Krein-Hermitian Schrieffer-Wolff transformation and band touchings in bosonic BdG Hamiltonians

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Krein-Hermitian Hamiltonians have emerged as an important class of non-Hermitian Hamiltonians in physics, encompassing both single-particle bosonic Bogoliubov-de Gennes (BdG) Hamiltonians and so-called “PT-symmetric” non-Hermitian Hamiltonians. In particular, they have attracted considerable scrutiny owing to the recent surge in interest for boson topology. Motivated by these developments, we formulate a perturbative Krein-unitary Schrieffer-Wolff transformation for finite-size dynamically stable Krein-Hermitian Hamiltonians, yielding an effective Hamiltonian for a subspace of interest. The effective Hamiltonian is Krein-Hermitian and, for sufficiently small perturbations, also dynamically stable. As an application, we use this transformation to justify codimension-based analyses of band touchings in bosonic BdG Hamiltonians, which complement topological characterization. We use this simple approach based on symmetry and codimension to revisit known topological magnon band touchings in several materials of recent interest.

I. INTRODUCTION

Non-Hermitian Hamiltonians have become a central field of study in condensed-matter physics in the last decades [1]. Important examples of systems governed by non-Hermitian Hamiltonians are quadratic bosonic Bogoliubov-de Gennes (BdG) Hamiltonians [2,3], which have been the subject of renewed interest recently in the context of topological systems [4,13], and so-called “PT-symmetric” non-Hermitian Hamiltonians, which initially attracted interest because they could give rise to real spectra despite not being Hermitian [14,15]. Note that in the context of non-Hermitian Hamiltonians, “PT symmetry” has come to refer to any antilinear symmetry of a specific form [10], and not necessarily to space-time inversion symmetry. Both these examples fall into a class of non-Hermitian Hamiltonians called Krein-Hermitian [10,16,23], also referred to in the literature as “pseudo-Hermitian” [10,11,16,19,24] or “para-Hermitian” [25].

Krein-Hermitian Hamiltonians are Hermitian with respect to an indefinite, nondegenerate inner product, rather than the conventional positive-definite inner product [25]. They have spectral properties that enable them to describe stable physical systems: the phase diagram of a Krein-Hermitian Hamiltonian typically includes dynamically stable regions, in which the Hamiltonian is diagonalizable with real eigenvalues and with eigenvectors that are orthonormal with respect to the indefinite inner product. Lately, the mathematics of Krein-Hermitian Hamiltonians and Krein spaces more generally have seen growing interest and adoption among theoretical physicists as a tool to approach these specific non-Hermitian problems [10,11,22,25].

The Schrieffer-Wolff (SW) transformation [26], also known as the Löwdin partitioning method [27], has been the object of renewed interest in recent years. Novel non-perturbative approaches have yielded new results, like the expansion’s radius of convergence and closed-form expressions to all orders [26]. Moreover, the SW approach has been generalized to obtain non-unitary similarity transformations of (non-Hermitian) Liouvillian operators in order to perturbatively eliminate fast degrees of freedom in dissipative quantum systems [28,29].

Previously, perturbative transformations have been used in bosonic BdG Hamiltonians to eliminate boson pairing terms [5,30,33]. In Sec. II, we formulate a general perturbative SW transformation for dynamically stable, finite-dimensional Krein-Hermitian Hamiltonians, yielding a reduced effective Hamiltonian that is Krein-Hermitian in a reduced space and is sure to be Krein-unitarily diagonalizable. Unlike previous work on general non-Hermitian SW transformations [28,29], our transformation is explicitly Krein-unitary; further, we highlight the implications of Krein stability theory on the effective Hamiltonian and its diagonalizability. In particular, it is safe to perturbatively study degenerate and near-degenerate states as long as they have the same (nonzero) Krein signature, since small perturbations cannot drive them to dynamical instability.

Besides the practical applications of a SW transformation for Krein-Hermitian Hamiltonians, our results allow a justification for the use of reduced Hamiltonians describing a subset of contiguous energy bands in a Krein-Hermitian system, as discussed in Sec. IV. In particular, we clarify why adjacent positive-energy bands of thermodynamically stable systems can simply be described by a Hermitian reduced Hamiltonian, even though the larger Hamiltonian they originate from is Krein-Hermitian.

We use this observation to justify codimension-based arguments for band touchings in bosonic BdG Hamiltonians, focusing on magnons for concreteness. Such arguments are well known for Hermitian Hamiltonians [34]. We then revisit known results on topological band touchings and the consequences of space-time inversion symmetry in magnon systems, based solely on codimension and symme-
try arguments. In short, the behavior hinges on the fact that space-time inversion squares to +1 for bosons [35]. We focus on Dirac points and gapless lines in the magnon spectrum of Cu₂TeO₆ [35–37] and gapless lines in the magnon spectrum of CoTiO₃ [38–39], both part of a recent drive to identify topological band touchings in bosonic systems.

Appendix A contains details on the SW transformation for Krein-Hermitian matrices, and Appendix C discusses magnons in linear spin-wave theory as well as the implementation of spin space group symmetries on the linear spin-wave Hamiltonian.

To avoid confusion with the aforementioned notion of “PT symmetry” in the context of non-Hermitian Hamiltonians, we refer to space-time inversion symmetry as magnetic inversion symmetry rather than “PT symmetry”. The Krein Hermicity—equivalent to so-called “PT symmetry” [10]—of bosonic BdG Hamiltonians stems solely from the bosonic commutation relations and holds regardless of the system’s physical symmetries.

II. BOSONIC BDG HAMILTONIANS

In this section, we review the mathematics of quadratic BdG Hamiltonians of bosons, which will be our main focus in this work, though our results have broader applicability. This keeps the article self contained, and allows us to introduce necessary notions and definitions. Consider a bosonic Fock space made up of \( n \) single-particle states, and a quadratic Hermitian Hamiltonian \( \hat{H} \) in that space. Though the second-quantized Hamiltonian \( \hat{H} \) is Hermitian and the bosonic Fock space is necessarily of infinite dimension, the “single-particle Hamiltonian” that governs the time evolution and determines the spectrum of the non-interacting bosons is finite dimensional and in general, as we will see, Krein-Hermitian. For concreteness, we assume the system has translational invariance, allowing us to write

\[
\hat{H} = \frac{1}{2} \sum_k \tau^3 \Phi^\dagger_k \hat{H}_k \Phi_k
\]

where \( \Phi_k = [b_{k,1}^\dagger, \ldots, b_{k,n}^\dagger, b_{-k,1}, \ldots, b_{-k,n}] \) is the Nambu spinor, and \( b_{k,\alpha} \) is the annihilation operator for state \( \alpha \) in the unit cell and with wavevector \( \mathbf{k} \). The extension of our results to systems without translational invariance presents no difficulties.

The redundancy inherent in the Nambu formalism is eliminated by choosing the Hermitian coefficient matrix \( H_k \) to satisfy the particle-hole (PH) constraint, \( \tau^3 \hat{H}_k \tau^{-1} = H_k^\tau \). (For clarity, we use hats on Hilbert-space operators, and not on coefficient matrices.)

Note that if the system is particle-conserving, \( H_k \) is block-diagonal in the Nambu space, in which case the spectrum of \( \hat{H} \) and the system’s time evolution are simply determined by the unitary eigendecomposition of \( \hat{H}_k \).

A. Diagonalization

Unlike for fermions, a Bogoliubov transformation for bosons is not simply achieved by the eigendecomposition of the coefficient matrix \( H_k \), as such a transformation does not preserve the bosonic canonical commutation relations [2, 3, 40–42]. Writing the transformation to a new bosonic Nambu spinor \( \Gamma_k \) as \( \Phi_k = T_k \Gamma_k \), meaning

\[
\hat{H} = \frac{1}{2} \sum_k \tau^3 \Gamma^\dagger_k (T_k \hat{H}_k T_k^\tau) \Gamma_k,
\]

the \( 2n \times 2n \) transformation matrix \( T_k \) must fulfill

\[
T_k^\dagger \tau^3 T_k = T_k \tau^3 T_k^\tau = \tau^3
\]

in order to preserve the bosonic commutation relations. Here and throughout the article, \( \tau^\nu \), short for \( \tau^\nu \otimes 1_n \), are the Pauli matrices in Nambu space. Hence, in general, \( T_k \) is not unitary, and the transformation on \( \hat{H}_k \) is not a similarity transformation [43]. A matrix satisfying the constraint of Eq. [3] has been called paraunitary in the physics literature [2].

In order to give rise to the eigenmodes of \( \hat{H} \), the transformation \( T_k \) should be chosen such that \( T_k^\dagger \hat{H}_k T_k \) is diagonal with real entries. If this is possible, the Hamiltonian can be written in its eigenbasis as

\[
\hat{H} = \sum_k \sum_{\alpha=1}^n \epsilon_{\gamma,k,\alpha} \gamma_{\gamma,k,\alpha} + \gamma_{\gamma,k,\alpha} \gamma_{\gamma,k,\alpha}^\dagger \frac{1}{2}
\]

where we have used the fact that the particle-hole constraint ensures the modes at \( \mathbf{k} \) and \( -\mathbf{k} \) have the same energies and appropriately related eigenvectors. As we shall see in reviewing Krein theory, that \( H_k \) is positive definite, which we denote \( H_k > 0 \), is a sufficient condition for there to exist a paraunitary \( T_k \) such that \( T_k^\dagger \hat{H}_k T_k \) is diagonal with real, strictly positive entries [44].

The Hamiltonian \( \hat{H} \) is thermodynamically stable, meaning it is bounded below, if and only if \( H_k \geq 0 \) at all \( \mathbf{k} \) [11]. In a linear spin wave system, for example, \( H_k \geq 0 \) holds as long as the underlying classical ground state is a local minimum of the classical energy. In many physical systems for which \( H_k \) is positive semidefinite but not positive definite, the zero eigenspace corresponds to the Goldstone mode; in such systems, \( H_k > 0 \) for \( \mathbf{k} \neq 0 \) [3, 11].

Finally, we point out that the transformed coefficient matrix \( T_k^\dagger \hat{H}_k T_k \) can be rewritten using the paraunitarity constraint of Eq. [3]

\[
T_k^\dagger \hat{H}_k T_k = \tau^3 (T_k^{-1} (\tau^3 \hat{H}_k) T_k).
\]

Since \( \tau^3 \) is diagonal, this form shows that the spectrum and the transformation \( T_k \) can be found from the (nonunitary) eigendecomposition of the non-Hermitian matrix \( \tau^3 H_k \). Since it determines the spectrum and governs the system’s time evolution [10], we refer to \( \tau^3 H_k \) as the single-particle Hamiltonian. The properties of the single-particle Hamiltonian, and of Krein-Hermitian Hamiltonians more generally, are reviewed in Sec. IIIA.
B. Unitary transformations

We also review how a unitary transformation on the Hamiltonian $\hat{H}$ of Eq. 1 translates to a paraunitary transformation on the single-particle Hamiltonian $\tau^3 H_k$ \cite{[25, 47, 68]}. To see this, consider the transformed Hamiltonian $\hat{\tilde{H}} = e^{-\hat{W}} \hat{H} e^{\hat{W}}$, where $e^W$ is a unitary transformation in the Fock space generated by the skew-Hermitian generator $W$, and rewrite it using the following expansion:

$$\hat{\tilde{W}} = e^{-\hat{W}} \hat{W} e^{\hat{W}} = \hat{H} + [\hat{H}, \hat{W}] + \frac{1}{2!} [[\hat{H}, \hat{W}], \hat{W}] + \ldots \quad (6)$$

In order for the transformation to keep the Hamiltonian quadratic, its generator $W$ must itself be quadratic: $W = \frac{1}{2} \sum_k \Phi_k^\dagger W_k \Phi_k$, where $W_k$ is a skew-Hermitian $2n \times 2n$ matrix. Furthermore, imposing the PH constraint on $W_k$ (i.e. $\tau^1 W_k \tau^1 = W_k^\dagger$) will ensure the coefficient matrix for $\hat{\tilde{W}}$ is PH symmetric, in addition to eliminating the redundancy in $W_k$ intrinsic to the Nambu formalism.

