The impact of defects on low-energy excitations in two-dimensional bipartite uniaxial antiferromagnet insulators

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We address scattering of spin waves off independent defects in two-dimensional (2D) easy-axis antiferromagnet (AFM) insulators. Despite an on-site magnetic anisotropy leads gapped Goldstone modes, such that a long-range (AFM) order can be established in 2D, lattice imperfections have a tendency to weaken, and eventually destroy, the magnetic ordering. The impact of defects is considered within two limits, single and multiple defects. Using Green’s function, we perform self-consistent simulations to study magnon properties such as density of states and lifetime of induced resonances. Our findings show that repulsive defects decrease the magnon density of states while attractive ones may enhance it. We provide a comprehensive analysis of how defects can result in a reduction, and even closing, the anisotropy induced gap, which weakens the long-range (AFM) order parameter in the 2D state. We conclude that a small concentration of random defects can fill the gap of magnon spectrum.

I. INTRODUCTION

Magnetic fluctuations, like spin precession, are described by spin waves which can be regarded as dynamical magnetic eigenmodes. A quanta of spin waves, commonly known as magnons, are classified as low-energy Bosonic quasiparticles. Magnons carry linear and spin angular momentum as well as energy. Owing to the unique properties of magnons, an entirely new field has recently emerged, where the physics of magnons and their potential applications are investigated, aiming towards design of magnon-based devices for information technology [1, 2]. One of the important advantages of magnons is their long coherence length, or life time, which opens the possibility for transfer of data across distances much larger than what traditional electronic transfer technology is capable of [3–5]. For instance, data transfers carrying by magnons have been achieved over distances ranging from tens of micrometers [5] to several centimetres in the magnetic insulator Y3Fe5O12 [6].

Antiparallel alignment of spins on two adjacent sublattices in antiferromagnets (AFMs) generates a vanishing zero net macroscopic magnetization. It makes AFMs robust against external magnetic perturbations which protects data from being changed [7]. Besides, this feature gives the freedom to observe some effects like magnons with opposite circular polarizations useful to encode binary information [8], which are absent in ferromagnets (FMs) [9]. Moreover, the intrinsically fast magnetization dynamics in AFMs allows for operation at terahertz frequencies at room temperature [10–13], something which is desirable for ultrafast applications [11, 14–16].

Low-energy excitations of purely isotropic AFMs are governed by two degenerate modes with opposite helicities [17, 18], in contrast to magnons in FMs in which magnon chirality is only right-handed with reference to the FM magnetization. This extra aspect enables chiral logic computing [19], magnon-mediated spin Hall [20–22] and antiferromagnetic magnon field-effect transistor [8].

At nonzero temperature and owing to magnons, magnetic order is prevented in low dimensions; one (1D) and two dimensions (2D). In 1966, Hohenberg [23], and Mermin and Wagner [24], argued that the low-energy cost fluctuations of spins around their expectation values destroy magnetic order in 1(2)D systems which are described by the isotropic Heisenberg Hamiltonian. As a consequence, constructing 2D magnets becomes challenging unless the spin fluctuations at the bottom of energy spectrum are suppressed. Moreover, dimensionality influences the magnon lifetimes which is a critical characteristic for magnon-based devices [2, 25, 26].

The presence of an out-of-plane easy-axis magnetic anisotropy in magnetic materials can regenerate the long-range magnetic order in 1(2)D [27]. However, the revived magnetic order is sensitive to lattice imperfections which makes the order unstable. Thus, a noteworthy debate is the study of lattice defects in low-dimensional structure by which translational invariance is broken. In particular, non-magnetic impurities can significantly alter the properties of low-dimensional magnets [28–31]. Moreover, in addition to electron-magnon interactions, i.e., Landau damping [26], and spin-orbit coupling [32], another mechanism which affects the magnon lifetime is scattering off impurities [33].

