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Determination of the Range of Magnetic Interactions from the Relations between Magnon Eigenvalues at High-Symmetry k Points

Di Wang(王棣)[1,2], Jihai Yu(于济海)[1,2], Feng Tang(唐峰)[1,2], Yuan Li(李源)[3,4], and Xiangang Wan(万贤纲)[1,2*]

[1]*National Laboratory of Solid State Microstructures and School of Physics, Nanjing University, Nanjing 210093, China*
[2]*Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China*
[3]*International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China*
[4]*Collaborative Innovation Center of Quantum Matter, Beijing 100871, China*

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Magnetic exchange interactions (MEIs) define networks of coupled magnetic moments and lead to a surprisingly rich variety of their magnetic properties. Typically MEIs can be estimated by fitting experimental results. Unfortunately, how many MEIs need to be included in the fitting process for a material is unclear a priori, which limits the results obtained by these conventional methods. Based on linear spin-wave theory but without performing matrix diagonalization, we show that for a general quadratic spin Hamiltonian, there is a simple relation between the Fourier transform of MEIs and the sum of square of magnon energies (SSME). We further show that according to the real-space distance range within which MEIs are considered relevant, one can obtain the corresponding relationships between SSME in momentum space. By directly utilizing these characteristics and the experimental magnon energies at only a few high-symmetry k points in the Brillouin zone, one can obtain strong constraints about the range of exchange path beyond which MEIs can be safely neglected. Our methodology is also generally applicable for other Hamiltonian with quadratic Fermi or Boson operators.

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As one of the oldest scientific topics, magnetism is still of great interest.[1−4] Magnetic materials have already been widely used in electromechanical and electronic devices, and their applications in information technology are also continuously growing.[1−3] Especially magnons, as the quanta of spin waves, have received more and more research attention over the past few decades.[5,6] As an elementary excitations of magnetic systems, magnons became an interesting platform for the study of general wave dynamics,[7,8] Bose–Einstein condensation of magnon,[9−11] and so on. In addition, with the development of topological physics in electron systems, topology in magnon spectrum has also attracted significant interests,[12−14] including topological magnon insulators,[15,16] magnonic Dirac semimetals[17−21] and Weyl semimetals.[22−24] Besides fundamental research, magnons have also attracted great attention for applications of information transport and processing.[25−29] Analogous to spintronics, the application of magnon are connected with the ability to carry, transport and process information. Potentially, the spins can be manipulated without current, thereby overcoming an important fundamental limitation of conventional electronic devices, the dissipation of energy due to Ohmic losses. Magnon spintronics is therefore an emerging field of modern magnetism, which has spurred significant advances towards computing application recently and is believed to deliver a number of breakthrough developments in the future.[25−29] In order to quantitatively understand the rich phenomenon and wide applications in this highly interdisciplinary field, a microscopic magnetic model with proper parameters becomes extremely important.

Magnetic properties can be typically described by a quadratic spin Hamiltonian $H = \sum_{i,j} \boldsymbol{S}_i \cdot \boldsymbol{J}_{ij} \cdot \boldsymbol{S}_j = \sum_{i,j} J_{ij}^{\alpha\beta} S_i^{\alpha} S_j^{\beta}$, where $\boldsymbol{J}_{ij}$ represents the magnetic exchange interaction (MEI) between the spin at i site $\boldsymbol{S}_i$ and spin at j site $\boldsymbol{S}_j$ as shown in the following equation. The sum should take over all possible exchange paths with sizable MEIs. However, it turns out that extracting quantitative J_{ij} is a highly non-trivial task. By choosing the set of parameters that best fit the experimental results, such as temperature-dependent magnetization, magnetic susceptibility $\chi(T)$, magnetic excitation spectra $\omega(q)$, one can basically obtain J's.[1−4] It is well known that the J_{ij} usually decreases rapidly with increasing R_{ij}, the distance between magnetic moment at i and j sites, and the J's with sufficient distance are believed to be negligible. Thus only a number of J's within a cutoff range R_{cut} are needed to be considered. However,

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*Corresponding author. Email: xgwan@nju.edu.cn
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a priori knowledge about $R_{\rm cut}$ is unknown, while the number of MEI used to fit the experimental data obviously affect the obtained J's. This leads to the arbitrariness of fitting approach, consequently affected the accuracy of the estimated MEIs, and currently unambiguous fitting is basically impossible. For example, very similar inelastic neutron scattering (INS) experimental results can be fitted by considerably different MEI parameters.[20,21]

In addition to the above approach, theoretical calculations have also been used to evaluate the exchange interaction parameters.[30–38] A popular numerical method is to calculate the total energies of more than N magnetic configurations and map them using a spin Hamiltonian to extract N MEIs.[30] Unfortunately, this method also needs to assume a cutoff range $R_{\rm cut}$, which again leads to the arbitrariness about the calculated MEIs. An alternative method is based on combining magnetic force theorem and linear-response approach.[31–35] Working in the momentum space, this method indeed does not suffer from the problem about $R_{\rm cut}$. However, the Coulomb interaction, which has been incorporated by the parameter U in first-principles calculations, usually plays an important role in magnetic systems.[39,40] Thus these theoretical MEIs strongly depend on choice of the parameter U.[39,40]

Symmetry imposes constraints about the magnetic model, and one can also use symmetry to check if two exchange paths with the same bond length have the same MEI. Unfortunately, this powerful theoretical method cannot provide any clue about $R_{\rm cut}$. The general features, such as sum rule for the spectral weight of the spin correlation function,[41] which requires accurate cross-section measurements over the entire Brillouin zone (BZ), cannot also predict the variation of MEIs over distance. Certain important subjects on magnetism, such as quantum spin liquids arising from exactly solvable models,[42] novel properties from geometrically frustrated magnet,[43] etc., explicitly requires small $R_{\rm cut}$, hence gaining a wealth of knowledge for $R_{\rm cut}$ in a large set of known magnetic materials will also be empirically useful for assessing the relevance of such models.

In this work, based on linear spin-wave theory (LSWT), we find that for a general quadratic spin Hamiltonian, the sum of square of magnon energies (SSME) at arbitrary k point in BZ can be directly obtained by the Fourier transform of MEIs, consequently one can easily calculate SSME at arbitrary k point in BZ without diagonalization. Thus, different from conventional symmetry analysis which groups the magnon energies into symmetry-related k points, our method produces different relationships between the SSME at different high-symmetry k points subjected to different $R_{\rm cut}$. Thus, using the magnon energies at only several high-symmetry k points, which can be measured by inelastic neutron scattering accurately,[1–6] one can unambiguously assert up to which neighbor the MEIs becomes negligible. To demonstrate how our algorithm works, we show an example for the Heisenberg model with ferromagnetic (FM) configuration and give the discussion about general cases with DM interaction, single-ion anisotropy (SIA) as well as non-collinear magnetic ordering. Instead of exhaustively listing the SSME relationships for all magnetic space group (MSG), we provide a code for the typical model to show our approach. Based on our example code, one can easily extend our method to other magnetic systems. With the basic information about a magnetic material (i.e., space group, the positions and magnetic moments orientations of the magnetic ions), the code will deliver corresponding SSME relationships according to the input $R_{\rm cut}$. Thus through simply checking up to which $R_{\rm cut}$, the experimental SSME starts to deviate from the obtained theoretical relationships, one can determine the real-space range of sizable MEIs. Our method can be easily extended to other Hamiltonian with quadratic Fermi or boson operators, thus is useful for the characteristics of the electronic band structure, phonon spectrum, etc.

