rangle\langle \boldsymbol{k},2|s_{j'}^y|0\rangle = -i\frac{s}{L}u_{\boldsymbol{k}}^2e^{i\boldsymbol{k}(\boldsymbol{R}_j-\boldsymbol{R}_{j'})}$$
(36)

for j, j' in sublattice B. This implies

$$\operatorname{Im}\sum_{\eta=1,2} \langle 0|s_{i}^{x}|\boldsymbol{k},\eta\rangle\langle\boldsymbol{k},\eta|s_{i'}^{y}|0\rangle = \frac{s}{L}\cos(\boldsymbol{k}(\boldsymbol{R}_{i}-\boldsymbol{R}_{i'}))$$
$$\operatorname{Im}\sum_{\eta=1,2} \langle 0|s_{j}^{x}|\boldsymbol{k},\eta\rangle\langle\boldsymbol{k},\eta|s_{j'}^{y}|0\rangle = -\frac{s}{L}\cos(\boldsymbol{k}(\boldsymbol{R}_{j}-\boldsymbol{R}_{j'})),$$
(37)

and finally we get

$$\Omega_{mm'} = \mp \frac{1}{s} \frac{J^2}{J_{\rm H}^2} \frac{2}{L} \sum_{k}^{\rm mBz} \frac{\cos(k(R_{i_m} - R_{i_{m'}}))}{\omega(k)^2} , \qquad (38)$$

where the upper sign refers to $i_m, i_{m'}$ in sublattice A and the lower for $i_m, i_{m'}$ in sublattice B. Recall that $\Omega_{mm'} = 0$ if $i_m, i_{m'}$ belong to different sublattices.

Eq. (38) can be evaluated numerically. For D = 3, for example, we find

$$\Omega_{\rm loc} \approx -0.084 \frac{J^2}{J_{\rm H}^2} \tag{39}$$

for the local element of the SBC with $i_m = i_{m'}$ in sublattice A. Section F: Different dimensions and distance dependence. In the thermodynamic limit $L \to \infty$ (and in the isotropic case $\Delta = 1$), the convergence of the resulting integral in Eq. (38) over the magnetic Brillouin zone decisively depends on the lattice dimension D. We consider the critical contribution of the long-wave-length magnons by integrating over a D-dimensional ball around $\mathbf{k} = 0$ with small cutoff radius k_c , such that we can make use of Eq. (30), i.e., of the linearity and isotropy of the magnon dispersion for $k \to 0$:

$$\Omega_{mm'} \sim \lim_{\kappa \to 0} \int_{\kappa}^{k_c} dk \, k^{D-1} \frac{1}{\omega(k)^2} \propto \lim_{\kappa \to 0} \int_{\kappa}^{k_c} dk \, k^{D-1} \frac{1}{k^2} \,. \tag{40}$$

This yields

$$\Omega_{mm'} \sim \begin{cases} \kappa^{D-2} & \text{for } D \ge 3\\ \ln \kappa & \text{for } D = 2\\ 1/\kappa & \text{for } D = 1 \end{cases}$$
(41)

For $\kappa \to 0$, the spin-Berry curvature diverges for D = 1and D = 2. We conclude that a meaningful theory is obtained in dimensions $D \ge 3$ only.

The magnitude of the spin-Berry curvature decreases with increasing distance $\mathbf{R} \equiv \mathbf{R}_{i_m} - \mathbf{R}_{i_{m'}}$. For $D \geq 3$ its dependence in the large-R limit is governed by longwave-length magnon excitations, and we have:

$$\Omega(R) \propto \int_0^{k_c} dk \, k^{D-1} \int d\Omega \frac{\cos(kR\cos\theta)}{k^2} \,, \qquad (42)$$

where $\int d\Omega$ denotes the surface integral over the (D-1)dimensional unit sphere, and θ the angle between \mathbf{k} and \mathbf{R} . Furthermore, we made use of Eq. (30) for k smaller than the cutoff k_c . We note that the distance dependence at large R is isotropic. Substituting $kR \to k$ in the onedimensional k integral immediately yields

$$\Omega(R) \propto \frac{1}{R^{D-2}} \,. \tag{43}$$

For D = 3, we have $\Omega(R) \propto 1/R$. In the infinite-D limit, we expect a local spin-Berry curvature