In Ref. [34] it was shown that even at low concentrations of impurities in a ferromagnet, emergence of local oscillations can give rise to a decrease of the magnetization if the induced energy level arises at the bottom of spin wave spectrum. Furthermore, in a recent study of FMs on a honeycomb lattice [35], it was demonstrated that Dirac magnons arise and a local impurity induces a resonance in the magnon density of states, in a strong analogy with the effects of impurity scattering in graphene [36–40]. In addition, the position of the resonance approaches the Dirac point by increasing the impurity scattering potential.

In the current work, we investigate the impact of defects on the low-energy excitations in AFMs or a honeycomb lattice without and with a magnetic easy-axis anisotropy. We assume uncorrelated defects and consider them in two regimes, (i) sin-
ingle defect and (ii) multiple randomly distributed defects. By using the $T$-matrix technique, we develop the single particle dressed Green’s function and calculate low-energy magnon local density of states (MLDOS). In the first case, single de-
dressed Green’s function and calculate low-energy magnon
scattering processes off the single defect, thus, allowing for
an exact solution. In the second case, multiple impurities, we employ spatial averaging and calculate the lowest-order self-energy diagrams within the self-consistent Born approx-
imation, to evaluate the magnon lifetime and MLDOS. This second component of the article is justified since it provides
an averaged description of the physics, something which is
relevant for optical and neutron scattering measurements, as
well as any potential technology that might be exploited for
AFMs.

In summary, magnetic order in an interacting spin system
can be destroyed by magnonic collective excitations of the
structure. It essentially means that magnons quantize all pos-
sible spin deviations located in the lattice sites. Our results
show that the total magnon density of states distribute non-
homogeneously over the two sublattices in AFMs. Moreover,
it is seen that in the regime of a single defect with strong
enough attractive potential, magnon local density of states in-
creases compared to the MLDOS of a pristine lattice. By
contrast, the repulsive defect diminish the local density of
magnons which indicates that a repulsive defect can suppress
magnon effects in AFMs. In the case of easy-axis AFMs, an
attractive single defect can induce a new peak within the en-
ergy gap of the system. These findings determine a reason-
able range of impurity potentials by which the magnon gap
can be filled in the regime of randomly distributed defects.
It can be concluded that the existence of a diluted density of
uncorrelated defects in a 2D easy-axis AFMs can prevent est-
ablishment of a long-range order in AFMs due to easy-axis
magnetic anisotropy.

The organization of the paper is as follow: Section II re-
views the model Hamiltonian of typical isotropic and easy-
axis AFM insulators on a honeycomb lattice which is a non-
Bravais bipartite lattice. We obtain the lowest-order magnon
Hamiltonian by Holstein-Primakoff transformation. In section
III, we study the effects of defects in introduced systems ana-
lytically by evaluation of the single particle Green’s function
for the whole system including host and defect. Here, defects
are considered within two regimes, a single defect and ran-
domly distributed defects. Thereafter, in Sec. IV we present
our numerical findings of magnon density of states in the pres-
ence of defects. Finally, we conclude our results in Sec. V.
Furthermore, in Apps. A–C more details of calculations are
provided.

II. MODELLING THE ANTI-FERROMAGNETIC
STRUCTURE

A. Hamiltonian

An easy-axis AFM on a bipartite lattice can be modeled by,

$$H = I \sum_{\langle i,j \rangle} S_i \cdot S_j - K_c \sum_{i \in A, B} (S_i^z)^2,$$

(1)

where $S_{\langle i,j \rangle}$ denotes the spin vector at site $i(j)$ such that
$(S_{i \in A}) = (0 \ 0 \ S)$ and $(S_{i \in B}) = (0 \ -S)$, $A, B$ refer
to different sublattices. Here, $J$ is the isotropic exchange coupling
between the nearest neighbors, indicated by $(i, j)$, and
assumed to be anti-ferromagnetic, $J > 0$. Moreover, $K_c > 0$
denotes the easy-axis on-site anisotropy, forcing the spins to
be collinearly aligned perpendicular to the material surface.