Method. Usually the magnetic properties of crystal materials can be well described by a general pairwise magnetic model:[1–6]

$$H = \sum_{l,n,\alpha,l',n',\beta} J^{\alpha,\beta}_{\boldsymbol{R}_l+\boldsymbol{\tau}_n,\boldsymbol{R}_{l'}+\boldsymbol{\tau}_{n'}} S^{\alpha}_{ln} S^{\beta}_{l'n'}, \tag{1}$$

where $J^{\alpha,\beta}_{\boldsymbol{R}_l+\boldsymbol{\tau}_n,\boldsymbol{R}_{l'}+\boldsymbol{\tau}_{n'}}$, a 3×3 tensor, represents the spin exchange parameter. Here $\boldsymbol{R}_l$ and $\boldsymbol{\tau}_n$ represent the lattice translation vector and the position of magnetic ions in the lattice basis, while α and β denote the Cartesian components x, y or z. As a 3×3 real tensor, $\boldsymbol{J}_{\boldsymbol{R}_l+\boldsymbol{\tau}_n,\boldsymbol{R}_{l'}+\boldsymbol{\tau}_{n'}}$ could be expanded as three terms, and Eq. (1) could be written as

$$\begin{aligned} H = &\sum_{l,n,l',n'} J_{\boldsymbol{R}_l+\boldsymbol{\tau}_n,\boldsymbol{R}_{l'}+\boldsymbol{\tau}_{n'}} \boldsymbol{S}_{ln}\cdot\boldsymbol{S}_{l'n'} \\ &+ \sum_{l,n,l',n'} \boldsymbol{D}_{\boldsymbol{R}_l+\boldsymbol{\tau}_n,\boldsymbol{R}_{l'}+\boldsymbol{\tau}_{n'}}\cdot[\boldsymbol{S}_{ln}\times\boldsymbol{S}_{l'n'}] \\ &+ \sum_{l,n,l',n'} \boldsymbol{S}_{ln}\cdot\Gamma_{\boldsymbol{R}_l+\boldsymbol{\tau}_n,\boldsymbol{R}_{l'}+\boldsymbol{\tau}_{n'}}\cdot\boldsymbol{S}_{l'n'}. \end{aligned} \tag{2}$$

Here the first term describes the isotropic Heisenberg Hamiltonian with the scalar term $J_{\boldsymbol{R}_l+\boldsymbol{\tau}_n,\boldsymbol{R}_{l'}+\boldsymbol{\tau}_{n'}}$, the second one represents the antisymmetric Dzyaloshinskii–Moriya (DM) interactions with the vector term $\boldsymbol{D}_{\boldsymbol{R}_l+\boldsymbol{\tau}_n,\boldsymbol{R}_{l'}+\boldsymbol{\tau}_{n'}}$,[44,45] and the third one is the rest of anisotropic terms with the symmetric tensor term $\Gamma_{\boldsymbol{R}_l+\boldsymbol{\tau}_n,\boldsymbol{R}_{l'}+\boldsymbol{\tau}_{n'}}$.[45] DM interaction is often used to explain the interesting magnetic behaviors such as weak ferromagnets,[44,45] spin glasses,[46] and

skyrmion formation,[47] while the symmetric tensor Γ term also plays an important role in some magnetic systems.[48] It is commonly believed that the magnitude of the DM interaction and Γ term are proportional to spin-orbit coupling (SOC) strength λ and λ^2, respectively.[45] For materials with large λ, such as f electronic systems, multipolar interactions may become important,[49] and Eq. (1) may not be suitable. Meanwhile, it should be noted that Eq. (1) may also not be suitable for the case being orbitally degenerate.[50] Therefore, we restrict this work on the cases with small λ and then ignore the third term in Eq. (2), which is proportional to λ^2 in this study. It is worth pointing out that, using LSWT,[5] one can also take the Γ term into consideration through a scheme similar to our method shown below, and we will consider the effect of the symmetric tensor Γ term in future work. To take account for non-collinear cases, we use the polar angle θ_n and azimuthal angle ϕ_n for the spin orientation of magnetic ion at n site.

Following the LSWT,[5] we perform the Holstein–Primakoff transformation and the Fourier transformation, and Eq. (1) could be written as

$$\sum_{k} \psi^{\dagger}(\boldsymbol{k}) H(\boldsymbol{k}) \psi(\boldsymbol{k}), \tag{3}$$

with

$$\begin{aligned}\psi^{\dagger}(\boldsymbol{k}) = &[a_1^{\dagger}(\boldsymbol{k}), \ldots, a_i^{\dagger}(\boldsymbol{k}), \ldots, a_N^{\dagger}(\boldsymbol{k}),\\ &a_1(-\boldsymbol{k}), \ldots, a_i(-\boldsymbol{k}), \ldots, a_N(-\boldsymbol{k})],\end{aligned}$$

where $a_i^{\dagger}(\boldsymbol{k})$ and $a_i(\boldsymbol{k})$ represent the canonical boson creation and annihilation operators with wave vector $\boldsymbol{k}$ with i running from 1 to N, and N is the number magnetic ions per unit cells. The Hermitian matrix $H(\boldsymbol{k})$ in Eq. (3) is expressed as

$$H(\boldsymbol{k}) = \begin{bmatrix} h(\boldsymbol{k}) & h'(\boldsymbol{k}) \\ h'(\boldsymbol{k})^{\dagger} & h(-\boldsymbol{k})^{\top} \end{bmatrix}. \tag{4}$$

Here $h(\boldsymbol{k})$ and $h'(\boldsymbol{k})$ can be expressed as

$$\begin{aligned} h(\boldsymbol{k})_{n,n'} =& \sum_{l} S(A_{n,n'} J_{\boldsymbol{\tau}_n, \boldsymbol{\tau}_{n'}+\boldsymbol{R}_l} + \boldsymbol{O}_{n,n'} \cdot \boldsymbol{D}_{\boldsymbol{\tau}_n, \boldsymbol{\tau}_{n'}+\boldsymbol{R}_l}) \\ &\cdot e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l} - \delta_{n,n'} \sum_{l,n''} S(B_{n,n''} J_{\boldsymbol{\tau}_n, \boldsymbol{\tau}_{n''}+\boldsymbol{R}_l} \\ &+ \boldsymbol{P}_{n,n''} \cdot \boldsymbol{D}_{\boldsymbol{\tau}_n, \boldsymbol{\tau}_{n''}+\boldsymbol{R}_l}), \\ h'(\boldsymbol{k})_{n,n'} =& \sum_{l} S(C_{n,n'} J_{\boldsymbol{\tau}_n, \boldsymbol{\tau}_{n'}+\boldsymbol{R}_l} + \boldsymbol{Q}_{n,n'} \cdot \boldsymbol{D}_{\boldsymbol{\tau}_n, \boldsymbol{\tau}_{n'}+\boldsymbol{R}_l}) \\ &\cdot e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l}, \end{aligned} \tag{5}$$

where $\delta_{n,n'}$ is the Kronecker delta function, while $A_{n,n'}$, $B_{n,n'}$, $C_{n,n'}$, $\boldsymbol{O}_{n,n'}$, $\boldsymbol{P}_{n,n'}$ and $\boldsymbol{Q}_{n,n'}$ are the parameters related to the spin directions at n and n' sites [see the Supplemental Materials (SM) for details].

Considering the commutation relation of $\psi(\boldsymbol{k})$ and $\psi^{\dagger}(\boldsymbol{k})$, we need perform the following transformation (see the SM for details):

$$H_J(\boldsymbol{k}) = I_{-} H(\boldsymbol{k}). \tag{6}$$

Through numerically diagonalizing the $H_J(\boldsymbol{k})$ in Eq. (6), we can obtain the magnon energies $\omega_i(\boldsymbol{k})(i = 1, \ldots, N)$ at wave vector k. In contrary without diagonalization, SSME can be analytically expressed as

$$\begin{aligned} \sum_i \omega_i^2(\boldsymbol{k}) =& \frac{1}{2}\mathrm{Tr}([H_J(\boldsymbol{k})]^2) \\ =& \frac{1}{2}\mathrm{Tr}[h^2(\boldsymbol{k}) + h^2(-\boldsymbol{k})^{\top} - h'(\boldsymbol{k})h'(\boldsymbol{k})^{\dagger} \\ &- h'(\boldsymbol{k})^{\dagger}h'(\boldsymbol{k})]. \end{aligned} \tag{7}$$

As shown in Eq. (5), $h(\boldsymbol{k})$ and $h'(\boldsymbol{k})$ basically depend on the orientation of magnetic moments and the Fourier transformation of MEIs $\boldsymbol{J}_{\boldsymbol{R}_l+\boldsymbol{\tau}_n, \boldsymbol{R}_{l'}+\boldsymbol{\tau}_{n'}}$ and $\boldsymbol{D}_{\boldsymbol{R}_l+\boldsymbol{\tau}_n, \boldsymbol{R}_{l'}+\boldsymbol{\tau}_{n'}}$. Thus, for arbitrary k, $\sum_i \omega_i^2(\boldsymbol{k})$ can be expressed by a quadratic polynomial of MEIs. With the assumption of R_{cut}, which is related with how many MEIs have been considered, one can obtain simple relationships between SSMEs at different wave vectors k.