Using the bosonic commutation relations $[\Phi_k^\dagger, \Phi_p^\dagger] = (\tau^3)^{ab} \delta_{p,k}^b$, where $a$ and $b$ are $\{1, \ldots, 2n\}$, and the PH constraint $\tau^1 H_k \tau^1 = H^\dagger_{-k}$, one finds that the commutator is given by

$$[\hat{H}, \hat{W}] = \frac{1}{2} \sum_k \Phi_k^\dagger (H_k, W_k) \Phi_k, \quad (7)$$

where $(H_k, W_k) := H_k \tau^3 W_k - W_k \tau^3 H_k$ is a $\tau^3$-intertwined commutator, which arises from the bosonic commutation relations. Since $H_k$ and $W_k$ are PH symmetric, so is $(H_k, W_k)$; hence, the result of Eq. 7 can be iterated to find all orders of $\hat{\tilde{H}}$ and the transformed Hamiltonian of Eq. 6 takes the form

$$\hat{\tilde{H}} = \frac{1}{2} \sum_k \Phi_k^\dagger \left( H_k + (H_k, W_k) \ight) + \frac{1}{2!} ((H_k, W_k), W_k) + \ldots \Phi_k \quad (8)$$

In the last line, we have introduced the paramunitary transformation $T_k := e^{\tau^3 W_k}$; indeed, any $2n \times 2n$ paraunitary matrix can be generated in this way with a skew-Hermitian matrix $W_k$. Furthermore, the transformation $T_k$ inherits a particle-hole constraint from that of $W_k$, i.e. $\tau^1 T_k \tau^1 = T_k^\dagger$ \cite{45}.

Equation 8 shows that a unitary transformation $\hat{H} \rightarrow e^{-\hat{W}} \hat{H} e^{\hat{W}}$ on the second-quantized Hamiltonian has a paraunitary representation $\tau^3 H_k \rightarrow T_k^{-1} \tau^3 H_k T_k$ on the single-particle Hamiltonian. Since the single-particle Hamiltonian undergoes a similarity transformation, the invariance of the spectrum is manifest.

Had the ladder operators been fermionic and obeyed anticommutation relations rather than commutation relations, the unitary transformation on the second-quantized Hamiltonian would have had a more familiar unitary representation on the single-particle Hamiltonian.

III. KREIN-HERMITIAN HAMILTONIANS AND PERTURBATION THEORY

In this section, we show that the SW transformation can be used to formulate a Krein-unitary perturbation theory for finite-size Krein-Hermitian Hamiltonians within a dynamically stable phase. A Hamiltonian is dynamically stable \cite{10}, meaning the time evolution it generates is bounded, iff the Hamiltonian is diagonalizable with real eigenvalues \cite{10}.

Since single-particle BdG Hamiltonians $\tau^3 H_k$ and paraunitary transformations $T_k$ are respectively Krein-Hermitian and Krein-unitary with respect to $\tau^3$, our results allow for a perturbation theory perturbatively yielding bosonic eigenmodes as well as mode energies.

We begin by briefly reviewing necessary aspects of Krein spaces, and then present the perturbation theory.

A. Krein spaces

Though the single-particle Hamiltonian $\tau^3 H_k$ is not Hermitian, it is Hermitian with respect to an indefinite inner product with metric $\tau^3$, $\langle \phi, \psi \rangle_{\tau^3} := \langle \phi^\dagger \tau^3 \psi \rangle$, in the sense that $\langle \tau^3 H \phi, \psi \rangle_{\tau^3} = \langle \phi, \tau^3 H \psi \rangle_{\tau^3}$ for any vectors $\phi$ and $\psi \in \mathbb{C}^{2n}$. Vector spaces endowed with an indefinite, nondegenerate inner product in addition to a positive-definite inner product are called Krein spaces \cite{25, 47, 68}. Although $\tau^3 H_k$ may fail to be diagonalizable or to have real eigenvalues because it is non-Hermitian, these possibilities are narrowly constrained because of its Krein-Hermiticity.

Consider a Krein space of dimension $n_K$ with indefinite inner product $\langle \phi, \psi \rangle_{\eta} := \phi^\dagger \eta \psi$, where the Hermitian metric $\eta$ is indefinite and nondegenerate. The Krein adjoint of a matrix $A$ is given by

$$A^\eta := \eta^{-1} A^\dagger \eta, \quad (9)$$

since $\langle A \phi, \psi \rangle_{\eta} = \langle \phi, A^\eta \psi \rangle_{\eta}$ for any vectors $\phi$ and $\psi \in \mathbb{C}^{n_K}$. The concepts of Krein-Hermitian matrices ($K^2 = K$) and Krein-unitary matrices ($T^* T = T^T T^4 = 1$) follow. Note that a change of basis (to “normal coordinates”) can make $\eta$ diagonal with entries $\pm 1$; specifically, diagonalization followed by a scaling transformation \cite{49}. From here on, we assume the metric $\eta$ has this form, with $n_+ \rightarrow n_+ + n_-$ entries of $-1$, which considerably simplifies the treatment.

The Krein space that naturally arises in bosonic BdG theory has metric $\eta = \tau^3 \otimes \mathbb{I}_n$, with $n_+ = n_+ = n$: the
single-particle Hamiltonian $K = \tau^3 H$ and paraunitary transformations $T$ are respectively Krein-Hermitian and Krein-unitary with respect to $\tau^3$. The PH constraint of bosonic systems is not, however, a general feature of Krein-Hermitian Hamiltonians; indeed, the momentum-space single-particle Hamiltonian at a given $k$ does not in general obey such a constraint, unless an inversion-like symmetry relating $k$ and $-k$ is present.

**Dynamical stability and perturbations**  

The eigenvalues of a Krein-Hermitian matrix $K$ are either real or come in complex-conjugate pairs \cite{[20] [21] [22]}. An eigenvector $\psi$ corresponding to a non-real eigenvalue has null signature $(\langle \psi, \psi \rangle_\eta = 0)$, while one corresponding to a real eigenvalue can have positive $(\langle \psi, \psi \rangle_\eta > 0)$, negative $(\langle \psi, \psi \rangle_\eta < 0)$, or null signature. If all the eigenvectors in the eigenspace of an eigenvalue $\lambda$ have the same nonzero signature, the eigenspace is said to have definite signature; otherwise, it has indefinite signature. According to Krein stability theory \cite{[20] [21]}, if each eigenspace of $K$ has definite signature, a perturbed Hamiltonian $K + \epsilon K'$ for sufficiently small $\epsilon$ is diagonalizable with real eigenvalues; that is, it is dynamically stable. Furthermore, its eigenvectors can be chosen to be orthonormal with respect to the Krein inner product. Conversely, if $K$ has an indefinite eigenspace, either with or without nontrivial Jordan blocks, then $K$ either has non-real eigenvalues or there are arbitrarily small perturbations that make them non-real, meaning $K$ is either dynamically unstable or at a phase boundary of dynamical stability.

If $K = K^2$ is positive-definite with respect to the Krein inner product, i.e. $\langle \phi, K \phi \rangle_\eta > 0$ for any nonzero $\phi$, all its eigenspaces automatically have definite signature, so it is within a dynamically stable phase \cite{[20] [21] [23]}. Furthermore, it has $n_+$ eigenstates with positive signature and positive energy, and $n_- = n_K - n_+$ eigenstates with negative signature and negative energy. Taking $K = \tau^3 H$, $K$ is clearly positive definite with respect to $\tau^3$ iff $H > 0$. Once the eigenstates $\psi$ of $K$ are chosen to be orthonormal with respect to the Krein inner product, the claim made in Sec. II[A]—that $H > 0$ implies there is a paraunitary $T$ such that $T^\dagger HT$ is diagonal with real, positive entries—follows.

**B. Schrieffer-Wolff transformation for Krein-Hermitian Hamiltonians**

We now demonstrate that within a dynamically stable phase, the perturbative SW transformation can be generally formulated in terms of Krein-unitary transformations. Applied to single-particle boson Hamiltonians, the transformation yields a reduced single-particle Hamiltonian with proper bosonic eigenmodes.

The SW transformation is used to study the effect of a perturbation on a subset of contiguous energy states of a (traditionally) Hermitian Hamiltonian \cite{[20] [27]}. This subspace of interest is often, but not necessarily, made up of the low-energy states of the unperturbed Hamiltonian. The transformation is defined as a unitary rotation that block-diagonalizes the perturbed Hamiltonian; the block corresponding to the subspace of interest then yields an effective Hamiltonian for those states. The transformation as well as the effective Hamiltonian can be expressed perturbatively, order by order in terms of the perturbation. One of the considerable strengths of this method is its ability to deal on an equal footing with perturbations of degenerate as well as nondegenerate states, avoiding the complications that arise in Rayleigh-Schrödinger perturbation theory, for example \cite{[20] [51]}. The canonical transformations for Krein-Hermitian Hamiltonians are Krein-unitary transformations: they preserve Krein-Hermiticity, and leave eigenspace signatures unchanged. We adapt the SW procedure to Krein-Hermitian Hamiltonians within a dynamically stable regime, showing that it naturally yields a Krein-unitary transformation that block-diagonalizes the Krein-Hermitian Hamiltonian order by order in the perturbation, producing an effective Hamiltonian that is also Krein-Hermitian. Krein stability theory ensures that for sufficiently small perturbations, the effective Hamiltonian at any order is also dynamically stable. Applied to single-particle boson Hamiltonians, the transformation will yield canonical boson modes.

Consider a perturbed $\eta$-Krein-Hermitian $n_K$-by-$n_K$ Hamiltonian

$$K = K^0 + \epsilon K',$$

where $K^0$ is within a dynamically stable regime and has a known Krein-orthonormal eigendecomposition, $K^0 t_i = E^0 t_i$, with $t_i^\dagger \tau^3 t_j = \pm \delta_{ij}$, and $\epsilon \in \mathbb{R}$ controls the smallness of the perturbation. Let $S_0$ denote a subset of energy-contiguous eigenstates of $K^0$, comprised of $m_+$ positive-signature states and $m_-$ negative-signature states, and gapped from the rest of the spectrum. Let $P_0$ denote the subspace spanned by the eigenstates in $S_0$. We wish to block-diagonalize the perturbed Hamiltonian $K$ in the subspace $P_0$ using a Krein-unitary transformation (see the schematic depiction in Fig. 1). Associated with the subspace $P_0$ is a unique Krein-orthogonal projector $P_0 = P_0^\dagger P_0 = P_0^T$ \cite{[22]}, where

$$P_0 = \sum_{i \in S_0} t_i^\dagger \eta t_i.$$  

Schematically, in the eigenbasis of $K^0$, any matrix $A$ can be written

$$A = P_0 A P_0 + P_0 A P_0 + P_0 A P_0 + P_0 A P_0$$

$$= \begin{bmatrix} P_0 A P_0 & P_0 A P_0 \\ P_0 A P_0 & P_0 A P_0 \end{bmatrix},$$

where $P_0 = 1 - P_0$. We use the notation $A_0 := P_0 A P_0 + P_0 A P_0$ and $A_o := P_0 A P_0 + P_0 A P_0$ for the parts of $A$ that are respectively block-diagonal and block-off-diagonal in the subspace $P_0$ \cite{[23]}.
The parameter $W_0$, we find the following equations defining $W$:

\[ W_{b} = 0, \quad W_{2} = 1. \]

These equations are compatible with $W^{(j)^T} = -W^{(j)}$, i.e., with the assumption that $T$ is Krein-unitary at all orders. Indeed, the first few orders are explicitly solved in App. A, showing that the generator $W$ is indeed skew-Krein-Hermitian, and the effective Hamiltonian $P_{0}K_{0}P_{0}$ is Krein-Hermitian with respect to $P_{0}\eta P_{0}$.