In order to model Bosonic excitations in this structure, we
apply the Holstein-Primakoff (HP) transformation [41], which
for the AFM is given by [42–44],

$$S_i^z = a_i^\dagger a_i, \quad S_i^- = a_i^\dagger \sqrt{2S - a_i^\dagger a_i}, \quad S_i^+ = (S_i^-)^\dagger,$$

(2a)

$$S_j^z = -S + b_j^\dagger b_j, \quad S_j^- = \sqrt{2S - b_j^\dagger b_j}, \quad S_j^+ = (S_j^-)^\dagger,$$

(2b)

in which $a_i^\dagger (a_i)$ is the creation (annihilation) operator where
$i \in A$, and $b_j^\dagger (b_j)$ refers to the one where $j \in B$. The HP
transformation for AFMs stress that $a$ and $b$ carry opposite
spin angular momentum along $z$-axis on different sublattices.
At low enough temperature, the number of excitations is very
small, $\langle a_i^\dagger a_i \rangle, \langle b_j^\dagger b_j \rangle \ll 2S$, i.e., the spin fluctuations are small
around the classical direction, $|S^z| \approx |S|$. Using the HP transformation makes it possible to rewrite the spin Hamiltonian,
Eq. (1), in terms of Bosonic operators describing spin devia-
tions around the equilibrium state. By expanding the square
root in Eq. (2) in powers of $1/S$, we construct a quadratic
model $H = E^0 + H_b^{(2)}$. The classical energy of the ground
state is given by $E^0 = -NS^2(zJ/2 + K_c)$ at zero temperature,
where $N$ is the total number of sites in the lattice. For a lattice
with periodic boundary conditions, we introduce the Fourier
transformation as,

$$a_i = \sqrt{2 \over N} \sum_q e^{iqr} a_q, \quad i \in A,$$

(3a)

$$b_j = \sqrt{2 \over N} \sum_q e^{iqr} b_q, \quad j \in B,$$

(3b)

thereafter the quadratic Hamiltonian in reciprocal space is ob-
tained,

$$H_b^{(2)} = \sum_q \left[ \varepsilon_0 a_q^\dagger a_q + \varepsilon_0 b_q^\dagger b_q + S Z J \gamma_q a_q b_{-q} + S Z J \gamma_q b_q a_{-q}^\dagger \right],$$

(4)

where $\varepsilon_0 = S(zJ + 2K_c)$. Here, $\gamma_q = \sum_{\delta=\pm} e^{\delta q \delta}/2Z$ is lat-
tice structure factor where $Z$ denotes the number of nearest neighbours and $\delta_i$ is the distance vectors between the nearest neighbours in the honeycomb lattice. For small $\mathbf{q}$ around the $\Gamma$-point, identified by the most important magnons close to the center of Brillouin zone at enough low temperature, $|\gamma_q| \approx 1 - (aq)^2/4$ with lattice constant $a$. In the spinor basis $\Psi_q^i = \left(\begin{array}{c} a_q^i \\ \alpha_q^i \\ \beta_q^i \end{array} \right)$, we rewrite the Hamiltonian as $H^{(2)}_q = \sum_\mathbf{q} \Psi_q^i \hat{h}_\mathbf{q} \Psi_q^i \Psi_q^j$ where,

$$h_\mathbf{q} = \begin{pmatrix} \epsilon_0 \\ S Z J \gamma_{-\mathbf{q}} \\ \epsilon_0 \end{pmatrix}.$$ (5)