Results and Discussion. We illustrate the usage of our results by the following typical example. Without loss of generality, we choose space group $P4/n$ (SG 85) to present our discussion and set the ratio between lattice constant c/a as 0.8. We put the magnetic ions at three nonequivalent crystallographic sites: $4d$ (0, 0, 0), $2a$ (0.25, 0.75, 0) and $2c$ (0.25, 0.25, z) Wyckoff positions (WPs), as summarized in Table 1. While the $4d$ and $2a$ WPs have been completely determined by the spatial symmetry, the coordinates of $2c$ WP have a variable z and here we adopt it as $z = 0.1$. There are two generators for this space group: the four-fold rotation $\{4^{+}_{001}|1/2, 0, 0\}$ and inversion operation $\{\bar{1}|0, 0, 0\}$, where the left part represents the rotation, the right part means the lattice translation, and $\bar{1}$ denotes the inversion symmetry. We firstly consider the most simple case: the isotropic Heisenberg model with all the spins along z. Considering the orientations of the magnetic moments, the space group could be divided into four types of magnetic space groups. The case with this collinear ferromagnetic (FM) ordering belongs to the type-I magnetic space group (BNS 85.59), and its magnetic configuration does not reduce the spatial symmetry. Since all the spins along z direction, polar angle θ_n and azimuthal angle ϕ_n are equal to 0 as listed in Table 1, thus according to Eqs. (21)–(23) in the SM, the parameters $A_{n,n'}$, $B_{n,n'}$ and $C_{n,n'}$ in Eq. (5) for this collinear FM state becomes 1, 1 and 0, respectively. Consequently, the SSME at wave vec-

tor k could be written as

$$\sum_i \omega_i^2(\boldsymbol{k}) = \frac{1}{2}\mathrm{Tr}([H_J(\boldsymbol{k})]^2)$$
$$= S^2 \sum_{n\neq n',l,l'} J_{\boldsymbol{\tau}_n,\boldsymbol{\tau}_{n'}+\boldsymbol{R}_{l'}} J_{\boldsymbol{\tau}_n,\boldsymbol{\tau}_{n'}+\boldsymbol{R}_l} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_l-\boldsymbol{R}_{l'})}$$
$$+ S^2 \sum_n \Big[\sum_{n'',l} J_{\boldsymbol{\tau}_n,\boldsymbol{\tau}_{n''}+\boldsymbol{R}_l} + \sum_l J_{\boldsymbol{\tau}_n,\boldsymbol{\tau}_n+\boldsymbol{R}_l} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l}\Big]^2. \quad (8)$$

Table 1. The WPs and the coordinates of the 8 magnetic ions in the conventional unit cell basis vectors for the example shown here. The Wyckoff positions are labeled in the space group P4/n (SG 85). The polar angles θ_n and azimuthal angles ϕ_n of these magnetic ions in our selected collinear and non-collinear states are also provided.

WP	n	τ_n	(θ_n, ϕ_n)	
			Collinear	Non-collinear
$4d$	1	(0, 0, 0)	(0,0)	$(\theta, \pi/2)$
	2	(0.5, 0, 0)	(0,0)	$(\theta, -\pi/2)$
	3	(0, 0.5, 0)	(0,0)	$(\theta, \pi/2)$
	4	(0.5, 0.5, 0)	(0,0)	$(\theta, -\pi/2)$
$2a$	5	(0.75, 0.25, 0)	(0,0)	(0,0)
	6	(0.25, 0.75, 0)	(0,0)	(0,0)
$2c$	7	(0.25, 0.25, 0.1)	(0,0)	(0,0)
	8	(0.75, 0.75, −0.1)	(0,0)	(0,0)

As shown in the above formula, the key for SSME is the exchange path between magnetic ions $\boldsymbol{\tau}_n$ and $\boldsymbol{\tau}_{n'} + \boldsymbol{R}_{l'}$, and the related MEI $J_{\boldsymbol{\tau}_n,\boldsymbol{\tau}_{n'}+\boldsymbol{R}_{l'}}$. As shown in the right part of Table 1 in the SM, the first and second nearest neighbors have similar distances ($0.35a$ vs $0.36a$, a is the lattice parameter). Crystal symmetry imposes strong restrictions on the MEIs as shown in the SM, and according to the spatial symmetry in this space group, all the first nearest neighbor exchange paths have the same MEI value, and we denotes it as J_1, similarly we can label all the second nearest neighbor MEI as J_2. Considering only the first two NN interactions J_1 and J_2, the term of $J_{\boldsymbol{\tau}_n,\boldsymbol{\tau}_n+\boldsymbol{R}_l}$ does not exist, and only the k dependence of SSME comes from the first term in Eq. (8). Namely, we need to check the non-zero MEIs $J_{\boldsymbol{\tau}_n,\boldsymbol{\tau}_{n'}+\boldsymbol{R}_{l'}}$ and $J_{\boldsymbol{\tau}_n,\boldsymbol{\tau}_{n'}+\boldsymbol{R}_l}$, with the requirement of $\boldsymbol{R}_l \neq \boldsymbol{R}_{l'}$. As clearly shown in the right part of Table 1 in the SM, such a kind of exchange path also does not exist. Thus, although spin wave has dispersion at the entire BZ, we get a surprisingly simple result of $\sum_i \omega_i^2(\boldsymbol{k}) = C$ with considering only J_1 and J_2.

We further take into account the impact of longer-ranged exchange paths. With the third NN MEI J_3 being considered, there exist more than one exchange paths connect a pair of $\boldsymbol{\tau}_n$ and $\boldsymbol{\tau}_{n'} + \boldsymbol{R}_l$. For example, both $\boldsymbol{\tau}_1, \boldsymbol{\tau}_2$ pair and $\boldsymbol{\tau}_1, \boldsymbol{\tau}_2 + \boldsymbol{R}_{-100}$ pair belong to J_3 exchange path as shown in Table 1 of the SM. As a result, $\sum_i \omega_i^2(\boldsymbol{k})$ is no longer equal to constant. Thus, if the observed SSME shows very weak k dependence, one can asserts that the MEIs beyond J_2 are ignorable. Since for the high symmetry k points at BZ, $e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_l-\boldsymbol{R}_{l'})}$ usually has simple values (equal to ± 1 in this magnetic system), one can expect simple relation between SSME at these k points. We indeed get several simple relationships with the MEIs up to J_3: $\sum_i \omega_i^2(\Gamma) = \sum_i \omega_i^2(Z)$, $\sum_i \omega_i^2(X) = \sum_i \omega_i^2(R)$, $\sum_i \omega_i^2(M) = \sum_i \omega_i^2(A)$ and $2\sum_i \omega_i^2(X) = \sum_i \omega_i^2(\Gamma) + \sum_i \omega_i^2(M)$. It is interesting to see that these four simple relations about SSME remains after including the fourth nearest neighbor MEI J_4. The algorithm about SSME is simple, which allows us quickly analyze the effect of considering further MEI. We summarize the results in Table 2. Using the measured magnon energies at only six high-symmetry k points, one can unambiguous determine the real-space range within which the MEI is considerable based on Table 2.

Table 2. The obtained SSME relationship of the collinear FM example shown here (i.e., the case with BNS 85.59). The first column J_x represents up to the x-th NN MEI. The coordinates of six high-symmetry k points: $\Gamma(0,0,0)$, $X(\frac{1}{2},0,0)$, $M(\frac{1}{2},\frac{1}{2},0)$, $Z(0,0,\frac{1}{2})$, $R(\frac{1}{2},0,\frac{1}{2})$, and $A(\frac{1}{2},\frac{1}{2},\frac{1}{2})$.

$J_{\max}$	Relation
J_2	$\sum_i \omega_i^2(k) = C$
J_4	$\sum_i \omega_i^2(\Gamma) = \sum_i \omega_i^2(Z)$ $\sum_i \omega_i^2(X) = \sum_i \omega_i^2(R)$ $\sum_i \omega_i^2(M) = \sum_i \omega_i^2(A)$ $2\sum_i \omega_i^2(X) = \sum_i \omega_i^2(\Gamma) + \sum_i \omega_i^2(M)$
J_{12}	$\sum_i \omega_i^2(\Gamma) = \sum_i \omega_i^2(Z)$ $\sum_i \omega_i^2(X) = \sum_i \omega_i^2(R)$ $\sum_i \omega_i^2(M) = \sum_i \omega_i^2(A)$
J_{15}	$\sum_i \omega_i^2(\Gamma) - \sum_i \omega_i^2(Z) = \sum_i \omega_i^2(X) - \sum_i \omega_i^2(R) = \sum_i \omega_i^2(M) - \sum_i \omega_i^2(A)$
J_{22}	$2\sum_i \omega_i^2(X) - \sum_i \omega_i^2(\Gamma) - \sum_i \omega_i^2(M) = 2\sum_i \omega_i^2(R) - \sum_i \omega_i^2(Z) - \sum_i \omega_i^2(A)$