We note that if the Hamiltonian $K$ is purely real, the transformation yields a purely real effective Hamiltonian $K$ to all orders in the perturbation. This is verified explicitly for the first few orders in App. A and extends to all orders.

Our findings agree with prior results on the first-order contribution $K^{(1)}$ found by applying degenerate perturbation theory to two degenerate states of a para-Hermitian Hamiltonian [26,51]. We stress once again, however, that the SW approach does not have certain limitations of a Rayleigh-Schrödinger perturbation theory and treats degenerate, quasidegenerate, and nondegenerate states on the same footing [27,51].

b. Range of validity For Hermitian matrices, the perturbative SW transformation is well controlled as long as the subspace of interest is gapped from the rest of the spectrum [26,27]. For Krein-Hermitian matrices, we additionally require that the perturbed Hamiltonian remain within a dynamically stable region in order for eigenvalues to remain real, and for eigenvectors to be orthonormal with respect to the Krein inner product. Furthermore, at points of non-diagonalizability, eigenvectors have a non-analytic dependence on perturbations [57,58], and since dynamical stability phase boundaries are mostly composed of non-diagonalizable points (called exceptional points) [10], they can constitute an obstruction to the convergence of a perturbation series.

In previous work, ranges of validity for the SW transformation were determined in terms of bounds on the norm $\|H'\|$ of a perturbation $H'$ ensuring that the gaps between the subspace of interest and the rest of the spectrum remain sufficiently large [26]. This simple picture...
was possible because the eigenvalues of a Hermitian matrix $H$ (and for normal matrices more generally) shift at most by $\|H\|$ under the effect of a perturbation $H'$, regardless of the details of $H$ \cite{ref5} \cite{ref7} \cite{ref8}. Here, $\|\|$ is the operator norm, equal to the largest singular value.

In contrast, the eigenvalues of a non-normal matrix $A$ can shift by more than $\|A\|$ under the effect of a perturbation $A'$ \cite{ref28}, and the set of points at which the eigenvalues can even up depends on the details of $A$ \cite{ref57} \cite{ref58}. This makes the task of formulating sufficient conditions for the non-closing of relevant gaps more complex. In mathematics, the notion of *pseudospectra* explores this striking difference between normal and non-normal matrices in regards to perturbations and eigenvalues \cite{ref57} \cite{ref58}.

For a Krein-Hermitian matrix $K^0$ satisfying $\eta K^0 > 0$, there is a simple condition under which a perturbed Hamiltonian $K^0 + K'$ remains dynamically stable and Krein-unitarily diagonalizable \cite{ref11}: assuming $\|K'\| < \|(K^0)^{-1}\|^{-1}$, no eigenvalues of $K^0 + K'$ can reach zero, implying the perturbed Hamiltonian remains within a dynamically stable phase. Note that $\|(K^0)^{-1}\|^{-1}$ constitutes a lower bound for the smallest eigenvalues (in absolute value), but since $K^0$ is non-normal, it is not in general equal to the smallest absolute value.

The formulation of more general bounds on allowable perturbations $K'$, and the derivation of a radius of convergence such as that which exists for perturbative SW transformations on Hermitian Hamiltonians \cite{ref26}, are left for future work.

### IV. BAND TOUCHINGS AND CODIMENSION IN MAGNON SYSTEMS

In Hermitian systems, the standard SW transformation allows one to obtain, at least locally in momentum space, an effective Hamiltonian describing a contiguous subset of bands \cite{ref69} \cite{ref62}. The transformation, which can in principle be carried out to any order, also justifies the existence of an effective reduced Hamiltonian that exactly describes contiguous bands if sufficiently large gaps separate them from the rest of the spectrum, again, locally in momentum space.

In linear spin wave theory, magnons are generally described by a bosonic BdG Hamiltonian of the form of Eq. \[1\] with a Krein-Hermitian single-particle Hamiltonian (see App. \[C\] for an overview of linear spin-wave theory). The Krein-Hermitian SW transformation we formulate explains why such effective reduced descriptions can also be used for Krein-Hermitian systems, and clarifies the properties of the effective reduced Hamiltonian in such cases. With these facts in hand, we revisit results on the codimensions of generic band touchings (i.e., those not at high-symmetry momenta) of noninteracting magnon systems with and without magnetic inversion symmetry. We comment on high-symmetry momenta at the end of the section.

Quadratic magnon Hamiltonians in 3D with magnetic inversion symmetry are known to exhibit either topologically protected Dirac points or topologically protected gapless lines, depending on the classical spin order and on other symmetries of the system \cite{ref25}. This behavior makes them in part analogous to quadratic Hamiltonians of spinless electron in 3D, which also generically exhibit gapless lines in the presence of space-time-inversion symmetry \cite{ref74} \cite{ref69} \cite{ref68}. The source of this commonality is that both are integer-spin particles, for which space-time inversion squares to $+1$ \cite{ref67} \cite{ref68}; however, the magnon case can exhibit richer behaviour because of the larger set of possible symmetries. The symmetries of magnetically ordered systems and their implementation on magnon Hamiltonians are discussed in App. \[C\].

Since our findings justify an effective two-band model for bosonic BdG Hamiltonians, we can use simple codimension counting approaches familiar from fermionic systems \cite{ref34} \cite{ref69} \cite{ref70} to understand the emergence of generic gapless features in magnon spectra, giving a useful complimentary understanding of the topologically protection.

Given a Bloch coefficient matrix function $H_k$, we first maximally block-diagonalize it using all the $(k$-conserving) unitary symmetries of the Hamiltonian—for example, the spin-rotation symmetry in the example above (see App. \[C\] for a general discussion). This gives rise to “symmetryless” blocks $\{H_k^3\}$ whose dependence on $k$ should be generic. Then, we consider the action of magnetic inversion symmetries—which are antimititary—on the symmetryless blocks to understand the generic band touchings that occur within them.

#### A. Two-band effective Hamiltonian for magnon systems

Consider a symmetryless block as described above, at least of size $2 \times 2$. At a wavevector $k_0$ at which $H_{k_0} > 0$, the magnon spectrum at $k_0$ and neighboring wavevectors is given by the set of positive eigenvalues of the $\tau^3$-Krein-Hermitian matrix $\tau^3 H_k$. Assume two positive eigenvalues of $\tau^3 H_k$, spanning a subspace $P_0$, are separated from the rest of the spectrum by nonzero gaps. In the neighbourhood of $k_0$, we can write

$$\tau^3 H_k = \tau^3 H_{k_0} + \tau^3 (H_k - H_{k_0}),$$

with the second term on the right-hand side acting as a “small” perturbation of the first term.

For every $k$ in a sufficiently small neighborhood of $k_0$, the SW transformation for Krein-Hermitian Hamiltonians presented in the previous section gives an effective Hamiltonian $P_0 (\tau^3 H_k) P_0$ (as defined in and after Eq. \[13\] for the subspace $P_0$, which faithfully reproduces the band structure. We reiterate that the SW method is especially well suited for the study of band touchings and their neighbourhoods. Since $P_0$ contains only positive-signature bands, the effective Hamiltonian is Hermitian.
In the eigenbasis of \( \tau^3 H_{k0} \), it is given by

\[
P_0(\tau^3 H_{k}) P_0 = d^0_k \sigma^0 + d^0_k \cdot \vec{\sigma},
\]

where \((\sigma^0, \vec{\sigma})\) are the Pauli matrices in the two-dimensional subspace \( P_0 \) and where \( d^0_k, \mu \in \{0, 1, 2, 3\} \) are real.

Importantly, the expressions for the effective Klein-Hamiltonian Hamiltonian (App. A) reveal that if \( H_k \) is real, so is the effective Hamiltonian \( P_0(\tau^3 H_{k}) P_0 \), forcing the term proportional to \( \sigma^2 \) to vanish, and meaning that the two bands touch iff the functions \( d^0_k \) and \( d^1_k \) vanish simultaneously. In that case, except at high-symmetry momenta, band touchings that are stable against symmetry-preserving perturbations will generically have a codimension of two, with twofold degeneracy. Otherwise, they would have a codimension of three, with twofold degeneracy.

B. Constraint of magnetic inversion symmetry and examples

As shown in App. C, the constraint due to magnetic inversion in a magnon system is generally \( H_k = V^\dagger H^*_k V \), where \( V \) is paramunitary, unitary, particle-hole symmetric, and also symmetric. This implies that \( V V^\ast = +\mathbb{1} \), i.e. that magnetic inversion squares to \( +1 \) [67]; indeed, this must be the case for integer-spin excitations [33, 51], like the magnon. Furthermore, because \( V V^\ast = +\mathbb{1} \), there must exist a basis in which the constraint takes the simple form \( H_k = H^*_k \)—see App. C.

This basis, however, may not coincide with that in which \( H_k \) is maximally block-diagonalized into symmetryless blocks. If a symmetryless block \( H^a_k \) is mapped to itself \( (H^a_k = V^\dagger H^a_k V \) for some \( V \), then magnetic inversion admits a representation within that block, and its generic band touchings are twofold degenerate and have codimension two instead of three. If two blocks \( H^a_k \) and \( H^a_{k'} \) are mapped to each other \( (H^a_k = V^\dagger H^a_{k'} V \) for some \( V \)), then they have the same energy eigenvalues, so their generic band touchings are fourfold degenerate with codimension three.

We now discuss some examples of magnon band touchings from the literature and illustrate how the dimension approach can be useful for quickly understanding the generic features.

1. Magnetic inversion and spin rotation symmetries

The scenario considered in Ref. [35] is that of a 3D collinear antiferromagnetic spin system with magnetic inversion symmetry \( \{P|\tau\} T \) in Seitz notation [71], where \( P \) denotes inversion, \( T \) denotes time reversal, and \( \tau \) is some origin-dependent translation), with and without spin-rotation symmetry. If the system has a spin-rotation symmetry about an axis, say \( \hat{z} \), the excitations conserve the quantum number \( S_z \). This is a \( k \)-independent symmetry that allows a block-diagonalization of \( H_k \),

\[
H_k = \begin{bmatrix} H_k^+ \\ H_k^- \end{bmatrix},
\]

into sectors corresponding to excitations with \( S_z = \pm 1 \) [55] (see App. C for details). In this case, magnetic inversion interchanges \( +\hat{z} \) spins and \( -\hat{z} \) spins, hence mapping the two blocks to each other and making the spectrum everywhere doubly degenerate. Then, assuming the blocks are symmetryless, the generically occurring band touchings are fourfold-degenerate isolated points; as explained in Ref. [35] they are made up of Weyl points with opposite monopole charges, making them Dirac points.

If the spin-rotation symmetry is broken by certain spin-orbit-coupling (SOC) terms in the Hamiltonian or by canting of the spins, but the magnetic inversion symmetry is preserved, then \( H_k \) can no longer be block-diagonalized into definite-spin sectors. Assuming \( H_k \) is a symmetryless block, its generic gapless manifolds are doubly-degenerate lines.

Of course, an analysis based simply on the codimension of the generic gapless manifolds does not tell the whole story [34]. For instance, it does not capture the \( Z_2 \) monopole charge carried by the the Dirac nodes and gapless lines in this example [35], which explains why the two can evolve into each other, but cannot—contrary to other gapless lines—gap out without encountering an opposite charge [34, 33, 64]. Nonetheless, the simplicity of this analysis makes it complimentary to other approaches.

In Ref. [35] the authors propose Cu$_3$TeO$_6$ as a material nearly at the cusp between these two scenarios. Indeed, Heisenberg interactions (which have spin-rotation symmetry) appear to be dominant; thus, in the absence of subdominant interactions, we expect Dirac points in the bandstructure. However, weak SOC likely breaks the spin-rotation symmetry and deforms the Dirac points into small gapless lines. Indeed, Dirac points have recently been observed in experiment, though they may be gapless lines that are too small to be resolved with current resolutions [36, 37].