Conventionally, the magnon spectrum is considered by diagonalizing $H^{(2)}_q$ through the Bogoliubov transformation [45, 46]. An alternative approach is provided by retaining the reference to the sublattices and consider the equation of motion for the magnon Green’s function [47, 48]. This approach gives the opportunity to obtain excitation spectrum and the probability of spin deviations at each sublattices [49]. Considering spin excitations resolved in the sublattices is preferable here, since the AFMs we are interested in are non-homogeneous. It was demonstrated in [48] that the local density of magnon states cannot be easily extracted from a description of the magnons in terms of the Bogoliubov transformation and there is, therefore, no good option to remaining in the sublattice resolved representation. Our purpose in this work is the investigation of magnon density of states in bare and perturbed crystals, extract the contribution of different sublattices and the effect of defects. Regarding them, it is convenient that we continue with the Green’s function formalism. In appendix (A), we present the Bogoliubov transformation for the sake of clarity. The Green’s function is defined by,

$$G(\epsilon, \mathbf{q}, \mathbf{q}') = -i \langle \langle \Psi_{\mathbf{q}}^i | \Psi_{\mathbf{q}'}^{j*} \rangle \rangle = -i \begin{pmatrix} \langle a_{\mathbf{q}'}^\alpha \rangle \\ \langle b_{\mathbf{q}'}^\alpha \rangle \\ \langle a_{\mathbf{q}'}^\beta \rangle \end{pmatrix}.$$ (6)

where $\langle \langle ... \rangle \rangle$ denotes the magnon propagator in energy space. Applying the equation of motion in energy space given by $\epsilon \langle \langle AB \rangle \rangle = \langle \langle [A, B] \rangle \rangle + \langle \langle [A, H]B \rangle \rangle$ [50] where $H$ is the system Hamiltonian and $A, B$ are arbitrary operators results in the bare Green’s function

$$G_0(\epsilon, \mathbf{q}) = \begin{pmatrix} \epsilon - \epsilon_0 & -S Z J \gamma_q \\ S Z J \gamma_q & \epsilon + \epsilon_0 \end{pmatrix}^{-1} = \frac{1}{\epsilon^2 - \epsilon_0^2 + S Z J \gamma_q^2} \begin{pmatrix} \epsilon - \epsilon_0 & -S Z J \gamma_q \\ S Z J \gamma_q & \epsilon + \epsilon_0 \end{pmatrix}.$$ (7)

from this expression, it is vividly clear that the (diagonal) components representing the $\mathcal{A}$- and $\mathcal{B}$-sublattices are not equivalent; $G^{0AB}_q$ is evaluated from $G^{0AA}_q$ by $\epsilon \rightarrow -\epsilon$. This feature of AFMs is as opposed to the properties of FMs on honeycomb lattice in which both are identical [35]. Therefore, the free magnon Hamiltonian can be written as,

$$H^{(2)}_q = E_0^q + \sum_\mathbf{q} \epsilon_q^\alpha a_q^\alpha a_q^\alpha + \epsilon_q^\beta b_q^\beta b_q^\beta.$$ (8)

where $\alpha_q$ and $\beta_q$ are magnon eigenmodes which are mixtures of fluctuations on sublattice $\mathcal{A}$ and $\mathcal{B}$ in the collinear AFM. Additionally, the quantum correction to the ground-state energy is $E_0^q = -N \epsilon_0^2 / 2$. The dispersion of the free magnons ($\epsilon_0^\alpha$ and $\epsilon_0^\beta$) is obtained from the denominator of $G_0$, that is,

$$\epsilon_0^{\alpha/\beta} = \sqrt{\epsilon_0^2 - S^2 Z^2 J^2 |\gamma_q|^2}.$$ (9)

which are degenerate but can be distinguished by their opposite chirality as they conduct opposite spin angular momentum [20]. In summary, magnons in the AFM are circularly polarized even in the presence of an easy-axis anisotropy. Hence, an easy-axis anisotropy does not break the $U(1)$ symmetry, which, in the absence of external fields, leads to that magnons distribute over two degenerate bands with opposite helicities [17, 18, 51].