After collinear FM configuration, we now illustrate the applications for the non-collinear case. We still use the crystal structure mentioned above and fix the magnetic moments at $2a$ and $2c$ WPs still along z direction. While the azimuthal angle ϕ for magnetic moments at $4d$ WP is $\pm\pi$, we assume their polar angles as a free parameter θ as shown in Table 1. Although an isotropic Heisenberg Hamiltonian may not produce the above non-collinearity, we still use it to demonstrate our method and show the discussion about

anisotropic spin model later. This non-collinear magnetic state belongs to the type-I magnetic space group BNS 13.65. While the inversion symmetry $\{\bar{1}|0,0,0\}$ are maintained, the deviation from z direction reduces the four-fold rotation symmetry $\{4^+_{001}|1/2,0,0\}$ to the two-fold rotation operation $\{2_{001}|1/2,1/2,0\}$. As a result, many symmetry-related exchange paths in collinear spin ordering case become inequivalent. For example, as shown in Table 1 of the SM, the eight first NN exchange paths in collinear spin ordering are no longer equivalent and divided into two groups, which are labeled as J_1 and J_2 for this non-collinear magnetic case. The parameters in Eq. (5) are also dependent on the magnetic moment directions, thus non-collinearity results in different relationships between SSMEs, which are listed in Table 3. We also want to mention that for the localized magnetic systems, the MEIs should not be sensitive to the magnetic configurations. For such cases, one can still use the symmetry operations in collinear instead of in the non-collinear case to determine equivalent exchange path. Namely, if this non-collinear magnetism is very localized, the MEIs will still approximately satisfy the relation of the right part in Table 1 of the SM instead of the left part. Based on this consideration, we apply our method to this non-collinear case with localized magnetism and list the results in the right part of Table 3. As shown in Table 3, the free parameter θ about directions of the magnetic moments explicitly appear in the relationship about SSMEs. Thus, for localized non-collinear magnetic materials, one may determine the magnetic moments directions based on the magnon energies at three wave vectors (i.e., Γ, X and M) in the case that MEIs further than J_3 are ignorable.

Table 3. The obtained results about SSME for the non-collinear case shown in this work (i.e., the case with symmetry of BNS 13.65). We also give the result for the same non-collinear configuration with the magnetism localized in the right part. For the localized magnetism case, the MEIs are not sensitive to the spin ordering, thus one can use the symmetry of SG 85 to determine if the exchange paths have the same MEIs, namely use the results given in the right part of Table 1 in the SM. The x in J_x still represents up to the x-th NN MEI, and the coordinations of six high-symmetry points have been shown in Table 2.

$J_{\max}$	Relation	$J_{\max}$	Relation
J_4	$\sum_i \omega_i^2(k) = C$	J_2	$\sum_i \omega_i^2(k) = C$
J_5	$\sum_i \omega_i^2(\Gamma) = \sum_i \omega_i^2(Z)$ $\sum_i \omega_i^2(X) = \sum_i \omega_i^2(R) = \sum_i \omega_i^2(M) = \sum_i \omega_i^2(A)$	J_3	$\sum_i \omega_i^2(\Gamma) = \sum_i \omega_i^2(Z)$ $\sum_i \omega_i^2(X) = \sum_i \omega_i^2(R)$ $\sum_i \omega_i^2(M) = \sum_i \omega_i^2(A)$ $[1+\cos(2\theta)]\sum_i \omega_i^2(X) = \omega_i^2(\Gamma) + \cos(2\theta)\sum_i \omega_i^2(M)$
J_{24}	$\sum_i \omega_i^2(\Gamma) = \sum_i \omega_i^2(Z)$ $\sum_i \omega_i^2(X) = \sum_i \omega_i^2(R)$ $\sum_i \omega_i^2(M) = \sum_i \omega_i^2(A)$	J_{12}	$\sum_i \omega_i^2(\Gamma) = \sum_i \omega_i^2(Z)$ $\sum_i \omega_i^2(X) = \sum_i \omega_i^2(R)$ $\sum_i \omega_i^2(M) = \sum_i \omega_i^2(A)$
J_{28}	$\sum_i \omega_i^2(\Gamma) - \sum_i \omega_i^2(Z) = \sum_i \omega_i^2(X) - \sum_i \omega_i^2(R)$ $= \sum_i \omega_i^2(M) - \sum_i \omega_i^2(A)$	J_{15}	$\sum_i \omega_i^2(\Gamma) - \sum_i \omega_i^2(Z) = \sum_i \omega_i^2(X) - \sum_i \omega_i^2(R)$ $= \sum_i \omega_i^2(M) - \sum_i \omega_i^2(A)$
		J_{19}	$2\sum_i \omega_i^2(X) - \sum_i \omega_i^2(\Gamma) - \sum_i \omega_i^2(M)$ $= 2\sum_i \omega_i^2(R) - \sum_i \omega_i^2(Z) - \sum_i \omega_i^2(A)$

It is worth mentioning that our method is also valid for the materials with considerable DM interactions.[44,45] One can still calculate SSME by Eq. (7) and directly use the example program provided in the SM to explore the relationship between them. The magnetic anisotropy may also come from the SIA.[1–3] With the SIA considered, the Hamiltonian becomes $H_{\text{total}} = H + H_{\text{SIA}}$, where H is the term shown in Eq. (2) while H_{SIA} represents the term of SIA. Here we adopt a popular form $H_{\text{SIA}} = \sum_{l,n} K(S^z_{ln})^2$,[3] with K being the strength of SIA. Based on the standard LSWT, one can easily obtain the spin Hamiltonian at arbitrary wave vector k to be $H_{\text{total}}(k) = H_J(k) + 2SKI_-$. Adding the SIA term into the case of the Heisenberg model with collinear FM magnetic ordering given in this work, the SSME could be written as

$$\begin{aligned}\sum_i \omega_i^2(\boldsymbol{k}) =& \frac{1}{2}\text{Tr}[[H_{\text{total}}(\boldsymbol{k})]^2] \\ =& \frac{1}{2}\text{Tr}[[H_J(\boldsymbol{k})]^2] + 4NS^2K^2 + 4S^2K \\ & \cdot \sum_n \Big[\sum_{n'',l} J_{\boldsymbol{\tau}_n,\boldsymbol{\tau}_{n''}+\boldsymbol{R}_l} + \sum_l J_{\boldsymbol{\tau}_n,\boldsymbol{\tau}_n+\boldsymbol{R}_l} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l}\Big]. \end{aligned} \tag{9}$$

Based on Eq. (9), one can easily prove that including SIA will not affect the results given in Table 2.

In summary, an appropriate magnetic model play a crucial role in investigating various magnetic properties. Unfortunately the current methods for extracting MEIs face a severe limitation about how many MEIs need to be included in the spin Hamiltonian. In this work, we circumvent this methodological bottleneck by noticing that for quadratic spin Hamiltonian, there is a simple connection between SSME and the considered MEIs. Namely, there is R_{cut}-related relationship between SSME at high-symmetry points. By efficient measurements of magnon energies only at several high-symmetry k points, one can check up to which the experimental SSME R_{cut} starts to devi-

ate from the obtained $R_{\rm cut}$-related results, and subsequently determine the real-space range beyond which MEIs can be safely neglected. For the localized non-collinear magnetic systems, our results may also be used to determine the directions of magnetization. We also provide an example program, directly utilizing it, one can get the relationship of SSME for the typical magnetic model in this study. Meanwhile, one can easily extend our method to other magnetic systems described by Hamiltonian with pairwise spin based on our example code. Besides the well used symmetry analysis for the symmetry-related k points, we expect that similar generic $R_{\rm cut}$-sensitive results also exist in other Hamiltonians with only quadratic Fermi or boson operators.