2. Effective magnetic inversion and Heisenberg ferromagnets

We can contrast the scenario of Sec. IV B 1 with one in which the magnetic inversion symmetry is replaced with an effective magnetic inversion symmetry that leaves the spin direction unchanged, an example of which is considered in Ref. [72]. Such a symmetry is possible in the absence of certain SOCs, and necessarily acts differently in position space and spin space. Using a modified Seitz notation (see App. C), we denote the effective magnetic inversion as \( h = \{P|Q|\tau\} T \)—here \( Q \) is a spin rotation by \( \pi \) about some suitable axis that serves to return the spin to its original direction.
If spin rotational symmetry about an axis is present, the Bloch Hamiltonian can again be block-diagonalized into spin-conserving sectors, as in Eq. \[18\]. However, rather than interchanging the sectors, \( h \) now maps each sector to itself. Therefore, the intra-sector band touchings will generically have codimension two and twofold degeneracy (assuming each sector is symmetryless). Of course, inter-sector band touchings can also occur; since they involve bands with different spin quantum numbers, their touchings will generically be of codimension one with twofold degeneracy.

On the other hand, if the spin rotation symmetry is broken, leaving the Bloch Hamiltonian symmetryless, any codimension-one band touchings either gap out or are reduced to codimension two.

The situation considered in Ref. \[72\] a spin model with Heisenberg interactions and ferromagnetic order, falls within this category. The effective magnetic inversion \( h = \{ P; R(\pi \hat{n}) | \tau \} T \) — where \( R(\pi \hat{n}) \) is a spin rotation of \( \pi \) about \( \hat{n} \) and \( \hat{n} \) is any axis perpendicular to the spin direction — protects the nodal lines. As the authors mention, certain SOCs, like the Dzyaloshinskii-Moriya (DM) interaction, would gap out the nodal lines completely or downgrade them to Weyl points. In our present language, it is those interactions that are incompatible with the symmetry \( h \) that will generically gap out nodal lines.

3. Nodal lines in a stacked honeycomb quantum magnet

We next discuss a concrete model Hamiltonian of a stacked honeycomb quantum magnet. A recent example of such a quantum magnet is provided by CoTiO\(_3\). CoTiO\(_3\) has an ilmenite structure and space group group \( \text{R}32 \); its magnetic Co\(^{2+}\) ions form stacked honeycomb layers with ABC-type stacking \[38, 39, 73\]. It becomes magnetically ordered below \( T_N \approx 38 \) K, with ferromagnetic order within each layer and antiferromagnetic stacking of the layers. The ordering direction is in plane \[38, 39, 73\].

The onset of magnetic order considerably lowers the symmetry: the corresponding magnetic space group is \( PS I \), which contains only inversions, magnetic inversions, and magnetic translations \[38, 39, 71, 73\].

The dominant exchange interactions are not rotation invariant about the ordering direction, since they have an easy-plane anisotropy \[38, 39\]. Hence, there is no approximate spin-rotation symmetry, and we expect gapless lines to be generically stable because of the magnetic inversion symmetry \( h_{\text{MI}} \) present in \( PS I \). Indeed, seemingly gapless lines have been reported in recent experiments \[38, 39\].

4. XXZ model of a stacked honeycomb quantum magnet

Let us now consider a simple spin model for CoTiO\(_3\) whose linear spin-wave theory has been found to capture all but the fine details of the magnon spectrum, including the observed gapless lines \[38, 39\]. It consists of effective spin-one-half moments on the Co\(^{2+}\) ions, coupled by easy-plane XXZ interactions; see App. \[B\] for details.

The effect of including additional symmetry-allowed SOC terms, which are not rotationally symmetric about the \( \hat{z} \) axis, is to eliminate certain extraneous symmetries of the XXZ interactions. The strength of the various spin interactions in CoTiO\(_3\) and other honeycomb magnets, including Kitaev, Gamma, and DM interactions, is still a subject of active research \[38, 39, 73\]. Therefore, rather than predicting the aspect of the gap closures in the presence of all such subdominant SOC terms, we merely focus on the general effects of lowering the symmetry. For this purpose, we use the DM interaction to illustrate the general effects of lowering the XXZ model symmetries, while recognizing that this is not the dominant SOC term relevant to CoTiO\(_3\). The four magnetic Co\(^{2+}\) ions per magnetic unit cell \[39, 73\] give rise to four magnon bands, which we label 1, 2, 3, and 4 in order of increasing energy.

a. Pure XXZ model With no additional interactions present, the XXZ model has more symmetry than required by the magnetic space group \( PS I \); in particular, the ordering direction can be freely rotated about the stacking axis \( \hat{z} \) at no energy cost \[39\]. Consequently, for a fixed in-plane order, the model’s spin-space group (see App. \[C\]) includes the unitary symmetry \( g = \{ 1; R(\pi \hat{z}) | \tau_g \} \), where the translation \( \tau_g \) connects like sublattices of the honeycomb in adjacent layers. The coefficient matrix \( H_k \) can hence be block-diagonalized into two sectors corresponding to the eigenvalues of \( g \), and the band touchings from different sectors are generically surfaces (codimension one) \[76\]. Indeed, with the parameters of App. \[B\] we find that gapless surfaces occur between bands 1 and 2 as well as between bands 3 and 4.

Another consequence of the additional symmetry of the XXZ model is the presence of an effective magnetic inversion symmetry \( h_{\text{EMI}} = \{ P; R(\pi \hat{z}) | \tau_h \} T \), distinct from the true magnetic inversion \( h_{\text{MI}} \) present in \( PS I \). Indeed, \( h_{\text{EMI}} \) interchanges sites with the same ordering directions, while \( h_{\text{MI}} \) interchanges sites with opposite ordering directions. Both magnetic inversions work \( \text{within} \) the sectors that arise from the symmetry \( g \), meaning either can stabilize magnon gapless lines, and both would have to be broken in order to destroy the gapless lines in the model, which occur between bands 2 and 3 (these are the gapless lines described in Refs. \[38, 39\]. We emphasize, however, that \( h_{\text{MI}} \), which is part of \( PS I \), is model independent, presuming the magnetic space group has been accurately identified \[39, 73\].

b. Adding SOC terms The addition of the DM interaction breaks the symmetries \( g \) and \( h_{\text{EMI}} \) of the pure XXZ model (see App. \[B\] for further details). The remaining magnetic inversion symmetry \( h_{\text{MI}} \) stabilizes gapless lines, which are shown in blue in Fig. \[2\] for the parameter set given in App. \[B\]. The gapless spirals already present in the pure XXZ model \[38, 39\] are qualitatively unchanged, and appear between bands 2 and 3 (Fig. \[2\]). This is expected, since here the DM interaction is a relatively small perturbation to the XXZ interaction, and the nodal
(a) Gap closings between bands 1 and 2.  (b) Gap closings between bands 2 and 3.  (c) Gap closings between bands 3 and 4.

**FIG. 2:** Magnonic gap closings in a stacked honeycomb magnet modelled with an XXZ interaction together with a weak DM interaction, with parameter values given in App. B. As argued in the text, the gap closings in the presence of magnetic inversion should generically be gapless lines, and indeed a plethora of gapless lines (shown in blue) are found. If magnetic inversion symmetry is broken (see main text and App. B), the gap closings are Weyl points and are shown in red.

lines are stable against small symmetry-preserving perturbations. On the other hand, the gapless lines between bands 1 and 2 (Fig. 2a, blue lines) and 3 and 4 (Fig. 2c, blue lines) are new and are the remnants of the gapless surfaces of the pure XXZ model, which have been reduced to lines by the DM interaction. We expect that including other symmetry-allowed subdominant interactions would significantly alter these gapless lines, though they would still appear as the remnants of the gapless surfaces as long as the subdominant interactions are small.

If the magnetic inversion symmetry $h_{MI}$ were somehow broken, gapless lines would no longer be stable, and since no spin rotation symmetry is present, the generically occurring band touching would become Weyl points. To demonstrate this, we introduce a small Zeeman field on one of the four atoms in the magnetic unit cell (see App. B), hence explicitly breaking $h_{MI}$. (Incidentally, this perturbation also breaks inversion symmetry and the magnetic translation symmetry.) The remaining band touchings—all Weyl points—are shown in red in Fig. 2; some of the gapless lines have been reduced to Weyl points, while others have fully disappeared.

c. Easy-axis XXZ model It is informative to contrast the easy-plane XXZ model discussed above with its easy-axis counterpart, in which the ordering direction is parallel to $\hat{z}$, with the order otherwise unchanged. The magnetic space group associated with this order is $R_{I}\bar{3}$ [39], which also contains a model-independent magnetic inversion symmetry $h_{MI}$.

As in the easy-plane case, the easy-axis XXZ model gives rise to an additional, effective magnetic inversion symmetry $h_{EMI}$. Crucially, whereas the easy-plane case has no spin rotation symmetry, the present model has spin-rotation symmetry about the $\hat{z}$ axis, meaning $H_{k}$ can be block-diagonalized as in Eq. 18. Since $h_{MI}$ interchanges the blocks $H_{k}^{+}$ and $H_{k}^{-}$, it causes them to have the same eigenvalues, making the bands everywhere at least doubly degenerate. Since $h_{EMI}$ maps each block to itself, its effect is to generically give rise to gapless lines rather than gapless points.

The symmetries $h_{MI}$ and $h_{EMI}$ can be broken independently using different Zeeman fields on the four sublattices of the magnetic unit cell. The effects of breaking either or both of these symmetries are presented in Table I. The explicit form of the Hamiltonian and the parameters used in the numerics are presented in App. B.

The previous examples all pertain to band touchings at generic momenta, i.e., not at high-symmetry points of the Brillouin zone. Of course, as is commonly done in fermion systems [34, 77], these methods can also be applied specifically to high-symmetry lines or planes, which are left invariant by additional unitary symmetries [42]. Within these manifolds, the additional symmetries can give rise to a block structure different from that at generic momenta.

V. CONCLUSION

In summary, after reviewing Krein-Hermitian Hamiltonians, particularly those arising as single-particle bosonic BdG Hamiltonians, we formulated a Krein-unitary SW transformation, paying special attention to the consequences of Krein stability theory and to the form of
We then reviewed this line of reasoning in the context of This simplification works well for many magnetic materi-
systems with strong quantum fluctuations [78], [79]. Sys-
als [78], though it can fail even at zero temperature for
Hamiltonian are taken to be long-lived quasiparticles.
bosons are neglected and the eigenstates of the quadratic
adopted here, interaction between the Holstein-Primakoff
emphasizing differences with electron systems.
magnon systems using examples from the literature, and
is easily predicted, much as for Hermitian Hamiltonians.
energy bands, the generic codimension of band touchings
• In numerics, gapless lines are observed between the
two pairs of degenerate bands.

| \( h_{EMI} \) unbroken | \( h_{EMI} \) broken |
|-----------------------|---------------------|
| • All bands are at least doubly degenerate because of \( h_{MI} \). |
| • Band touchings within each sector are generically lines because of \( h_{EMI} \). |
| • In numerics, gapless lines are observed between the two pairs of degenerate bands. |
| • The two sectors \( H^+ \) and \( H^- \) are independent. |
| • Global double degeneracy is gone, and bands from different sectors generically cross on surfaces (codi-
mension one). |
| • Band touchings within each sector are generically lines because of \( h_{EMI} \). |
| • In numerics, gapless surfaces are observed between bands 2 & 3; gapless lines are observed between bands 1 & 2 and 3 & 4. |

The two sectors \( H^+ \) and \( H^- \) are independent. Global double degeneracy is gone, and bands from different sectors generically cross on surfaces (codimension one).
Band touchings within each sector are generically points.
In numerics, gapless surfaces were found between each pair of adjacent bands.

| \( h_{MI} \) broken |
|-------------------|
| • All bands are at least doubly degenerate because of \( h_{MI} \). |
| • Band touchings within each sector are generically points. |
| • In numerics, no gapless lines are observed between the two pairs of degenerate bands. |

The two sectors \( H^+ \) and \( H^- \) are independent. Global double degeneracy is gone, and bands from different sectors generically cross on surfaces (codi-
mension one).
Band touchings within each sector are generically points.
In numerics, gapless surfaces are observed between each pair of adjacent bands.