From Eq. (9), it is clear that for an isotropic AFM ($\mathcal{K}_c = 0$), the energy dispersion is linear, $\epsilon_q = \zeta q / \sqrt{2}$, where $\zeta = S Z J a$, as shown in Fig. 1 (a), where the magnon energy of the isotropic AFM is plotted as function of $q$ near $\Gamma$. In this case, magnons are massless with group velocity depending on the exchange interaction as $v_g = \zeta / \sqrt{2}$. These aspects are universal fingerprints of Dirac-type materials [52]. Note that the gapless band structure of magnons sustain the emergence of Goldstone excitations, corresponding to spin deviations around the equilibrium, which can occur without any cost of energy. Hence, at finite temperatures, such easily excited fluctuations destroy long range order in 2D isotropic AFMs.

However, from Eq. (9) it is, furthermore, clear that a finite easy-axis anisotropy, $\mathcal{K}_c > 0$, induces a gap at the bottom of the magnon spectrum around the $\Gamma$-point. The gap opening is accompanied by the introduction of a non-linearity of the energy dispersion, which is shown in Fig. 1 (b). The gap opening stabilizes the system and revive long range magnetic order in the 2D structure. In this case, the AFM resonance frequency, evaluated at $q = 0$, is given by $\omega_{RAFM} = 4 Z J K_c + 4 K_c^2$.

The dispersion relation in Eq. (9), moreover, shows that despite $\epsilon_q^{\alpha/\beta}$ depends on the lattice structure factor $\gamma_q$, which is unique for the lattice, in general, the magnon dispersion
is qualitatively similar in square and honeycomb lattices for \( q \to 0 \), that is, an additional bipartite structure of the lattice does not change the linear energy dispersion near the \( \Gamma \)-point. For small \( q \) and sufficiently weak anisotropy, \( \mathcal{K}_z \ll J \), the magnon bands are defined through the relations,

\[
\varepsilon^\alpha_q \approx 2S \sqrt{ZJ} \mathcal{K}_z \left( 1 + \frac{ZJo^2}{16\mathcal{K}_z q^2} \right),
\]

\[
\varepsilon^\beta_q \approx -2S \sqrt{ZJ} \mathcal{K}_z \left( 1 + \frac{ZJo^2}{16\mathcal{K}_z q^2} \right).
\]

Here, due to the anisotropy, the non-zero effective mass and group velocity of magnons are, respectively,

\[
|m|^2 = h^2 \left( \frac{\partial^2 \varepsilon}{\partial q^2} \right)^{-1} = \frac{4\hbar^2}{\zeta a} \sqrt{\frac{\mathcal{K}_z}{ZJ}},
\]

\[
|v_x| = \frac{\partial \varepsilon}{\partial q} = \frac{\zeta a}{4} \sqrt{\frac{ZJ}{\mathcal{K}_z} q}.
\]

**B. Bare magnon local density of states**

We finish this section by a further analysis of Eq. (7), from which we obtain the magnon local density of states for bare systems in both isotropic and easy-axis AFMs.

In general, the local density of states is evaluated from the relation \( n(\varepsilon, \mathbf{q}) = -\text{Im} \text{Tr} G(\mathbf{q}, \varepsilon) \pi \), where the trace runs over sublattice degrees of freedom. The bipartite structure allows us to write \( n(\varepsilon, \mathbf{q}) = \sum_{\alpha} n^\alpha(\varepsilon, \mathbf{q}) \), where \( n^\alpha(\varepsilon, \mathbf{q}) = -\text{Im} \text{Tr}^{\alpha}_\varepsilon \pi \), \( x = A, B \), indicating how the two sublattices contribute to the total MLDOS.

Magnons are eigenmodes of the spin wave spectrum, and should be regarded as a collective behaviour of the structure. In this sense, they involve all the spin deviations in the lattice. However, here we are interested in how the magnon LDOS is distributed over the two sublattices. Hence, in order to address the LDOS of the bare structures, we consider the on-site Green’s function given by \( g_0(\varepsilon) = \sum_{\mathbf{q}} G_0(\mathbf{q}, \varepsilon)/N \) [53]. In the following, we express magnon LDOS for unperturbed isotropic and easy-axis AFMs.