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Supplemental Materials for "Determining the range of magnetic interactions from the relations between magnon eigenvalues at high-symmetry k points"

Di Wang(王棣),[1,2] Jihai Yu(于济海),[1,2] Feng Tang(唐峰),[1,2] Yuan Li(李源),[3,4] and Xiangang Wan(万贤纲)[1,2,*]

[1] *National Laboratory of Solid State Microstructures and School of Physics, Nanjing University, Nanjing 210093, China*
[2] *Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China*
[3] *International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China*
[4] *Collaborative Innovation Center of Quantum Matter, Beijing 100871, China*

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A. The symmetry restrictions on the magnetic interactions

As mentioned in the maintext, the microscopic magnetic model with proper parameters is extremely important. Note that the crystal symmetry impose restrictions on the magnetic model and its parameters. Here we consider a general pairwise spin model as shown in the maintext

$$H = \sum_{l,n,l',n'} \mathbf{S}_{ln} \cdot \mathbf{J}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}} \cdot \mathbf{S}_{l'n'} \tag{1}$$

where $\mathbf{J}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}}$, a 3×3 tensor, represents the spin exchange parameters. R_l and τ_n represent the lattice translation vector and the position of magnetic ions in the lattice basis, and $\mathbf{S}_{l'n'}$ means the spin at the site of $\mathbf{R}_l+\boldsymbol{\tau}_n$ Translation symmetry will restrict $\mathbf{J}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}}$ to be only related to $\mathbf{J}_{\boldsymbol{\tau}_n,\boldsymbol{\tau}_{\boldsymbol{n}'}+\mathbf{R}_{l''}}$ where $R_{l''} = R_{l'} - R_l$, irrespective of the starting unit cell. Other spatial symmetries will also give restrictions on the magnetic exchange interactions (MEIs). We consider a general space group element $\{\alpha|\mathbf{t}\}$, where the left part represents the rotation and the right part means the lattice translation. Supposing under this symmetry operator, $\mathbf{R}_m+\boldsymbol{\tau}_p$ and $\mathbf{R}_{m'}+\boldsymbol{\tau}_{\boldsymbol{p}'}$ transfer to $\mathbf{R}_l+\boldsymbol{\tau}_n$ and $\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}$, respectively, meanwhile the transformation of spin becomes $\mathbf{S}_{mp} = M(\alpha)\mathbf{S}_{ln}$, where $M(\alpha)$ is the representation matrix of the proper rotation part of the operation α in the coordinate system, we get the following expression:

$$\begin{aligned} H &= \sum_{l,n,l',n'} \mathbf{S}_{ln} \cdot \mathbf{J}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}} \cdot \mathbf{S}_{l'n'} \\ &= \sum_{l,n,l',n'} \mathbf{S}_{ln} M^\dagger(\alpha)M(\alpha)\mathbf{J}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}} M^\dagger(\alpha)M(\alpha)\mathbf{S}_{l'n'} \\ &= \sum_{m,p,m',p'} \mathbf{S}_{mp} \cdot M(\alpha)\mathbf{J}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}} M^\dagger(\alpha) \cdot \mathbf{S}_{m'p'} \end{aligned} \tag{2}$$

Then the exchange interactions should satisfy the following condition:

$$\mathbf{J}_{\mathbf{R}_m+\boldsymbol{\tau}_p,\mathbf{R}_{m'}+\boldsymbol{\tau}_{\boldsymbol{p}'}} = M(\alpha)\mathbf{J}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}} M^\dagger(\alpha) \tag{3}$$

After decomposing the 3×3 tensor $\mathbf{J}$ into scalar Heisenberg term J and vector DM term D as in the maintext, we obtain the following results:

$$\begin{aligned} J_{\mathbf{R}_m+\boldsymbol{\tau}_p,\mathbf{R}_{m'}+\boldsymbol{\tau}_{\boldsymbol{p}'}} &= J_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}} \\ \mathbf{D}_{\mathbf{R}_m+\boldsymbol{\tau}_p,\mathbf{R}_{m'}+\boldsymbol{\tau}_{\boldsymbol{p}'}} &= M(\alpha)\mathbf{D}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}} \end{aligned} \tag{4}$$

Meanwhile, it is should be noted that the Heisenberg and DM interactions obey the following commutation relations

$$\begin{aligned} J_{\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'},\mathbf{R}_l+\boldsymbol{\tau}_n} &= J_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}} \\ \mathbf{D}_{\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'},\mathbf{R}_l+\boldsymbol{\tau}_n} &= -\mathbf{D}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n}'}} \end{aligned} \tag{5}$$

According to the above equations (i.e. Eq. (4) and (5)), one can obtain the symmetry restricted MEIs for any space group. Similarly, for the magnetic space group, the symmetry restriction on MEIs can also be easily obtained. The collinear ferromagnetic system shown in maintext (i.e. BNS 85.59 case) have two generators: the four-fold rotation $\{4^+_{001}|1/2,0,0\}$ and inversion operation $\{\bar{1}|0,0,0\}$. The magnetic ion located at τ_1 position has only two nearest neighbors, i.e. $(\boldsymbol{\tau}_1, \boldsymbol{\tau}_5+\mathbf{R}_{-100})$ pair and $(\boldsymbol{\tau}_1, \boldsymbol{\tau}_6+\mathbf{R}_{0-10})$ pair as shown in Table I. These two bonds are equivalent by the inversion symmetry $\{\bar{1}|0,0,0\}$. Meanwhile, performing the four-fold rotation symmetry for the above two pairs, we can get other six pairs in a unit cell, and there are in total eight NN in a unit cell. Based on Eq. (4), it is also easy to prove all of these eight NN exchange paths has the same Heisenberg term, which we denote as J_1 as shown in Table I. The non-collinearity shown in maintext reduces the four-fold rotation $\{4^+_{001}|1/2,0,0\}$ to the two-fold rotation operation $\{2_{001}|1/2,1/2,0\}$, as a result the eight NN exchange path is no longer equivalent as indicated in Table I. Similarly, one can obtain the symmetry restriction on the DM interactions, as also shown in Table I.

For simplicity, we only list the corresponding MEIs for longer range with the collinear FM example (i.e. the case with symmetry of BNS 85.59) and non-collinear example

* The corresponding author: xgwan@nju.edu.cn.

TABLE I. The distances and the bond information of corresponding MEIs (with $R_{cut} = 0.5\ a$) for the non-collinear magnetic example in the maintext (i.e. the case with symmetry of BNS 13.65). We also list the results by using the symmetry of BNS 85.59, which is applicable for the collinear FM case as well as the non-collinear case with localized magnetism in the right part.

distance(a)	n	n'	R_l	BNS 13.65		BNS 85.59	
0.35	1	5	$(-1,0,0)$	J_1	(D_1^x, D_1^y, D_1^z)	J_1	(D_1^x, D_1^y, D_1^z)
	1	6	$(0,-1,0)$	J_1	(D_1^x, D_1^y, D_1^z)	J_1	(D_1^x, D_1^y, D_1^z)
	2	5	$(0,0,0)$	J_2	(D_2^x, D_2^y, D_2^z)	J_1	$(-D_1^y, D_1^x, D_1^z)$
	2	6	$(0,-1,0)$	J_2	(D_2^x, D_2^y, D_2^z)	J_1	$(-D_1^y, D_1^x, D_1^z)$
	3	5	$(-1,0,0)$	J_2	$(-D_2^x, -D_2^y, D_2^z)$	J_1	$(D_1^y, -D_1^x, D_1^z)$
	3	6	$(0,0,0)$	J_2	$(-D_2^x, -D_2^y, D_2^z)$	J_1	$(D_1^y, -D_1^x, D_1^z)$
	4	5	$(0,0,0)$	J_1	$(-D_1^x, -D_1^y, D_1^z)$	J_1	$(-D_1^x, -D_1^y, D_1^z)$
	4	6	$(0,0,0)$	J_1	$(-D_1^x, -D_1^y, D_1^z)$	J_1	$(-D_1^x, -D_1^y, D_1^z)$
0.36	1	7	$(0,0,0)$	J_3	(D_3^x, D_3^y, D_3^z)	J_2	(D_2^x, D_2^y, D_2^z)
	1	8	$(-1,-1,0)$	J_3	(D_3^x, D_3^y, D_3^z)	J_2	(D_2^x, D_2^y, D_2^z)
	2	7	$(0,0,0)$	J_4	(D_4^x, D_4^y, D_4^z)	J_2	$(-D_2^y, D_2^x, D_2^z)$
	2	8	$(0,-1,0)$	J_4	(D_4^x, D_4^y, D_4^z)	J_2	$(-D_2^y, D_2^x, D_2^z)$
	3	7	$(0,0,0)$	J_4	$(-D_4^x, -D_4^y, D_4^z)$	J_2	$(D_2^y, -D_2^x, D_2^z)$
	3	8	$(-1,0,0)$	J_4	$(-D_4^x, -D_4^y, D_4^z)$	J_2	$(D_2^y, -D_2^x, D_2^z)$
	4	7	$(0,0,0)$	J_3	$(-D_3^x, -D_3^y, D_3^z)$	J_2	$(-D_2^x, -D_2^y, D_2^z)$
	4	8	$(0,0,0)$	J_3	$(-D_3^x, -D_3^y, D_3^z)$	J_2	$(-D_2^x, -D_2^y, D_2^z)$
0.5	1	2	$(0,0,0)$	J_5	(D_5^x, D_5^y, D_5^z)	J_3	(D_3^x, D_3^y, D_3^z)
	1	2	$(-1,0,0)$	J_5	(D_5^x, D_5^y, D_5^z)	J_3	(D_3^x, D_3^y, D_3^z)
	1	3	$(0,0,0)$	J_6	(D_6^x, D_6^y, D_6^z)	J_3	$(-D_3^y, D_3^x, -D_3^z)$
	1	3	$(0,-1,0)$	J_6	(D_6^x, D_6^y, D_6^z)	J_3	$(-D_3^y, D_3^x, -D_3^z)$
	2	4	$(0,0,0)$	J_6	$(D_6^x, D_6^y, -D_6^z)$	J_3	$(-D_3^y, D_3^x, D_3^z)$
	2	4	$(0,-1,0)$	J_6	$(D_6^x, D_6^y, -D_6^z)$	J_3	$(-D_3^y, D_3^x, D_3^z)$
	3	4	$(0,0,0)$	J_5	$(D_5^x, D_5^y, -D_5^z)$	J_3	$(D_3^x, D_3^y, -D_3^z)$
	3	4	$(-1,0,0)$	J_5	$(D_5^x, D_5^y, -D_5^z)$	J_3	$(D_3^x, D_3^y, -D_3^z)$