We argued that, in a translation-invariant Krein-
Hermitian system, the SW transformation we formulated
justifies the description of adjacent bands by reduced
effective Hamiltonians, at least locally in momentum
space. For a single-particle bosonic Hamiltonian \( \tau^3 H^*_k \)
with \( H^*_k > 0 \), a subset of contiguous positive-energy
bands that is gapped from the rest of the spectrum near
\( k_0 \) can locally be described by a Hermitian reduced Hamiltonian. In particular, by considering two adjacent positive-energy bands, the generic codimension of band touchings is easily predicted, much as for Hermitian Hamiltonians. We then reviewed this line of reasoning in the context of magnon systems using examples from the literature, and emphasizing differences with electron systems.

In the linear spin-wave approximation, which we have adopted here, interaction between the Holstein-Primakoff bosons are neglected and the eigenstates of the quadratic Hamiltonian are taken to be long-lived quasiparticles. This simplification works well for many magnetic materials [78], though it can fail even at zero temperature for systems with strong quantum fluctuations [78], [79]. Systems in which magnon interactions play an essential role are at the forefront of the field of topological magnons [79]. On the other hand, whereas electrons can be spinless only in an approximate sense, for magnons and other bosonic particles, space-time inversion truly squares to +1 regardless of additional material details [80].

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Appendix A: Details of perturbative SW transformation

This section provides more details on the perturba-
tively defined transformation presented in Sec. III B. The presentation follows that of Ref. [27] adapting it to Krein-Hermitian matrices.

We seek an effective Hamiltonian \( \tilde{K} \) that is block-
diagonal in the subspace \( P_0 \), meaning \( \tilde{K}_0 = 0 \), and that reproduc-
est the spectrum of \( K \) order by order in the perturbation \( K' \)—see Eq. [14]. We assume that there exists a skew-Krein-unitary \( W = -W^\dagger \) that block-diagonalizes the perturbed Hamiltonian \( K \) order-by-order in the perturbation \( K' \), and later confirm our assumption by establishing

TABLE I: The effects of the symmetries \( h_{MI} \) and \( h_{EMI} \) on the band touchings in the easy-axis stacked honeycomb XXZ model, which has spin-rotation symmetry about the \( \hat{z} \) axis. See Sec. IV B 4 c for details and App. [8] for parameter values.
that explicit expressions for such a \( W \) can be found to all orders.

We further assume that \( W \) is block-off-diagonal; i.e., \( W_{bb} = 0 \). Because of this, \([A_b, W]\) is purely block-off-diagonal and \([A_o, W]\) is purely block-diagonal for any \( A \). Hence, the transformed Hamiltonian can be split into block-diagonal and block-off-diagonal parts:

\[
\tilde{K}_b = \sum_{l=0}^{\infty} \frac{1}{(2l)!} [K_b, W]^{(2l)} + \sum_{l=0}^{\infty} \frac{1}{(2l+1)!} [K_o, W]^{(2l+1)},
\]

(A1a)

\[
\tilde{K}_o = \sum_{l=0}^{\infty} \frac{1}{(2l)!} [K_o, W]^{(2l)} + \sum_{l=0}^{\infty} \frac{1}{(2l+1)!} [K_b, W]^{(2l+1)},
\]

(A1b)

where

\[
[A, B]^{(l)} := \ldots [A, B, B, \ldots, B].
\]

(A2)

We then further constrain the generating matrix \( W \) by demanding that \( \tilde{K}_o = 0 \); order by order in the perturbation \( K' \), making the transformed Hamiltonian \( \tilde{K} = \tilde{K}_b \) purely block diagonal. Letting \( W = W_0 + W_2 + \ldots \), this requirement leads to the constraints of Eq. 15. As noted in the main text, these constraints are compatible with the assumption that \( W \) is skew-Krein-Hermitian to all orders.

Working in the eigenbasis of \( K^0, K^0_{t_i} = E^0_{t_i}, \) Eq. 15 can be solved order by order. For instance,

\[
[K^0, W^{(1)}] = -K'
\]

\[
\Leftrightarrow \sum_c \left( K^0_{ac} W^{(1)}_{cb} - W^{(1)}_{ac} K^0_{cb} \right) = -(K')_{ab}
\]

(A3a)

\[
\Leftrightarrow \left( E^0_a - E^0_b \right) W^{(1)}_{ab} = -(K')_{ab}
\]

Letting \( m \) index states in \( \mathcal{P}_0 \) and \( l \) index states not in \( \mathcal{P}_0 \) (or vice versa), we may then write

\[
W^{(1)}_{ml} = -\frac{K'_{ml}}{E^0_m - E^0_l}, \quad W^{(1)}_{mm} = W^{(1)}_{l0} = 0.
\]

(A3b)

By the same token, one can find the expressions to all orders:

\[
W^{(2)}_{ml} = \frac{1}{E^0_m - E^0_l} \left( \sum_{m'} K'_{mm} K'_{ml} - \sum_{l'} K'_{ml} K'_{l'l} \right)
\]

(A4)

Using these expressions and that for \( \tilde{K} = \tilde{K}_b \), we find the effective Hamiltonian \( \tilde{P}_0 \tilde{K} \tilde{P}_0 \), whose matrix elements are \( \tilde{K}_{mm'} \), order by order:

\[
\tilde{K}^{(0)}_{mm'} = K^0_{mm'}
\]

(A5a)

\[
\tilde{K}^{(1)}_{mm'} = K'_{mm'}
\]

(A5b)

\[
\tilde{K}^{(2)}_{mm'} = \frac{1}{2} \sum_l K'_{ml} K'_{l'm} \left( \frac{1}{E^0_m - E^0_l} + \frac{1}{E^0_{m'} - E^0_{l'}} \right)
\]

(A5c)

The zeroth- and first-order expressions are manifestly Krein-Hermitian with respect to \( \mathcal{P}_0 \); the higher orders, which involve mixing with states outside \( \mathcal{P}_0 \), are too, as can be seen using \( K'_{ab} = \eta_{ab} K'_{ba} \eta_{bb} \) and the fact that \( \eta \) is diagonal with entries \( \pm 1 \).

The formulae for \( W^{(j)} \) and \( \tilde{K}^{(j)} \) at all orders have the same form as those for a Hermitian Hamiltonian, more of which are given in Refs. 27 and 26. The expansion is controlled as long as the perturbation is small compared to energy separations between states in \( \mathcal{P}_0 \) and states outside \( \mathcal{P}_0 \).

Appendix B: Details and parameter values for XXZ model

This section provides more details on the XXZ spin model and parameter values used in Sec. [VB.4]. As explained in the main text, it is based on models of CoTiO\(_3\) wherein effective spin 1/2 moments at each Co\(^{2+}\) ion are coupled by XXZ interactions [38, 39]. In general, the Hamiltonian has the form

\[
H_{XXZ} = \sum_{i<j} \left( J_{ij} \left( S^x_i S^x_j + S^y_i S^y_j \right) + J_{ij}^z S^z_i S^z_j \right),
\]

(B1)

where \( i \) and \( j \) label spins and “\( i < j \)” indicates that pairs of spins are not double counted. In the stacked honeycomb geometry under study, the \( \hat{z} \) direction is taken to be the stacking direction (see Fig. 3). Hence, an XXZ interaction is of easy plane if \( |J| > |J^z| \), and of easy axis if \( |J| < |J^z| \); the magnetic ground-state order depends on the relative strength of the nonzero interactions and their coordination numbers.

a. Easy plane Our choice of which spins to couple with the interactions of Eq. (31) is loosely based on Refs. [38] and [39], which model the magnon dispersion of CoTiO\(_3\). An additional, weak coupling, \( J_9 \), is included to avoid accidental degeneracies along six lines in the Brillouin zone [31]. The couplings are as follows:

- Between NN in-plane spins: \( J_1 = -1 \) and \( J_1^z = 0.25 J_1 \) (see Ref. [38] for schematic representation);
- Between NNN sites in adjacent layers: \( J_2 = 0.5, J_2^z = 0.25 J_2 \) (see Ref. [38]);
- Between NN sites in adjacent layers: \( J_3 = 0.5, J_3^z = 0.25 J_3 \) (see Ref. [38]).
With these parameter values, the magnetic order is manifestly in the magnetic unit cell (see Fig. 3), in the direction with magnitude $0_1$. Two layers are shown, both as a 3D illustration in panel (a) and as a projection along the stacking direction $\hat{z}$ in panel (b). The crystal’s primitive lattice vectors $a_1$, $a_2$, and $a_3$ are shown; the magnetic order doubles the third one to $2a_3$. Sublattice indices 1, 2, 3, and 4 of the magnetic unit cell are shown in panel (a).

- Between NN sites three layers apart: $J_3 = 0.02$, $J_9^+ = J_9$.  

With these parameter values, the magnetic order is manifestly in plane, with ferromagnetic order within each layer and antiferromagnetically stacked layers. The ordering direction is chosen to be $\hat{x}$ (see Fig. 3), and the Holstein-Primakoff transformation is carried out as shown in App. C.

b. Easy-plane XXZ with DM As explained in Sec. IV B 4, a weak DM interaction,
\begin{equation}
H_{\text{DM}} = \sum_{i<j} D_{ij} \cdot (S_i \times S_j),
\end{equation}
is added to the easy-plane XXZ model to break certain extraneous symmetries of the pure XXZ model.

In the space group $R\bar{3}$ of the stacked honeycomb CoTiO$_3$, the geometry of which we are using here, inversion centers forbid DM interactions on the intra-layer NN bonds. Hence, the simplest choice is to include it on the intra-layer NN bonds; this leaves the magnetic order unchanged. The vector $D_{ij}$ on one such bond is not constrained by symmetry—we choose it to be in the $\hat{x}$-$\hat{y}$ plane and perpendicular to the bond direction, pointing toward the center of each hexagonal plaquette, and with magnitude 0.25. The interactions on different bonds are constrained by the threefold rotation, inversion, and translation symmetries of $R\bar{3}$. The gapless lines of the associated linear spin wave dispersion are represented in Fig. 2.

In order to break the magnetic inversion symmetry $h_{\text{MI}}$ and destabilize the gapless lines, a Zeeman field $B_1 = B_1\hat{x}$, with $B_1 = 0.0008$, is introduced on sublattice 1 in the magnetic unit cell (see Fig. 3), in the direction of the ground-state magnetic moment. This lifts the line degeneracies, leaving behind gapless points, as shown in Fig. 2.

c. Easy-axis XXZ In Sec. IV B 4c we consider an easy-axis version of the model of Eq. (B1) using the following parameters:

- Between NN in-plane spins: $J_1 = -1$ and $J_1^+ = 1.5 J_1$;
- Between NN sites in adjacent layers: $J_2 = 0.5$, $J_2^+ = 1.5 J_2$;
- Between NN sites in adjacent layers: $J_3 = 0.5$, $J_3^+ = 1.5 J_3$;
- Between NN sites three layers apart: $J_9 = 0.02$, $J_9^+ = J_9$.

With these values, the magnetic order is clearly parallel to the stacking direction $\hat{z}$, with ferromagnetic order within each layer and antiferromagnetically stacked layers. The Holstein-Primakoff transformation is carried out as shown in App. C.