To compute the local element m = m' of the spin-Berry curvature Eq. (38) in this limit, we start from the representation

$$\Omega_{\rm loc} = -\frac{1}{s} \frac{J^2}{J_{\rm H}^2} \int_{-\infty}^{\infty} dx \,\rho_D(x) \frac{1}{z^2 \Delta^2 - Dx^2} \,, \qquad (44)$$

where, for dimension D, we have defined the density function

$$\rho_D(x) = \frac{2}{L} \sum_{\boldsymbol{k}}^{\text{mBz}} \delta(x - \gamma_{\boldsymbol{k}} / \sqrt{D}) , \qquad (45)$$

and where we have used Eq. (29). We have z = 2D for the *D*-dimensional hypercubic lattice and, in the Heisenberg

limit of the Hubbard model, $J_{\rm H} = 4t^2/U = 4t^{*2}/DU$, when using the scaling $t = t^*/\sqrt{D}$ with $t^* = \text{const.}$ In the limit $D \to \infty$, this scaling of the hopping ensures that the kinetic energy of the Hubbard model remains nontrivial and balances the interaction term [59]. Moreover, the density function converges to a Gaussian [59]:

$$\rho_D(x) \to \rho_\infty(x) = \frac{1}{2\sqrt{\pi}} \exp\left(-\frac{x^2}{4}\right).$$
(46)

In the Heisenberg limit and with the scaled hopping, we thus have

$$\Omega_{\rm loc}(D) = -\frac{1}{s} \frac{J^2 U^2}{16t^{*4}} \int_{-\infty}^{\infty} \frac{dx \rho_D(x)}{4\Delta^2 - x^2/D} , \qquad (47)$$

which for $D \to \infty$, and assuming s = 1/2 and $\Delta = 1$ converges to

$$\Omega_{\rm loc}(\infty) = -\frac{1}{32t^{*4}}J^2U^2.$$
(48)

This represents the mean-field value of the (lcoal) spin-Berry curvature in the antiferromagnetic state at large U. To compare with the result obtained for D = 3, we must use the same scaling of the hopping. This yields

$$\Omega_{\rm loc}(3) \approx -0.084 \frac{J^2 U^2}{16{t^*}^4} D^2 \bigg|_{D=3} \approx 1.51 \cdot \Omega(\infty).$$
(49)

For lattice dimensions D > 3 we find: $\Omega_{\rm loc}(4) \approx 1.22 \,\Omega(\infty), \,\Omega_{\rm loc}(5) \approx 1.16 \,\Omega(\infty), \,\Omega_{\rm loc}(6) \approx 1.12 \,\Omega(\infty).$ Hence, given the standard scaling of the hopping with D, the absolute value of $\Omega_{\rm loc}(D)$ increases with decreasing D and finally, for D = 2 diverges.

Finally, when addressing the dimensional crossover [61–63], we consider the Heisenberg model given by Eq. (19) again, but with spatially anisotropic nearest-neighbor exchange couplings $J_{\rm H} \equiv J_{\rm H,x} = J_{\rm H,y} \geq J_{\rm H,z}$. Proceeding analogously to Sec. C, one ends up with a modified magnon dispersion only:

$$\omega(\mathbf{k}) = \sqrt{(z_{\text{eff}}\Delta)^2 - \gamma_{\mathbf{k}}'^2} \,. \tag{50}$$

Here, we have defined an effective coordination number $z_{\rm eff} = 2(J_{\rm H,x} + J_{\rm H,y} + J_{\rm H,z})/J_{\rm H,x}$. Furthermore, $\gamma'_{k} := 2(J_{\rm H,x}\cos k_x + J_{\rm H,y}\cos k_y + J_{\rm H,z}\cos k_z)/J_{\rm H,x}$.