TABLE II. The corresponding MEIs for the collinear FM example (i.e. the case with symmetry of BNS 85.59) and non-collinear example (i.e. the case with symmetry of BNS 13.65) shown in maintext.

BNS 85.59	BNS 13.65
J_1	J_1, J_2
J_2	J_3, J_4
J_3	J_5, J_6
J_4	J_7, J_8
J_5~J_7	J_9~J_{14}
J_8	J_{15}, J_{16}
J_9, J_{10}	J_{17}~J_{20}
J_{11}, J_{12}	J_{21}~J_{24}
J_{13}~J_{15}	J_{25}~J_{28}
J_{16}	J_{29}, J_{30}
J_{17}, J_{18}	J_{32}~J_{34}
J_{19}	J_{35}, J_{36}
J_{20}, J_{21}	J_{37}~J_{40}
J_{22}	J_{41}, J_{42}
J_{23}	J_{43}, J_{44}
J_{24}~J_{27}	J_{45}~J_{52}

in the maintext (i.e. the case with symmetry of BNS 13.65), as shown in Table II.

It is worth mentioning that Eq. (3) can also give symmetry restrictions on SIA. The general quadratic expression of SIA could be written as $\sum_{l,n,\alpha,\beta} K^{\alpha,\beta}_{\mathbf{R}_l+\boldsymbol{\tau}_n} S^{\alpha}_{ln} S^{\beta}_{ln}$. Note that the SIA term should be naturally symmetric, i.e. $K^{\alpha,\beta}_{\mathbf{R}_l+\boldsymbol{\tau}_n} = K^{\beta,\alpha}_{\mathbf{R}_l+\boldsymbol{\tau}_n}$. According to Eq. (3), when the action of symmetry operation $\{\alpha|t\}$ keeps the position $R_l + \tau_n$ unchanged, we have $K_{\mathbf{R}_l+\boldsymbol{\tau}_n} = M(\alpha) K_{\mathbf{R}_l+\boldsymbol{\tau}_n} M^{\dagger}(\alpha)$. For the typical FM collinear magnetic material (BNS 85.59) in the maintext, the SIA term for magnetic ions located at $2a$ and $2c$ Wyckoff positions should satisfy that

$$K_{\mathbf{R}_l+\boldsymbol{\tau}_n} = \begin{bmatrix} K^{xx}_{\mathbf{R}_l+\boldsymbol{\tau}_n} & & \\ & K^{xx}_{\mathbf{R}_l+\boldsymbol{\tau}_n} & \\ & & K^{zz}_{\mathbf{R}_l+\boldsymbol{\tau}_n} \end{bmatrix}$$

which is actually the usual form $H_{SIA} = \sum_{l,n} K_{\mathbf{R}_l+\boldsymbol{\tau}_n} (S^z_{ln})^2 + C$ where $K_{\mathbf{R}_l+\boldsymbol{\tau}_n} = K^{zz}_{\mathbf{R}_l+\boldsymbol{\tau}_n} - K^{xx}_{\mathbf{R}_l+\boldsymbol{\tau}_n}$ and C represents the constant term. However, the symmetry does not give restrictions on the SIA term of magnetic ions at $4d$ position. In the maintext, we adopt the usual form $H_{SIA} = \sum_{l,n} K (S^z_{ln})^2$ for simplicity.

B. The parameters $A_{n,n'}$, $B_{n,n'}$, $C_{n,n'}$, $\mathbf{O}_{n,n'}$, $\mathbf{P}_{n,n'}$ and $\mathbf{Q}_{n,n'}$

In the maintext, considering the spin model including the Heisenberg and DM interactions, we perform the standard LSWT and obtain spin Hamiltonian as Eq. (4) in the maintext, where the parameters $A_{n,n'}$, $B_{n,n'}$, $C_{n,n'}$, $\mathbf{O}_{n,n'}$, $\mathbf{P}_{n,n'}$ and $\mathbf{Q}_{n,n'}$ are related to the spin directions at n and n' sites. Here $A_{n,n'}$, $B_{n,n'}$ and $C_{n,n'}$

could be written as:

$$\begin{aligned}A_{n,n'} = &\frac{1}{4}\cos(\theta_n-\theta_{n'})-\frac{1}{4}\cos(\theta_n+\theta_{n'})+\frac{1}{2}\cos(\phi_n-\phi_{n'})\\&+\frac{1}{8}\cos(\theta_n-\theta_{n'}+\phi_n-\phi_{n'})\\&+\frac{1}{8}\cos(\theta_n+\theta_{n'}+\phi_n-\phi_{n'})\\&+\frac{1}{8}\cos(\theta_n-\theta_{n'}-\phi_n+\phi_{n'})\\&+\frac{1}{8}\cos(\theta_n+\theta_{n'}-\phi_n+\phi_{n'})\\&+\frac{i}{4}\sin(\theta_n+\phi_n-\phi_{n'})+\frac{i}{4}\sin(\theta_{n'}+\phi_n-\phi_{n'})\\&-\frac{i}{4}\sin(\theta_n-\phi_n+\phi_{n'})-\frac{i}{4}\sin(\theta_{n'}-\phi_n+\phi_{n'})\end{aligned}\quad(6)$$

$$B_{n,n'} = \sin\theta_n\sin\theta_{n'}\cos(\phi_n-\phi_{n'})+\cos\theta_n\cos\theta_{n'}\quad(7)$$

$$\begin{aligned}C_{n,n'} = &\frac{1}{4}\cos(\theta_n-\theta_{n'})-\frac{1}{4}\cos(\theta_n+\theta_{n'})-\frac{1}{2}\cos(\phi_n-\phi_{n'})\\&+\frac{1}{8}\cos(\theta_n-\theta_{n'}+\phi_n-\phi_{n'})\\&+\frac{1}{8}\cos(\theta_n+\theta_{n'}+\phi_n-\phi_{n'})\\&+\frac{1}{8}\cos(\theta_n-\theta_{n'}-\phi_n+\phi_{n'})\\&+\frac{1}{8}\cos(\theta_n+\theta_{n'}-\phi_n+\phi_{n'})\\&-\frac{i}{4}\sin(\theta_n+\phi_n-\phi_{n'})+\frac{i}{4}\sin(\theta_{n'}+\phi_n-\phi_{n'})\\&+\frac{i}{4}\sin(\theta_n-\phi_n+\phi_{n'})-\frac{i}{4}\sin(\theta_{n'}-\phi_n+\phi_{n'})\end{aligned}\quad(8)$$