In the results presented in the main text, Zeeman fields pointing along the moments are used to selectively break the symmetries $h_{\text{MI}}$ and $h_{\text{EMI}}$. Labelling the four sublattices in the magnetic unit cell as shown in Fig. 3, the Zeeman fields are $B_1 = B_1\hat{z}$, $B_2 = B_2\hat{z}$, $B_3 = -B_3\hat{z}$, and $B_4 = -B_4\hat{z}$. Since $h_{\text{MI}}$ constrains $B_1 = B_4$ and $B_2 = B_3$, and $h_{\text{EMI}}$ constrains $B_1 = B_2$ and $B_3 = B_4$, the symmetries can be selectively broken in the following way:

- $B_1 = B_2 = 0.01$ and $B_3 = B_4 = 0$ to break $h_{\text{MI}}$;
- $B_1 = B_3 = 0.01$ and $B_2 = B_4 = 0$ to break $h_{\text{EMI}}$;
- $B_1 = B_3 = 0.01$ and $B_2 = B_4 = 0.03$ to break both $h_{\text{MI}}$ and $h_{\text{EMI}}$.

Appendix C: Implementation of symmetries in magnon Hamiltonians

In this section, we provide an overview of how symmetries of a spin Hamiltonian translate to symmetries of the magnon Hamiltonian in a compatible ordered state. We highlight the constraints that unitary and antiunitary symmetries place on the single-particle Bloch Hamiltonian (Eqs. C19 and C28). We show that, in the right basis, magnetic inversion symmetry constrains the single-particle magnon Hamiltonian to be purely real.

1. Overview

The spin space group of a spin Hamiltonian together with a compatible classical ground state is the set of symmetries of the Hamiltonian which also leave the classical order invariant [71,82,84]. Such symmetries have
a well-defined implementation in the magnon Hamiltonian, which describes excitations above a specific classical ground state. Symmetries of the spin-space group come in two types: those that include the operation of time reversal and those that do not \([6][7]\). Time reversal alone is never part of the spin-space group.

Spin space groups are closely related to, though distinct from, magnetic space groups—a magnetic space group is the symmetry group of a crystal structure endowed with a magnetic order \([71]\). For example, since an effective spin Hamiltonian can have more symmetry than the physical system it models, the spin space group may contain symmetries not present in the magnetic space group. In particular, unlike the magnetic space group, the spin space group can have symmetries that act differently on spin and position space. We will denote such operations using a modified Seitz notation \([71]\): \(g = \{Q_g; Q_g^*; \tau_g\}\), where the first entry denotes the O(3) operation acting in position space. Given a spin labeled \(i\), we refer to the site to which \(i\) is mapped by \((g)\) \(g(i)\): \(x_{g(i)} = \{Q_g|x_i|\tau_g\}\). We will find that in the local frame, transformations in the spin-space group are of the form

\[
\hat{S}_i \rightarrow \hat{S}'_i = \begin{bmatrix} \ast & \ast & 0 \\ \ast & \ast & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{S}^x_i \\ \hat{S}^y_i \\ \hat{S}^z_i \end{bmatrix}.
\]

(C1)

Hence, these symmetry transformations mix together only the components transverse to the local classical order.

2. Spin Hamiltonian

We begin with a spin Hamiltonian with a corresponding classical ground state. Spin interactions beyond bilinear order can also be included, and would not change our conclusions at the level of noninteracting bosons.

\[
\hat{H} = \frac{1}{2} \sum_{ij} \hat{S}^\dagger_i M_{ij} \hat{S}_j - \sum_i \hat{B}^\dagger_i \hat{S}_i.
\]

(C2)

We may choose \(M_{ij} = M^\dagger_{ji}\). Furthermore, the Hermicity of \(\hat{H}\) and the assumption of time-reversal symmetry (absent the Zeeman term) makes \(M_{ij} = M^\dagger_{ji}\) real for all \(i\) and \(j\).

Consider a classical ground state compatible with the spin Hamiltonian. To carry out the Holstein-Primakoff transformation, each spin is expressed in a local basis whose \(\hat{z}\) direction (and quantization axis) is aligned with the classical ordering direction of that spin. Hence, we let

\[
\hat{S}_i = R_i \hat{S}_i, \quad \hat{S}_i = \begin{bmatrix} \hat{S}^x_i \\ \hat{S}^y_i \\ \hat{S}^z_i \end{bmatrix}^\dagger,
\]

where \(R_i\) is an appropriate SO(3) rotation matrix. There is, of course, freedom in the choice of \(R_i\). The Hamiltonian becomes

\[
\hat{H} = \frac{1}{2} \sum_{ij} \hat{S}^\dagger_i M_{ij} \hat{S}_j - \sum_i \hat{B}^\dagger_i \hat{S}_i, \quad \text{(4a)}
\]

\[
\begin{aligned}
\tilde{M}_{ij} := & \; R_i^\dagger M_{ij} R_j = \tilde{M}_{ji}^\dagger, \\
\tilde{B}_i := & \; R_i^\dagger B_i.
\end{aligned}
\]

(C4b)

The stability of the classical order implies that linear contributions (in \(\hat{S}^x_i\) and \(\hat{S}^y_i\)) to the Hamiltonian vanish.

We now proceed to rewrite the spin operators in terms of Holstein-Primakoff bosons. Letting \(\phi_i = \begin{bmatrix} b_i & b_i^\dagger \end{bmatrix}^\dagger\), in the linearized Holstein-Primakoff transformation, the spin operators become

\[
\begin{aligned}
\tilde{S}^+_i := & \; \sqrt{2S_i} b_i + \ldots, \\
\tilde{S}^-_i := & \; \sqrt{2S_i} b_i^\dagger + \ldots, \\
\tilde{S}^z_i := & \; S_i - b_i b_i^\dagger = S_i + \frac{1}{2} - \frac{1}{2} \phi_i^\dagger \phi_i,
\end{aligned}
\]

(C5)

where \(\phi_i := \tilde{S}^z_i \pm i \tilde{S}^y_i\) are the raising and lowering operators in the local bases, and \(S_i\) is the spin magnitude at site \(i\), formally considered a large parameter controlling the expansion. This way of writing \(\tilde{S}^z_i\) is key in ensuring it is invariant under symmetries. Discarding terms beyond quadratic in boson operators, the linearized Hamiltonian takes the form

\[
\hat{H} = E_{cl} + \frac{1}{2} \sum_{ij} \phi_i^\dagger h_{ij} \phi_j + O(\phi^3),
\]

where \(E_{cl}\) is the classical energy and the \(h_{ij}\) are \(2 \times 2\) coefficient matrices. Note that \(h_{ij} = h_{ji}^\dagger\) as a consequence of \(\tilde{M}_{ij} = \tilde{M}_{ji}^\dagger\). Furthermore, the particle-hole symmetry of \(h_{ij}\), i.e. \(h_{ij} = \tau^1 h_{ji}^\dagger \tau^1\), stems from the reality of \(\tilde{M}_{ij}\) and the symmetric way of writing \(\tilde{S}^z_i\). This constraint leaves no redundancy in \(h_{ij}\).

\textit{Quadratic boson Hamiltonian in Fourier space}

The Fourier transformation is a paraunitary (and unitary) transformation that partially diagonalizes the Hamiltonian. Letting \(i = (R, \alpha)\), where \(R\) denotes the magnetic unit cell (of which there are \(N\)) and \(\alpha\) denotes the magnetic sublattice (of which there are \(n\)),

\[
\phi_{k\alpha} := \begin{bmatrix} b_{k\alpha} \\ b_{k\alpha}^\dagger \end{bmatrix} = \frac{1}{\sqrt{N}} \sum_R e^{-i k \cdot x_{R\alpha}} \phi_{R\alpha}, \quad \text{(7a)}
\]

\[
\phi_{R\alpha} = \frac{1}{\sqrt{N}} \sum_k e^{i k \cdot x_{R\alpha}} \phi_{k\alpha}. \quad \text{(7b)}
\]
With this notation, the Hamiltonian becomes
\[
\hat{H} = E_{cl} + \frac{1}{2} \sum_{ij} \phi_{ij}^\dagger h_{ij} \phi_j = E_{cl} + \frac{1}{2} \sum_{\alpha\beta} \sum_{\alpha\beta} \phi_{\alpha i}^\dagger h_{R\alpha} R_{\alpha\beta} \phi_{\beta j}.
\] (C8)

Using the translational invariance of the magnetic lattice (and assuming the SO(3) matrices \( R_i = R_\alpha \) were chosen with the same translational invariance), we define \( h_{R - R'; \alpha\beta} := h_{R; \alpha\beta} \), as well as its Fourier transform
\[
h_{k; \alpha\beta} := e^{-ik \cdot (\delta_{\alpha\beta} - \delta_{\alpha\beta})} \sum_R e^{-ik \cdot R} h_{R; \alpha\beta}.
\] (C9)

Note that \( h_{ij} = h_{ji}^\dagger \) implies that \( h_{k; \alpha\beta} = h_{k; \beta\alpha} \), and that the particle-hole symmetry \( h_{ij} = \tau^1 h_{ij}^\dagger \tau^1 \) manifests itself in momentum space as \( \tau^1 h_{k; \alpha\beta}^\dagger \tau^1 = h_{-k; \alpha\beta} \).

Finally, the magnon Hamiltonian becomes
\[
\hat{H} = E_{cl} + \frac{1}{2} \sum_k \phi_{k; \alpha}^\dagger h_{k; \alpha\beta} \phi_{\beta k} = E_{cl} + \frac{1}{2} \sum_k \phi_{k; \alpha}^\dagger h_k \Phi_k, \quad \Phi_k := \begin{bmatrix} \phi_{kA} \\ \phi_{kB} \\ \vdots \end{bmatrix},
\] (C10a)
\[
\phi_{kA} = e^{-ik \cdot \delta_{\alpha\beta}} \sum_R e^{-ik \cdot R} h_{R; \alpha\beta}.
\] (C10b)

where we have introduced the spinor \( \Phi_k \) and the \( 2n \times 2n \) coefficient matrix \( H_k \). The matrix \( H_k \) is Hermitian and (assuming the classical order is stable) positive semidefinite. Also, the PH symmetry now takes the form \( \tau^1 H_k^\dagger \tau^1 = H_{-k} \).

### 3. Unitary symmetries

Let \( g \) be a unitary symmetry of the spin-space group, with unitary Hilbert-space implementation \( U_g \). These are the operations of the spin-space group that do not contain time reversal. In modified Seitz notation, we let \( g = \{ Q_g; Q_g^\dagger \} \). Letting \( S'_i \) denote the transformed spin at site \( i \),
\[
S'_i = U_g S_i U_g^\dagger = (\det Q_g) Q_g^\dagger S_{g^{-1}i}.
\] (C11)

Because spins are axial vectors, they transform with \( (\det Q_g) Q_g^\dagger \), which is always an SO(3) rotation matrix.

By definition of spin-space group symmetries, the transformed spin \( S'_i \) has the same “classical” direction as \( S_i \); therefore, \( S'_i = R_i S'_i \), like \( S_i = R_i S_i \). This way, in the transformation in the local basis from \( S_i \) to \( S'_i \),
\[
\tilde{S}_i = U_g \tilde{S}_i U_g^\dagger = \tilde{Q}_g \tilde{S}_{g^{-1}i},
\] (C12a)
\[
\tilde{Q}_g := R_i (\det Q_g) Q_g^\dagger R_{g^{-1}i},
\] (C12b)

\( \tilde{Q}_g \) is just a rotation about the local \( \tilde{z} \) axis.

Denoting the rotation angle at site \( i \) about the local \( \tilde{z} \) axis as \( \theta^i_g \), the ladder operators transform as \( U_g \tilde{S}_g^\dagger U_g^\dagger = e^{i\theta^i_g} \tilde{S}\), while \( U_g \tilde{S}_g U_g^\dagger = \tilde{S}_{g^{-1}i} \). The rotation angle \( \theta^i_g \) is determined by \( g \) and the rotation matrices \( \{ R_i \} \). The bosons transform as
\[
U_g \phi_i U_g^\dagger = u^i_g \phi_{g^{-1}i}.
\] (C13a)
\[
u^i_g = \begin{bmatrix} e^{i\theta^i_g} & e^{-i\theta^i_g} \end{bmatrix} = e^{i\theta^i_g} \cos \theta^i_g + i \tau^3 \sin \theta^i_g.
\] (C13b)

Note that in addition to being unitary, \( u^i_g \) is paraunitary (a unitary matrix that commutes with \( \tau^3 \) is also paraunitary), so it gives valid boson operators. Furthermore, \( u^i_g \) is particle-hole symmetric, \( \tau^1 (u^i_g)^\dagger \tau^1 = u^i_g \), so the transformed Hamiltonian will be particle-hole symmetric, as it must.