Section G: Spin dynamics. The equations of motion Eq. (1) for the classical spins comprise the conventional (Hamiltonian) and the geometrical spin torque, see Eq. (2). In the weak-J limit, the former results from the local direct exchange J as well as from the indirect RKKY-type exchange. We have:

$$\dot{\boldsymbol{S}}_{m} = J \langle \boldsymbol{s}_{i_{m}} \rangle^{(0)} \times \boldsymbol{S}_{m} + J^{2} \sum_{m'} \underline{\chi}_{i_{m}i_{m'}}(0) \boldsymbol{S}_{m'} \times \boldsymbol{S}_{m} + \sum_{\alpha} \sum_{m'\alpha'} \Omega_{m'm,\alpha'\alpha}(\boldsymbol{S}) \dot{\boldsymbol{S}}_{m'\alpha'} \boldsymbol{e}_{\alpha} \times \boldsymbol{S}_{m} , \qquad (51)$$

where $\langle \dots \rangle^{(0)}$ denotes the expectation value at J = 0. For the non-vanishing components of the spin susceptibility and of the spin-Berry curvature on sublattice A we have

$$\chi_{ii'} \equiv \chi_{ii',xx}(0) = \chi_{ii',yy}(0) = -\frac{z\Delta}{J_{\rm H}} \frac{2}{L} \sum_{\boldsymbol{k}}^{\rm mBz} \frac{\cos \boldsymbol{k}(\boldsymbol{R}_i - \boldsymbol{R}_{i'})}{\omega(\boldsymbol{k})^2}$$
(52)

and

$$\Omega_{mm'} \equiv \Omega_{mm',xy} = -\Omega_{mm',yx} = -\frac{1}{s} \frac{J^2}{J_{\rm H}^2} \frac{2}{L} \sum_{k}^{\rm mBz} \frac{\cos(k(R_{i_m} - R_{i_{m'}}))}{\omega(k)^2} \,.$$
(53)

Specializing Eq. (51) for M = 1, i.e., for a single classical spin, we get

$$\dot{\boldsymbol{S}}_1 = \boldsymbol{T}_1^{(\mathrm{H})} \times \boldsymbol{S}_1 + \Omega_{11} (\boldsymbol{e}_z \times \dot{\boldsymbol{S}}_1) \times \boldsymbol{S}_1 , \qquad (54)$$

where

$$\boldsymbol{T}_{1}^{(\mathrm{H})} = J \langle \boldsymbol{s}_{i_{1}} \rangle^{(0)} + J^{2} \chi_{i_{1}i_{1}}(\boldsymbol{e}_{z} \times \boldsymbol{S}_{m}) \times \boldsymbol{e}_{z} .$$

$$(55)$$

With

$$\underline{T}_{1}^{(\mathrm{H})} = \begin{pmatrix} 0 & -T_{1,z}^{(\mathrm{H})} & T_{1,y}^{(\mathrm{H})} \\ T_{1,z}^{(\mathrm{H})} & 0 & -T_{1,x}^{(\mathrm{H})} \\ -T_{1,y}^{(\mathrm{H})} & T_{1,x}^{(\mathrm{H})} & 0 \end{pmatrix}$$
(56)

the cross product can be written as a matrix-vector product, $\boldsymbol{T}_{1}^{(\mathrm{H})} \times \boldsymbol{S}_{1} = \underline{T}_{1}^{(\mathrm{H})} \boldsymbol{S}_{1}$, and the equation of motion reads:

$$\dot{\boldsymbol{S}}_{1} = \frac{1}{1 - \Omega_{11} S_{1z}} \underline{T}_{1}^{(\mathrm{H})} \boldsymbol{S}_{1} .$$
(57)

The classical spin undergoes a purely precessional dynamics around the z axis, but with a renormalized precession frequency. The renormalization is due to the local spin-Berry curvature $\Omega_{\text{loc}} = \Omega_{11}$ and is the strongest for $\Omega_{\text{loc}} = \mathcal{O}(1)$. Right at $\Omega_{\text{loc}} = 1/S_{1z}$, the precession frequency diverges. This implies that the spin dynamics is no longer adiabatic and the theory breaks down.

In case of two classical spins, M = 2, the equations of motion (51) can be cast into the form

$$\dot{\boldsymbol{S}}_{1} = \boldsymbol{T}_{1}^{(\mathrm{H})} \times \boldsymbol{S}_{1} + \boldsymbol{T}_{1}^{(\mathrm{geo})} \times \boldsymbol{S}_{1} , \dot{\boldsymbol{S}}_{2} = \boldsymbol{T}_{2}^{(\mathrm{H})} \times \boldsymbol{S}_{2} + \boldsymbol{T}_{2}^{(\mathrm{geo})} \times \boldsymbol{S}_{2} ,$$