Meanwhile, the parameters $\mathbf{O}_{n,n'} = (O^x_{n,n'}, O^y_{n,n'}, O^z_{n,n'})$, $\mathbf{P}_{n,n'} = (P^x_{n,n'}, P^y_{n,n'}, P^z_{n,n'})$ and $\mathbf{Q}_{n,n'} = (Q^x_{n,n'}, Q^y_{n,n'}, Q^z_{n,n'})$ related to the spin directions at n and n' sites could be written as:

$$\begin{aligned}O^x_{n,n'} = &\frac{1}{2}[-\cos\theta_n\sin\theta_{n'}\sin\phi_n+\sin\theta_n\cos\theta_{n'}\sin\phi_{n'}\\&+i(\sin\theta_n\cos\phi_{n'}+\sin\theta_{n'}\cos\phi_n)]\end{aligned}\quad(9)$$

$$P^x_{n,n'} = \sin\theta_n\cos\theta_{n'}\sin\phi_n-\cos\theta_n\sin\theta_{n'}\sin\phi_{n'}\quad(10)$$

$$\begin{aligned}Q^x_{n,n'} = &\frac{1}{2}[-\cos\theta_n\sin\theta_{n'}\sin\phi_n+\sin\theta_n\cos\theta_{n'}\sin\phi_{n'}\\&+i(\sin\theta_n\cos\phi_{n'}-\sin\theta_{n'}\cos\phi_n)]\end{aligned}\quad(11)$$

$$\begin{aligned}O^y_{n,n'} = &\frac{1}{2}[-\cos\theta_n\sin\theta_{n'}\cos\phi_n+\sin\theta_n\cos\theta_{n'}\cos\phi_{n'}\\&+i(-\sin\theta_n\sin\phi_{n'}+\sin\theta_{n'}\sin\phi_n)]\end{aligned}\quad(12)$$

$$P^y_{n,n'} = \sin\theta_n\cos\theta_{n'}\cos\phi_n-\cos\theta_n\sin\theta_{n'}\cos\phi_{n'}\quad(13)$$

$$\begin{aligned}Q^y_{n,n'} = &\frac{1}{2}[-\cos\theta_n\sin\theta_{n'}\cos\phi_n+\sin\theta_n\cos\theta_{n'}\cos\phi_{n'}\\&+i(-\sin\theta_n\sin\phi_{n'}-\sin\theta_{n'}\sin\phi_n)]\end{aligned}\quad(14)$$

$$\begin{aligned}O^z_{n,n'} = &\frac{1}{2}[(1+\cos\theta_n\cos\theta_{n'})\sin(\phi_n-\phi_{n'})\\&-i(\cos\theta_n+\cos\theta_{n'})\cos(\phi_n-\phi_{n'})]\end{aligned}\quad(15)$$

$$P^z_{n,n'} = \sin\theta_n\sin\theta_{n'}\sin(\phi_n-\phi_{n'})\quad(16)$$

$$\begin{aligned}Q^z_{n,n'} = &\frac{1}{2}[(-1+\cos\theta_n\cos\theta_{n'})\sin(\phi_n-\phi_{n'})\\&-i(\cos\theta_n-\cos\theta_{n'})\cos(\phi_n-\phi_{n'})]\end{aligned}\quad(17)$$

If the ground state of this magnetic system is collinear, which means that $\theta_n = \theta_{n'}$ (when magnetic ions at n and n' sites are ferromagnetic) or $\theta_n = \theta_{n'} + \pi$ (when magnetic ions at n and n' sites are antiferromagnetic) and $\phi_n = \phi_{n'}$, the parameters $A_{n,n'}$, $B_{n,n'}$, $C_{n,n'}$ can be simplified as

$$A_{n,n'} = \frac{\zeta_{n,n'}+1}{2}\quad(18)$$

$$B_{n,n'} = \zeta_{n,n'}\quad(19)$$

$$C_{n,n'} = \frac{\zeta_{n,n'}-1}{2}\quad(20)$$

where $\zeta_{n,n'}$ equals to 1 when the spins for the n and n' sites are parallel, otherwise $\zeta_{n,n'}$ equals to -1. More specially, when the ground state of this magnetic system is assumed to be collinear ferromagnetic [PS: do not need to be along z-direction], which means that $\theta_n = \theta_{n'}$ and $\phi_n = \phi_{n'}$, the parameters $A_{n,n'}$, $B_{n,n'}$, $C_{n,n'}$ can be simplified as

$$A_{n,n'} = 1\quad(21)$$

$$B_{n,n'} = 1\quad(22)$$

$$C_{n,n'} = 0\quad(23)$$

C. The eigenvalue problem of magnon eigenvalues

As shown in the maintext, following the LSWT, a general pairwise spin Hamiltonian could be written as Eq. (3) in the maintext. However, it should be noted that the operators in $\psi^\dagger(\mathbf{k}) = [a_1^\dagger(\mathbf{k}), ..., a_N^\dagger(\mathbf{k}), a_1(-\mathbf{k}), ..., a_N(-\mathbf{k})]$ in the Eq. (3) of the maintext satisfy the commutation relation

$$[\psi(k), \psi^\dagger(k)] = \begin{bmatrix} I & \\ & -I \end{bmatrix} = I_-\quad(24)$$

where I represents N×N identity matrix, and N represents the number of magnetic ions in an unit cell. To diagonalize the boson pairing Hamiltonian, we can solve the eigenvalue problem of the general Hamiltonian $H_J(\mathbf{k}) = I_- H(\mathbf{k})$ (i.e., Eq. (6) of the maintext). The first N diagonal elements are the energies of the normal spin wave modes $\omega_{k,n}$ and the last N eigenvalues are equal to the first N eigenvalues multiplied by minus one.

D. Instructions on the program of general relations between magnon eigenvalues

As shown in the maintext, a general pairwise spin model could be expanded as the isotropic Heisenberg Hamiltonian, the DM interactions, and the anisotropic symmetric terms, as shown in Eq. (2) in the maintext. We ignore the third term and perform LSWT to obtain the quadratic spin Hamiltonian as shown in Eq. (3) in the maintext. Note that there is a simple relation between the Fourier transform of MEIs and the SSME, consequently one can easily calculate SSME at arbitrary k point in BZ. Thus, different with the conventional group symmetry analysis, which give the relationship between the magnon energies at the symmetry-related k points, our method produces the relationships between the SSME at high symmetry k points subjected to R_{cut}. We propose a method to obtain the relations between SSME of different high-symmetry k-points. For the given magnetic system in the maintext, the algorithm of the proposed method is implemented in the Mathematica notebook "SR.nb". Using this code, one should first enter the information of magnetic materials, including: (1) the primitive basis and conventional basis; (2) the positions of magnetic atoms; (3) the (magnetic) space group; (4) the spin directions of magnetic atoms; (5) the range of MEIs to be considered (including Heisenberg and DM interactions); (6) whether to consider SIA; (7) the interested k-points. Then the relations between SSME can be automatically obtained. To catch your eye, we have used red color to indicate that the following variable should be specified in the notebook "SR.nb".

The typical magnetic system has the magnetic structure with the magnetic space group (BNS 85.59). As shown in Table I in the maintext, the lattice constant c/a is 0.8. The magnetic ions are located at three nonequivalent crystallographic sites: $4d$ (0, 0, 0), $2a$ (0.25, 0.75, 0) and $2c$ (0.25, 0.25, z) WP and the positions for these eight magnetic ions are summarized in Table I in the maintext. While the $4d$ and $2a$ WP had been completely determined by the symmetry, the coordinates of $2c$ WP have a variable z and here we adopt it as $z = 0.1$. The magnetic state is a collinear ferromagnetic order with spin along the z direction. This case belongs to the type-I magnetic space group (BNS 85.59), and all of the the polar angle and azimuthal angles are equal to 0.

In this notebook "SR.nb", one should specify the parameters as input information, such as:

(*input parameters:*)
(*primitive lattice basis*)
A = {{1, 0, 0}, {0, 1, 0}, {0, 0, 0.8}};
(*conventional lattice basis*)
AA = {{1, 0, 0}, {0, 1, 0}, {0, 0, 0.8}};
(*input positions of magnetic atoms based on conventional lattice basis vectors*)
atoms=8;
$\boldsymbol{\tau}$ = {{0, 0, 0},
{0.5, 0, 0},
{0, 0.5, 0},
{0.5, 0.5, 0},
{0.75, 0.25, 0.},
{0.25, 0.75, 0.},
{0.25, 0.25, 0.1},
{0.75, 0.75, -0.1}};
(*input the serial number of space group or the magnetic space group (in BNS notation).*)
msg=85.59;
(*spin directions of magnetic atoms in spherical coordinates (θ_n, ϕ_n) with the polar angles θ_n and azimuthal angles ϕ_n.*)
ang = {{0, 0}, {0, 0}, {0, 0}, {0, 0}, {0, 0}, {0, 0}, {0, 0}, {0,0}};
(*the range of Heisenberg and DM interactions to be considered, respectively*)
Jmax = 3;
Dmax = 2;
(*set DIA = "True" or "False" to indicate whether to consider single ion anisotropy.*)
DIA = False;
(*high-symmetry points*)
kk[1] = {0, 0, 0};
kk[2] = {0.5, 0, 0};
kk[3] = {0.5, 0.5, 0};
kk[4] = {0, 0, 0.5};
kk[5] = {0.5, 0, 0.5};
kk[6] = {0.5, 0.5, 0.5};
kname = {"Γ", "X", "M", "Z", "R", "A"};

In the following, we would like to give a description of these parameters one by one:

(1) the primitive basis and conventional basis of Bravais lattice

One should input them in Cartesian coordinates. As the example in the maintext, the space group P4/n (No. 85) crystallizes in a tetragonal lattice, and its primitive basis A and conventional basis AA of Bravais lattice are both $\{\{1,0,0\},\{0,1,0\},\{0,0,0.8\}\}$.