In Fourier space

Next, we consider the transformation in Fourier space. Though \( \tau_g \), the translational part of \( g \), appears in the transformation for \( \phi_{k\alpha} \), it will not appear in the constraint on the Hamiltonian at the quadratic level. For notational convenience, let \( g = g^{-1} (R) \), meaning \( x_{R'\alpha'} = (Q_g)_{g^{-1}} x_{R,\alpha} \). We will use the fact that the rotation matrix \( R_i = R_\alpha \) (and hence \( u^i_g = u^i_{g^{-1}} \)) does not depend on \( R \), but only on \( \alpha \), and also that the transformed sublattice index \( \alpha' \) depends only on \( \alpha \) (and not on \( R \)). For this reason, we can think of the action of \( g \) (or \( g^{-1} \)) on the \( n \) sublattice indices \( \alpha \) as a permutation.

\[
U_g \phi_{k\alpha} U_g^\dagger = \frac{1}{\sqrt{N}} \sum_{R} e^{-ik \cdot R_{\alpha}} U_g \phi_{R_{\alpha}U_g} U_g^\dagger u^\alpha_{g^{-1}} \phi_{R'\alpha'}.
\] (C14)
\[
= \frac{u^\alpha_{g^{-1}}}{\sqrt{N}} \sum_{R} e^{-ik \cdot (Q_g)_{\alpha} R_{\alpha'} \cdot x_{R'\alpha'}} \phi_{R'\alpha'}.
\] (C15)
\[
= \frac{u^\alpha_{g^{-1}}}{\sqrt{N}} \sum_{R} e^{-ik \cdot (Q_g)_{\alpha} R_{\alpha'} \cdot \tau_g} \phi_{R'\alpha'}.
\] (C16)

We can sum over \( R' \) instead of \( R \) because the relation between \( R \) and \( R' \) is bijective:

\[
U_g \phi_{k\alpha} U_g^\dagger = e^{-ik \cdot \tau_g} \frac{u^\alpha_{g^{-1}}}{\sqrt{N}} \sum_{R'} e^{-i(Q_g k)_{\alpha} R_{\alpha'} \cdot \tau_g} \phi_{R'\alpha'}.
\] (C17)
\[
= e^{-i\theta^i_g} u^\alpha \phi_{Q_g k,\alpha'}.
\] (C18)

In terms of the \( 2n \times 2n \) component spinor \( \Phi_k \),
\[
U_g \Phi_k U_g^\dagger = e^{-ik \cdot \tau_g} V_g \phi_{Q_g k,\alpha'}.
\] (C19)
In the above, $F_{g^{-1}}$ is the $n \times n$ permutation matrix for the permutation of sublattices $g^{-1}(\alpha)$, with components

$$P^{\alpha\beta}_{g^{-1}} = \delta^{\alpha\beta} g^{-1}(\alpha),$$

and $C_g$ and $S_g$ are $n \times n$ diagonal matrices with entries $\{\cos \theta^\alpha_g\}$ and $\{\sin \theta^\alpha_g\}$, respectively.

Finally, we find the transformed magnon Hamiltonian:

$$U_g H U_g^\dagger = E_{cl} + \frac{1}{2} \sum_k \left( U_g \Phi^\dagger_k U_g^\dagger \right) H_k \left( U_g \Phi_k U_g^\dagger \right)$$

$$= E_{cl} + \frac{1}{2} \sum_k \left( \Phi^\dagger_k V^\dagger_g H_k V_g \Phi_k \right)$$

(C18)

so the constraint on $H_k$ due to $g$ is

$$H_k = V^\dagger_g H_{Q,g,k} V_g.$$  

(C19)

For a unitary symmetry with $Q_g = 1$, the Nambu-Bloch Hamiltonian can be block-diagonalized at each $k$ into sectors corresponding to the eigenvalues of $V_g$.

4. Antiunitary symmetries

Let $h$ be an antiunitary symmetry in the spin-space group. Such a transformation is made up of a spatial transformation (with unitary implementation $U_h$) along with time reversal. Let $\Theta_h = U_h T$ be the antiunitary operator that implements it in the Hilbert space. In modified Seitz notation, $h = \{Q_h, \Theta_h\} T$. Since $\Theta_h^{-1} = T^{-1} U_h^\dagger$ and spin is odd under time reversal, we have

$$S'_i = \Theta_h S_i \Theta_h^{-1}$$

$$= U_h T S_i U_{-h} = - (\det Q_h^\prime) S_{h^{-1}i}.$$  

(C20)

Once again, $S'_i$ has the same classical direction as $S_i$, so $S'_i = R_i S'_i$, like $S_i = R_i S_i$—this is the key point that allows a well-defined implementation of $h$ on the magnon Hamiltonian and enables us to write the transformation for $S_i$:

$$\tilde{S}'_i = \Theta_h \tilde{S}_i \Theta_h^{-1} = \tilde{Q}_h \tilde{S}_{h^{-1}i},$$

$$\tilde{Q}_h := - R_{h}^\dagger (\det Q_k^\prime) Q_h R_{h^{-1}}.$$  

(C21a)

(C21b)

In this case, the transformation $\tilde{Q}_h$ is an improper rotation about the local $\tilde{z}$ axis; i.e., an $O(3)$ matrix with determinant $-1$ that leaves the $\tilde{z}$ direction invariant.

Nevertheless, the ladder operators transform as

$$\Theta_h \tilde{S}_{h^{-1}} = e^{i \theta^\alpha_h} \tilde{S}_{h^{-1}},$$

while

$$\Theta_h \tilde{S}_{h^{-1}} = \tilde{S}_{h^{-1}},$$

where the parameter $\theta^\alpha_h$ is determined by $h$ and by the SO(3) matrices $\{R_i\}$. The bosons transform as

$$\Theta_h \phi_{\alpha} \Theta_h^{-1} = u^\alpha_i \phi_{h^{-1}i},$$

$$u_h^\alpha = \begin{bmatrix} e^{i \theta^\alpha_h} \\ e^{-i \theta^\alpha_h} \end{bmatrix} = \tau^0 \cos \theta^\alpha_h + i \tau^3 \sin \theta^\alpha_h.$$  

(C22a)

(C22b)

Like $u^\alpha_g$, $u_h^\alpha$ is paramutary, unitary, and particle-hole symmetric.

In Fourier space

Next, we consider the effect in Fourier space. Again, for notational convenience, we let $\{R^{\prime \alpha} \prime\} = h^{-1}(R^{\prime \alpha})$, meaning $x_{R^{\prime \alpha} \prime} = \{Q_h | R^{\prime \alpha} \prime\}^{-1} x_{R^{\prime \alpha}}$.

$$\Theta_h \phi_{\alpha \alpha'} \Theta_h^{-1} = \frac{1}{\sqrt{N}} \sum_{R^{\prime \alpha} \prime} e^{i k \cdot x_{R^{\prime \alpha} \prime}} \phi_{h^{\prime \alpha} \alpha'} u^\alpha_h,$$

$$= \frac{1}{\sqrt{N}} \sum_{R^{\prime \alpha} \prime} e^{i k \cdot \{Q_h | R^{\prime \alpha} \prime \} x_{R^{\prime \alpha} \prime}} \phi_{h^{\prime \alpha} \alpha'}$$

$$= \frac{1}{\sqrt{N}} \sum_{R^{\prime \alpha} \prime} e^{i k \cdot \{Q_h | R^{\prime \alpha} \prime \} \cdot \tau^0 \cdot x_{R^{\prime \alpha} \prime}} \phi_{R^{\prime \alpha} \prime}$$

$$= e^{i k \cdot \tau_h} \frac{1}{\sqrt{N}} \sum_{R^{\prime \alpha} \prime} e^{-i \{Q_h | R^{\prime \alpha} \prime \} \cdot \tau^0 \cdot x_{R^{\prime \alpha} \prime}} \phi_{R^{\prime \alpha} \prime},$$

(C23)

where in the last line, we have changed summation variable from $R$ to $R^{\prime}$. Hence, we find

$$\Theta_h \phi_{\alpha \alpha'} \Theta_h^{-1} = e^{i k \cdot \tau_h} u^\alpha_h \phi_{h^{\prime \alpha} \alpha'},$$

(C24a)

$$\Theta_h \phi_{\alpha \alpha'} \Theta_h^{-1} = e^{-i k \cdot \tau_h} \phi_{h^{\prime \alpha} \alpha'} u^\alpha_h.$$  

(C24b)

In terms of the 2n-component spinor $\Phi_k$,

$$\Theta_h \Phi_k \Theta_h^{-1} = e^{i k \cdot \tau_h} V_h \Phi_{h^{\prime \alpha} \alpha'},$$

$$\Theta_h \phi_{\alpha \alpha'} \Theta_h^{-1} = e^{-i k \cdot \tau_h} \phi_{h^{\prime \alpha} \alpha'} u^\alpha_h,$$

(C25a)

(C25b)

where $V_h$ is a $2n \times 2n$ unitary, paramutary, and particle-hole-symmetric matrix:

$$V_h = C_h P_{h^{-1}} \otimes \tau^0 - i S_h P_{h^{-1}} \otimes \tau^3,$$

(C26)

where $P_{h^{-1}}$, $C_h$, and $S_h$ are defined in analogy with the unitary case.

Finally, the transformed magnon Hamiltonian is

$$\Theta_h \hat{H} \Theta_h^{-1} = E_{cl} + \frac{1}{2} \sum_k \left( \Theta_h \Phi_k \Theta_h^{-1} \right) \hat{H}_k \left( \Theta_h \Phi_k \Theta_h^{-1} \right)$$

$$= E_{cl} + \frac{1}{2} \sum_k \left( \Phi^\dagger_{h^{\prime \alpha} \alpha',k} V_h^\dagger \right) \hat{H}_k \left( V_h \Phi_{h^{\prime \alpha} \alpha',k} \right)$$

$$= E_{cl} + \frac{1}{2} \sum_k \Phi^\dagger_k V_h^\dagger H^*_{h^{\prime \alpha} \alpha',k} V_h \Phi_k,$$

(C27)
so the constraint on $H_k$ due to $h$ is

$$H_k = V_h^\dagger H^*_Q V_h.$$  \hfill (C28)

\begin{itemize}
  \item \textit{When is $V_h$ symmetric?}
\end{itemize}

Here, we identify necessary and sufficient conditions for $V_h = V_h^T$ (or equivalently, $V_h V_h^* = +1$).