$$(58)$$

where

$$\Gamma_{1}^{(\mathrm{H})} = J \langle \mathbf{s}_{i_{1}} \rangle^{(0)} + J^{2} \chi_{i_{1}i_{1}}(\mathbf{e}_{z} \times \mathbf{S}_{1}) \times \mathbf{e}_{z} + J^{2} \chi_{i_{1}i_{2}}(\mathbf{e}_{z} \times \mathbf{S}_{2}) \times \mathbf{e}_{z} ,$$

$$\Gamma_{2}^{(\mathrm{H})} = J \langle \mathbf{s}_{i_{2}} \rangle^{(0)} + J^{2} \chi_{i_{2}i_{2}}(\mathbf{e}_{z} \times \mathbf{S}_{2}) \times \mathbf{e}_{z} + J^{2} \chi_{i_{2}i_{1}}(\mathbf{e}_{z} \times \mathbf{S}_{1}) \times \mathbf{e}_{z} .$$
(59)

and

Here, we have assumed that the two spins couple to sites in the same sublattice, as otherwise the spin-Berry curvature vanishes. The local spin-Berry curvature term can be treated in the same way as in the M = 1 case, while the nonlocal term can be written as a matrix-vector product:

$$(1 - \Omega_{11}S_{1z})\dot{\boldsymbol{S}}_{1} = \boldsymbol{T}_{1}^{(\mathrm{H})} \times \boldsymbol{S}_{1} - \Omega_{12}\underline{\mathcal{A}}_{1}^{(z)}\dot{\boldsymbol{S}}_{2} ,$$

$$(1 - \Omega_{22}S_{2z})\dot{\boldsymbol{S}}_{2} = \boldsymbol{T}_{2}^{(\mathrm{H})} \times \boldsymbol{S}_{2} - \Omega_{12}\underline{\mathcal{A}}_{2}^{(z)}\dot{\boldsymbol{S}}_{1} ,$$
(61)

with

$$\underline{\mathcal{A}}_{m}^{(z)} = \begin{pmatrix} -S_{mz} & 0 & 0\\ 0 & -S_{mz} & 0\\ S_{mx} & S_{my} & 0 \end{pmatrix} .$$
(62)

This allows us to cast the equations of motion into an explicit system of ordinary differential equations:

$$\begin{pmatrix} \dot{\boldsymbol{S}}_1 \\ \dot{\boldsymbol{S}}_2 \end{pmatrix} = \mathcal{M}^{-1} \begin{pmatrix} \boldsymbol{T}_1^{(\mathrm{H})} \times \boldsymbol{S}_1 \\ \boldsymbol{T}_2^{(\mathrm{H})} \times \boldsymbol{S}_2 \end{pmatrix} .$$
 (63)

Here, the 6×6 matrix

$$\mathcal{M} = \begin{pmatrix} (1 - \Omega_{11}S_{1z})\mathbf{1} & \Omega_{12}\underline{\mathcal{A}}_1^{(z)} \\ \Omega_{12}\underline{\mathcal{A}}_2^{(z)} & (1 - \Omega_{22}S_{2z})\mathbf{1} \end{pmatrix}$$
(64)

is given in terms of the components of the spin-Berry curvature tensor. Eq. (63) demonstrates that the effect of the geometrical spin torque is not simply additive and hence does not directly compete with the conventional spin torque, but enters the spin dynamics as a multiplicative (matrix) factor.

The determinant of \mathcal{M} can be computed analytically:

$$\det \mathcal{M} = (1 - \Omega_{11}S_{1z})(1 - \Omega_{11}S_{2z}) \left[(1 - \Omega_{11}S_{1z})(1 - \Omega_{22}S_{2z}) - \Omega_{12}^2S_{1z}S_{2z} \right]^2.$$
(65)

The theory breaks down if det $\mathcal{M} = 0$. We consider det \mathcal{M} as a function of the local elements $\Omega_{\text{loc}} = \Omega_{11} = \Omega_{22}$ and assume that the nonlocal elements are small, $\Omega_{\text{nonloc}} = |\Omega_{12}| \ll \Omega_{\text{loc}}$. We immediately see that the zeros of det \mathcal{M} are of the order of unity. This implies that anomalous spin dynamics, which is substantially affected by the geometrical spin torque, is expected if $\Omega_{\text{loc}} = \mathcal{O}(1)$ and thus close to, but yet different from the zeros of \mathcal{M} .