1. **Isotropic AFM**

For AFMs without anisotropy, the \( g_0^{\mathcal{A}A} = g_0^{\mathcal{A}A}(\varepsilon) \) component of on-site Green’s function reduces to,

\[
g_0^{\mathcal{A}A} = \frac{\varepsilon + ZJS}{W^2} \left( \ln \left| \frac{\varepsilon^2}{\varepsilon^2 - \varepsilon^2} \right| - i\pi \text{sgn}(\varepsilon) \Theta(\varepsilon^2 q_c^2/2 - \varepsilon^2) \right),
\]

where \( \text{sgn}(\varepsilon) \) refers to the sign function, and \( q_c \) denotes the cut-off wave vector which relates to the magnon band width, \( W \), through the relation of \( W = v_x q_c \). Moreover, \( \Omega = 1/S \), where \( S = 3\sqrt{3}a^2/2 \), is the area of the hexagonal unit cell, such that we can set \( W^2 = 4\pi\Omega a^2 \) [53]. The bare magnon

![FIG. 2. Real and imaginary part of on-site Green’s function, \( g_0^{\mathcal{A}A} \) and \( g_0^{BB} \), where we set in (a) \( \mathcal{K}_z = 0 \) and in (b) \( \mathcal{K}_z = 0.05J \). The other parameters are \( J = 1 \), \( S = 1 \), \( a = 1 \) nm. The solid and dotted lines illustrate the imaginary and real part of on-site Green’s function.

LDOS in the \( \mathcal{A} \)- and \( \mathcal{B} \)-sublattice are obtained from the imaginary part of Eq. (7), hence, giving

\[
n_0^{\mathcal{A}}(\varepsilon, \mathbf{q}) = \frac{\varepsilon + ZJS}{W^2} \text{sgn}(\varepsilon) \Theta(\varepsilon^2 q_c^2/2 - \varepsilon^2),
\]

\[
n_0^{\mathcal{B}}(\varepsilon, \mathbf{q}) = -\frac{\varepsilon + ZJS}{W^2} \text{sgn}(\varepsilon) \Theta(\varepsilon^2 q_c^2/2 - \varepsilon^2).
\]

These expressions suggest that \( n_0^{\mathcal{A}} \) and \( n_0^{\mathcal{B}} \) increases and decreases, respectively, with increasing energy. Indeed, a comparison of the imaginary parts of \( g_0^{\mathcal{A}A} \) and \( g_0^{BB} \) (negative of the densities \( n_0^{\mathcal{A}} \) and \( n_0^{\mathcal{B}} \)), which are plotted in Fig. 2 (a), along with their corresponding real parts, as a function of the energy, \( \varepsilon \), indicates that the MLDOS for two sublattices are completely different, which is in stark contrast to FM honeycomb lattices [35]. This behaviour arises from the fact that there is an antiferromagnetic exchange interaction between sublattices which is also displayed through the HP transformation, Eq. (2).

2. **Easy-axis AFM**

A non-vanishing easy-axis anisotropy, \( \mathcal{K}_z > 0 \), opens up a low energy gap in the magnonic structure. This property can be seen from the Green’s functions of sublattice \( \mathcal{A} \) and \( \mathcal{B} \), which are given by the expression

\[
g_0^{\mathcal{A}A} = -\frac{\varepsilon + \varepsilon_0}{W^2} \left[ \ln \left| 1 - \frac{\varepsilon^2 q_c^2/2}{\varepsilon^2 - \mathcal{K}} \right| + i\pi \text{sgn}(\varepsilon) \Theta(\varepsilon^2 q_c^2/2 - \varepsilon^2 - \mathcal{K}) \right],
\]