(*primitive lattice basis*)
A = {{1, 0, 0}, {0, 1, 0}, {0, 0, 0.8}};
(*conventional lattice basis*)
AA = {{1, 0, 0}, {0, 1, 0}, {0, 0, 0.8}};

(2) the number and the Wyckoff positions of magnetic atoms (based on conventional lattice basis vectors)

(*input positions of magnetic atoms based on conventional lattice basis vectors*)
atoms=8;
$\boldsymbol{\tau}$ = {{0, 0, 0},
{0.5, 0, 0},
{0, 0.5, 0},
{0.5, 0.5, 0},
{0.75, 0.25, 0.},
{0.25, 0.75, 0.},
{0.25, 0.25, 0.1},

{0.75, 0.75, -0.1}};

(3) the (magnetic) space group of the magnetic system. When the magnetic moments are quite localized, magnetic interactions may still satisfy the symmetries of its space group. In this case, one can enter the serial number of its space group. Otherwise, one should enter the serial number of its magnetic space group (in BNS notation). As the example for collinear ferromagnetic state in the maintext, the magnetic space group (BNS 85.59) has the same symmetries as the space group (SG. 85). In this case, the results of the input "msg=85" and "msg=85.59" are equivalent. Note that if the input parameter is an integer "X", we would use the symmetry of this space group (No. X), otherwise, we will use the symmetry of the magnetic space group as "BNS X.Y".

(*input the serial number of space group or the magnetic space group (in BNS notation).*)

msg=85.59;

(4) the spin directions of magnetic atoms. One should input them in spherical coordinates (θ_n, ϕ_n) with the polar angles θ_n and azimuthal angles ϕ_n. As the example in the maintext, the FM (001) state should be

(*spin directions of magnetic atoms in spherical coordinates (θ_n, ϕ_n) with the polar angles θ_n and azimuthal angles ϕ_n.*)

ang = {{0, 0}, {0, 0}, {0, 0}, {0, 0}, {0, 0}, {0, 0}, {0, 0}, {0,0}};

(5) One should set up the range of magnetic interactions to be considered. You can set the range of Heisenberg and DM interactions respectively.

(*the range of Heisenberg and DM interactions to be considered, respectively*)

Jmax = 3;

Dmax = 2;

For example, we set Jmax = 3 and Dmax = 2, which means that we consider the range of Heisenberg interactions up to J_3, while the DM interactions are considered up to $\mathbf{D}_2$.

(6) Then one should set up whether to consider SIA by setting DIA = "True" or "False".

(*set DIA = "True" or "False" to indicate whether to consider single ion anisotropy.*)

DIA = False;

(7) Last, one should input the information of high-symmetry points to be considered, including the positions of these high-symmetry points and the labeled names of these high-symmetry points.

(*high-symmetry points*)

kk[1] = {0, 0, 0};
kk[2] = {0.5, 0, 0};
kk[3] = {0.5, 0.5, 0};
kk[4] = {0, 0, 0.5};
kk[5] = {0.5, 0, 0.5};
kk[6] = {0.5, 0.5, 0.5};
kname = {"Γ", "X", "M", "Z", "R", "A"};

After entering the above parameters, our program would output the following information, including:

TABLE III. The Heisenberg and DM interactions for the NNs of the typical material in the maintext for collinear FM state (BNS 85.59) restricted by the crystal symmetry.

distance(a)	n	n'	R_l	J	D
0.35	1	5	$(-1,0,0)$	J_1	(D_1^x, D_1^y, D_1^z)
	1	6	$(0,-1,0)$		(D_1^x, D_1^y, D_1^z)
	2	5	$(0,0,0)$		$(-D_1^y, D_1^x, D_1^z)$
	2	6	$(0,-1,0)$		$(-D_1^y, D_1^x, D_1^z)$
	3	5	$(-1,0,0)$		$(D_1^y, -D_1^x, D_1^z)$
	3	6	$(0,0,0)$		$(D_1^y, -D_1^x, D_1^z)$
	4	5	$(0,0,0)$		$(-D_1^x, -D_1^y, D_1^z)$
	4	6	$(0,0,0)$		$(-D_1^x, -D_1^y, D_1^z)$
0.36	1	7	$(0,0,0)$	J_2	(D_2^x, D_2^y, D_2^z)
	1	8	$(-1,-1,0)$		(D_2^x, D_2^y, D_2^z)
	2	7	$(0,0,0)$		$(-D_2^y, D_2^x, D_2^z)$
	2	8	$(0,-1,0)$		$(-D_2^y, D_2^x, D_2^z)$
	3	7	$(0,0,0)$		$(D_2^y, -D_2^x, D_2^z)$
	3	8	$(-1,0,0)$		$(D_2^y, -D_2^x, D_2^z)$
	4	7	$(0,0,0)$		$(-D_2^x, -D_2^y, D_2^z)$
	4	8	$(0,0,0)$		$(-D_2^x, -D_2^y, D_2^z)$
0.5	1	2	$(0,0,0)$	J_3	(D_3^x, D_3^y, D_3^z)
	1	2	$(-1,0,0)$		(D_3^x, D_3^y, D_3^z)
	1	3	$(0,0,0)$		$(-D_3^y, D_3^x, -D_3^z)$
	1	3	$(0,-1,0)$		$(-D_3^y, D_3^x, -D_3^z)$
	2	4	$(0,0,0)$		$(-D_3^y, D_3^x, D_3^z)$
	2	4	$(0,-1,0)$		$(-D_3^y, D_3^x, D_3^z)$
	3	4	$(0,0,0)$		$(D_3^x, D_3^y, -D_3^z)$
	3	4	$(-1,0,0)$		$(D_3^x, D_3^y, -D_3^z)$

(1) the symmetry of the (magnetic) space group.

output[symmetry]=
(x,y,z | mx,my,mz)
(-y+1/2,x,z | -my,mx,mz)
(y,-x+1/2,z | my,-mx,mz)
(-x+1/2,-y+1/2,z | -mx,-my,mz)
(-x,-y,-z | mx,my,mz)
(y+1/2,-x,-z | -my,mx,mz)
(-y,x+1/2,-z | my,-mx,mz)
(x+1/2,y+1/2,-z | -mx,-my,mz)

where the left part represents the symmetry operation for positions of magnetic atoms, while the right part means the symmetry operation for the orientation of magnetic moment.

(2) The program would also give the distance and the corresponding symmetry restricted MEIs, including the Heisenberg and DM interactions. For example, there are in total 24 MEIs in this magnetic system up to J_3, as summarized in the Table III. Meanwhile, the corresponding symmetry restricted DM interactions $\mathbf{D}(\boldsymbol{\tau}_n, \boldsymbol{\tau}_{n'}, \mathbf{R}_l)$ are also listed here. Note that for 5th NN MEIs, the symmetry makes $D_5^z = 0$, while for 7th NN MEIs, we have

$\mathbf{D}_7 = (0, 0, 0)$. These symmetry restrictions would also be automatically considered in our program.

(3) the main output: the relations between SSME at different high-symmetry k points.

output[relations]=

$M - A = 0$

$X - R = 0$

$\Gamma - Z = 0$

$\Gamma - 2X + M = 0$

where the label "M" means the quadratic sum of the magnon energies at M point "$\sum_i \omega_i^2(M)$", as well as the labels of other high-symmetry k points. We can see that, up to J_3, the quadratic sum of the magnon energies satisfy that $\sum_i \omega_i^2(\Gamma) = \sum_i \omega_i^2(Z)$, $\sum_i \omega_i^2(X) = \sum_i \omega_i^2(R)$, $\sum_i \omega_i^2(M) = \sum_i \omega_i^2(A)$ and $2\sum_i \omega_i^2(X) = \sum_i \omega_i^2(\Gamma) + \sum_i \omega_i^2(M)$, as shown in Table II in the maintext.

As shown above, by entering the information of the typical magnetic model, one can use this code to obtain the relations between magnon eigenvalues in this paper easily. Meanwhile, one can easily extend our method to other magnetic systems by simply modifying this example code.