First, since $V_h$ is block-diagonal in Nambu space, we can write it as a direct sum of its particle and hole sectors, $V_h = V_h^P \oplus V_h^h$; here, $(V_h^P)^{\alpha\beta} = e^{-i\theta_h^{\alpha}} \delta^{\beta,h^{-1}(\alpha)}$ and $V_h^h = (V_h^h)^*.$

\begin{itemize}
  \item \textit{Necessary condition} First, assume $V_h$ is symmetric. Then,
  \begin{equation}
  (V_h^P)^{\alpha\beta} \equiv (V_h^P)^{\beta\alpha} \quad \forall \alpha, \beta
  \end{equation}
  \begin{equation}
  \Leftrightarrow e^{-i\theta_h^{\alpha}} \delta^{\beta,h^{-1}(\alpha)} \equiv e^{-i\theta_h^{\beta}} \delta^{\alpha,h^{-1}(\beta)} \quad \forall \alpha, \beta. \tag{C29}
  \end{equation}

  Since the equality of two numbers implies the equality of their absolute values, we have

  \begin{equation}
  \Rightarrow \left| e^{-i\theta_h^{\alpha}} \delta^{\beta,h^{-1}(\alpha)} \right| = \left| e^{-i\theta_h^{\beta}} \delta^{\alpha,h^{-1}(\beta)} \right| \quad \forall \alpha, \beta
  \end{equation}

  \begin{equation}
  \Leftrightarrow \delta^{\beta,h^{-1}(\alpha)} \equiv \delta^{\alpha,h^{-1}(\beta)} \quad \forall \alpha, \beta
  \end{equation}

  \begin{equation}
  \Leftrightarrow \delta^{\beta,h^{-1}(\alpha)} \equiv \delta^{\alpha,h^{-1}(\beta)} \quad \forall \alpha, \beta
  \end{equation}

  \begin{equation}
  \Leftrightarrow h^{-1}(\alpha) \equiv h(\alpha) \quad \forall \alpha
  \end{equation}

  \begin{equation}
  \Leftrightarrow h^2(\alpha) \equiv \alpha \quad \forall \alpha. \tag{C30}
  \end{equation}

  In other words, the permutation engendered on the sublattice indices by $h$ must square to identity (called a transposition), i.e., it must be a permutation with only 1-cycles and 2-cycles.

  Hence, the condition becomes

  \begin{equation}
  (e^{-i\theta_h^{\alpha}} - e^{-i\theta_h^{\beta}}) \delta^{\beta,h^{-1}(\alpha)} \equiv 0 \quad \forall \alpha, \beta. \tag{C31}
  \end{equation}

  \begin{itemize}
    \item For $h^{-1}(\alpha) = \alpha$ (a 1-cycle), there is no constraint on $e^{-i\theta_h^{\alpha}}$.
    \item For $h^{-1}(\alpha) = \beta$ and $h^{-1}(\beta) = \alpha$ (a 2-cycle),
  \end{itemize}

  $e^{-i\theta_h^{\alpha}} = e^{-i\theta_h^{\beta}}$.

  Hence, if $V_h$ is symmetric, the permutation is a transposition (i.e., made up of 1-cycles and 2-cycles) and the phases $e^{-i\theta_h^{\alpha}}$ are the same within each cycle of the permutation.

  \begin{itemize}
    \item \textit{Sufficient condition} Assuming the permutation is a transposition and the phases $e^{-i\theta_h^{\alpha}}$ are the same within each cycle of the permutation, it is straightforward to see that $V_h$ is symmetric.
  \end{itemize}

\section{Examples}

\begin{itemize}
  \item \textit{Magnetic inversion symmetry}
  \end{itemize}

We consider magnetic inversion symmetry, i.e. $h = \{P^T \tau\} T$. In this case, $(\det R_h^\alpha) R_h^\alpha = (\det P^T) P = I$.

Consider a pair of sublattices $\alpha$ and $\alpha'$ related by $h$. We can always choose

\begin{equation}
\begin{cases}
R_\alpha = R(\eta_\alpha \hat{m}_\alpha), \\
R_{\alpha'} = R(\eta_\alpha + \pi \hat{m}_\alpha),
\end{cases} \tag{C32}
\end{equation}

where $\eta_\alpha$ and $\hat{m}_\alpha$ are an appropriate angle and unit vector, respectively. In the local frames, the transformation on the spins are

$$\tilde{Q}_h^\alpha = -R_{\alpha'}^\top R_{\alpha} = -R(\pi \hat{m}_\alpha), \tag{C33a}$$

$$\tilde{Q}_h^\alpha = -R_{\alpha'}^\top R_{\alpha} = -R(\pi \hat{m}_\alpha) = -R(\pi \hat{m}_\alpha), \tag{C33b}$$

where the last equality holds because SO(3) rotation matrices have period $2\pi$.

The fact that $\tilde{Q}_h^\alpha = \tilde{Q}_h^\alpha'$ implies that $\theta_h^\alpha = \theta_h^\alpha'$. Hence, because the sublattice permutation is made up of 2-cycles and the phases $\theta_h^\alpha$ are the same within each cycle, the matrix $V_h$ is symmetric based on Section C 4 a.

Hence, the constraint on the Hamiltonian is

$$H_k = V_h^\dagger H^*_k V_h, \quad V_h = V_h^T.$$  \hfill (C34)

\begin{itemize}
  \item \textit{Time reversal with spin rotation}
  \end{itemize}

For coplanar spins, time reversal with spin rotation yields a time-reversal-like constraint on the magnon Hamiltonian. Specifically, if we consider spins in the $y-z$ plane, $h = \{\mathbb{1}; R(\pi \hat{x})|0\} T$ and the rotation matrices can be chosen to be

$$R_\alpha = R(\eta_\alpha \hat{x}) = \begin{bmatrix}
\cos \eta_\alpha & -\sin \eta_\alpha \\
\sin \eta_\alpha & \cos \eta_\alpha
\end{bmatrix}. \tag{C35}$$

With this choice, the local transformation on the spins is

$$\tilde{Q}_h^\alpha = -R(\eta_\alpha \hat{x})^\top R(\pi \hat{x}) R(\eta_\alpha \hat{x}) \tag{C36a}$$

$$= -e^{\pi \hat{x}}. \tag{C36b}$$

After transforming to the basis of ladder operators, with this specific choice of $R_\alpha$, we find $\theta_h^\alpha = \pi$ for all $\alpha$ and

$$H_k = H_k^*. \tag{C37}$$

A different choice of $\{R_\alpha\}$ would have yielded different phases $\theta_h^\alpha$, and a more complicated matrix $V_h$.\]
c. Effective magnetic inversion symmetry

For coplanar spins with separate inversion and TR+spin rotation symmetries, one can have an effective magnetic inversion symmetry: $h = \{P; R_{h}^{\alpha}|\tau\}T$, with any appropriate $R_{h}$. 

For example, for spins in the $y$-$z$ plane, $h = \{P; R(\pi \hat{z})|\tau\}T$. Let $\alpha$ and $\alpha'$ denote a pair of sublattices related by $P$. These two sublattices have the same classical direction, so we can choose

$$R_{\alpha} = R_{\alpha'} = \begin{bmatrix} 1 & \cos \eta_{\alpha} & -\sin \eta_{\alpha} \\ \sin \eta_{\alpha} & \cos \eta_{\alpha} & 0 \end{bmatrix}. \quad (C38)$$

This choice gives us the exact same result as in Section [C5b] $\theta_{h}^{\alpha} = \theta_{h}^{\alpha'} = \pi$; more generally, we will find $\theta_{h}^{\alpha} = \theta_{h}^{\alpha'}$. Therefore,

$$H_{k} = V_{h}^{\dagger}H_{k}^{*}V_{h}, \quad V_{h} = V_{h}^{\dagger} \quad (C39)$$

because the permutations are all 2-cycles with the same phases within each cycle.

d. Translation with spin rotation

Suppose that translation followed by spin rotation is an element of the spin-space group; for example, $g = \{I; R(\pi \hat{z})|\tau\}$. Since this transformation has no spatial O(3) part, it acts locally in momentum space, and we get

$$H_{k} = V_{g}^{\dagger}H_{k}V_{g}, \quad V_{g} \text{ unitary.} \quad (C40)$$

But this is a unitary symmetry of the $H_{k}$ at a fixed momentum. This means that $H_{k}$ can be block-diagonalized, with the different blocks corresponding to different eigenvalues of $V_{g}$.

What does this additional structure correspond to, and why in this case does Fourier transforming leave local unitary symmetries? Suppose $g^{2}$ is a magnetic translation. Then, one way of understanding this is to note that one can define modified translation operators (containing a global spin rotation by $\pi$ about $\hat{z}$) whose eigenvalues span a Brillouin zone twice as large as the magnetic Brillouin zone. This is simply an alternate way of labelling the states, as it halves the bands and doubles the number of momenta.

e. Axial spin rotation symmetry

Consider a global spin-rotation symmetry $g$ about an axis—we can take it to be the $\hat{z}$ axis, in which case $g = \{I; R(\theta \hat{z})|0\}$ for any $\theta$. This implies the classical spin order is collinear, with spins pointing either in the $\hat{z}$ or $-\hat{z}$ directions.

It is easy to see that $\tilde{Q}_{g} = R(\theta \hat{z})$ and $\theta_{g}^{\alpha} = \theta$ if the spin at sublattice $\alpha$ points in $+\hat{z}$ direction, whereas $\tilde{Q}_{g} = R(-\theta \hat{z})$ and $\theta_{g}^{\alpha} = -\theta$ if the spin at sublattice $\alpha$ points in $-\hat{z}$ direction.

Hence, the associated matrix $H_{g}$ is diagonal with eigenvalues of $e^{i\theta}$ and $e^{-i\theta}$. This implies that the coefficient matrix $H_{k}$ is block diagonal, with the blocks corresponding to $S_{z}$-conserving sectors: one block contains annihilation operators for $+\hat{z}$ spins and creation operators for $-\hat{z}$ spins, and vice-versa for the other block.

6. Magnetic inversion and reality condition

We show that in the appropriate basis, the constraint imposed by magnetic inversion symmetry on the Bloch Hamiltonian $H_{k}$ is that it is purely real for each $k$. This is expected for integer-spin excitations like magnons [51]; we nonetheless discuss how this arises for completeness.

Consider any (effective) magnetic inversion symmetry $h = \{P; Q^{\dagger}|\tau\}T$, where $Q^{\dagger}$ is some O(3) operation and $\tau$ is some spatial translation. We have seen that the constraint on $H_{k}$ is local in momentum space, $H_{k} = V_{h}^{\dagger}H_{k}^{*}V_{h}$, with $V_{h}$ symmetric. Since $V_{h} = V_{h}^{\dagger} \oplus V_{h}^{*}$, this implies $V_{h} = (V_{h}^{\dagger})^{*}$ are symmetric. The symmetric unitary matrix $V_{h}^{\dagger}$ can be factorized as $V_{h}^{\dagger} = \ell^{\dagger} \ell$ using Autonne-Takagi decomposition, where $\ell$ is unitary. We then find $V_{h} = L^{\dagger} L$, where $L := \ell \oplus \ell^{*}$ is unitary, paraunitary, and particle-hole symmetric.

In the new basis defined by $\Phi_{k} = L^{\dagger} \phi_{k}$ the transformation $\Theta_{h} \phi_{k} \theta_{h}^{-1} = \epsilon^{ik} \tau \eta_{h} \phi_{k}$ becomes

$$\Theta_{h} L^{\dagger} \phi'_{k} \theta_{h}^{-1} = \epsilon^{ik} \tau L^{\dagger} \phi'_{k} \quad \Leftrightarrow \quad \Theta_{h} \phi'_{k} \theta_{h}^{-1} = \epsilon^{ik} \tau L^{\dagger} \phi'_{k}. \quad (C41)$$

Therefore,

$$V_{h}' = L^{*} V_{h} L^{\dagger} = L^{*} L^{\dagger} L L^{\dagger} = I, \quad (C42)$$

and the constraint due to magnetic inversion symmetry reads $H_{k}' = (H_{k})^{*}$. Hence, we have shown that there exists a ($k$-independent) change of basis such that in that basis, the constraint due to magnetic inversion is simply that $H_{k}'$ is purely real.

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[44] It seems this was initially proven in the physics literature and is usually true, since the tools from Krein theory are often used.

[45] The various expressions of PH symmetry all arise in the same way, from the redundancy of the Nambu spinors. On the (Hermitian) Bloch-BdG matrix, it reads \( \tau^3 H \tau = H \). On the transformation matrix, it reads \( \tau^3 T \tau = T \), making the transformed Bloch-BdG matrix F-H symmetric. On the (skew-Hermitian) generator \( W \), it reads \( \tau^3 W \tau^2 = W^{-1} \). Note that dynamical stability and thermodynamic stability are fully independent concepts: Krein-Hermitian Hamiltonians can be both, either, or neither.

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