\[
g_0^{BB} = -\frac{\varepsilon - \varepsilon_0}{W^2} \left[ \ln \left| 1 - \frac{\varepsilon^2 q_c^2/2}{\varepsilon^2 - \mathcal{K}} \right| + i\pi \text{sgn}(\varepsilon) \Theta(\varepsilon^2 q_c^2/2 - \varepsilon^2 + \mathcal{K}) \right],
\]

where \( \mathcal{K} = 4ZJ/\mathcal{K}_z S^2 \) and \( \varepsilon_0 = S(ZJ + 2\mathcal{K}_z) \). In Fig. 2 (b), the real and imaginary parts of the onsite Green’s function are plotted as a function of energy. Compared to the isotropic AFM, the properties of the magnonic structure are
here shifted to positive energies, reflecting the gap introduced by the anisotropy. It can also be noticed that the imaginary parts of the Green’s function are non-degenerate with respect to the sublattice degree of freedom already at the onset energy $\sqrt{K}$, which is another reflection of the non-vanishing anisotropy, c.f., the degenerate imaginary parts of the Green’s function at $\varepsilon = 0$ in the isotropic AFM, Fig. 2 (a).

III. IMPURITY EFFECTS

The existence of defects in materials can induce either localized modes or resonances in the energy spectrum. Specifically, a localized mode has a small, if any, overlap with the host band structure while a resonance resides inside the continuous part of the spectrum. Such resonances can, in magnon systems, be detected in experiments by optical measurements and neutron scattering [47]. The impurities can be considered in different regimes which are, here, theoretically investigated by using the single particle Green’s function. In this section, we first consider a single defect and study how the magnon lifetime of localized states generated by impurities. We finalize this section with a comprehensive analysis of the impact of defects on elementary excitations in AFMs.

A. Single defect

By manipulating one spin in one of the sublattices, such local perturbation can be considered as a local defect, which may influence the rest of the system. For sake of concreteness, we consider a single defect located at the coordinate $r_0$ in sublattice $\mathcal{A}$, modeled by $H_d = U_0(\sigma_0 + \sigma_3)a^\dagger_0a_0/2$. Here, $\sigma_a$, $a \in \{0, x, y, z\}$, define the $2 \times 2$ unit and Pauli matrices in pseudospin space. In the presence of the local defect, the Green’s function can be partitioned as

$$G(\varepsilon, \mathbf{q}, \mathbf{q}') = G_0(\varepsilon, \mathbf{q}, \mathbf{q}') + \delta G(\varepsilon, \mathbf{q}, \mathbf{q}')$$

where $G_0(\varepsilon, \mathbf{q}, \mathbf{q}')$ is the bare Green’s function, whereas $\delta G(\varepsilon, \mathbf{q}, \mathbf{q}')$ is the correction due to the local perturbation. The dressed Green’s function manifests a propagation of excitations through the perfect system in which scattering occurs by a local perturbation. Here, we calculate this correction using the $T$-matrix expansion,

$$\delta G(\varepsilon, \mathbf{q}, \mathbf{q}') = G_0(\varepsilon, \mathbf{q})T(\varepsilon)G_0(\varepsilon, \mathbf{q}')$$

where the $T$-matrix is given by

$$T(\varepsilon) = (H_d^{-1} - g_0(\varepsilon))^{-1} = H_d(\sigma_0 - g_0(\varepsilon)H_d)^{-1}$$

where $g_0(\varepsilon)$ is the on-site Green’s function [53]. After straightforward calculations, the diagonal components of the correction term, $\delta G(\varepsilon, \mathbf{q}) \equiv \delta G(\varepsilon, \mathbf{q}, \mathbf{q})$, are obtained,

$$\delta G^{\mathcal{A}\mathcal{A}}(\varepsilon, \mathbf{q}) = \frac{1}{U_0^{-1} - g_0^{\mathcal{A}\mathcal{A}}} \left( \frac{\varepsilon + \varepsilon_0}{(\varepsilon - \varepsilon_0 + S^2Z^2J^2|\gamma_q|^2)} \right)^2, \quad (18a)$$

$$\delta G^{\mathcal{B}\mathcal{B}}(\varepsilon, \mathbf{q}) = \frac{1}{U_0^{-1} - g_0^{\mathcal{B}\mathcal{B}}} \left( \frac{\varepsilon - \varepsilon_0 + S^2Z^2J^2|\gamma_q|^2}{(\varepsilon - \varepsilon_0 + S^2Z^2J^2|\gamma_q|^2)} \right)^2, \quad (18b)$$

providing the corrections to the MLDOS

$$\delta n^{\mathcal{A}}(\varepsilon, \mathbf{q}) = -\frac{1}{\pi} \frac{\text{Im} g_0^{\mathcal{A}\mathcal{A}}}{|U_0^{-1} - g_0^{\mathcal{A}\mathcal{A}}|^2} \left( \frac{\varepsilon + \varepsilon_0}{(\varepsilon - \varepsilon_0 + S^2Z^2J^2|\gamma_q|^2)} \right)^2, \quad (19a)$$

$$\delta n^{\mathcal{B}}(\varepsilon, \mathbf{q}) = -\frac{1}{\pi} \frac{\text{Im} g_0^{\mathcal{B}\mathcal{B}}}{|U_0^{-1} - g_0^{\mathcal{B}\mathcal{B}}|^2} \left( \frac{\varepsilon - \varepsilon_0 + S^2Z^2J^2|\gamma_q|^2}{(\varepsilon - \varepsilon_0 + S^2Z^2J^2|\gamma_q|^2)} \right)^2. \quad (19b)$$

From the above equations, we determine the energy of the impurity resonance by requiring

$$|U_0^{-1} - g_0^{\mathcal{A}\mathcal{A}}|^2(\varepsilon - \varepsilon_0 + S^2Z^2J^2|\gamma_q|^2)^2 = 0. \quad (20)$$

This condition implies either that $\text{Im} g_0^{\mathcal{A}\mathcal{A}} = 0$ and $\text{Re} g_0^{\mathcal{A}\mathcal{A}} = 1/U_0$, simultaneously, or $\varepsilon - \varepsilon_0 + S^2Z^2J^2|\gamma_q|^2 = 0$. The zeros arising from the former requirement correspond to impurity induced resonances in the magnon density, Eq. (19). For these resonances to arise in the density of the spin excitations, the defect has to be attractive, $U_0 < 0$ (for more details see App.(C)). By contrast, a negative scattering potential enhances the easy spin deviation on this sublattice, compared to attractive scattering potentials, which leads to a diminished production of magnons. Hence, a repulsive scattering potential tends to locally facilitate the formation of a gapped magnon density. However, this latter can only make a difference either in an already anisotropic AFM or in an isotropic AFM by giving rise to an effective easy axis anisotropy which can open a gap in the magnon spectrum.

B. Multiple defects

Beyond the case of a single defect, as a more realistic scenario, we consider here the effect of multiple defects randomly distributed on the honeycomb lattice. Considering a collection of randomly distributed impurities is motivated since many experimental techniques, as well as potential technological applications, sample the averaged properties of the AFMs, rather than the very local effects that can be addressed for single defects. Hence, by assuming a dilute concentration of defects, correlations between them can be neglected, while at the same time enables to consider averaged properties of the AFM. We investigate the problem of short-ranged scattering potentials, and we assume an equal number, $n$, of independent defects in the two sublattices constituting the volume $V$, all with the same scattering strength $U$. Under this assumption,
we model the defects through
\begin{align}
    cU\sigma_A &= \frac{nU\sigma_0 + \sigma_z}{V}, \quad (21a) \\
    cU\sigma_B &= \frac{nU\sigma_0 - \sigma_z}{V}. \quad (21b)
\end{align}

on sublattice \( A \) and \( B \), respectively, where \( c = n/V \) is the concentration of defects. In addition, the scattering potential is assumed to be \( \mathbf{q} \)-independent. Distributing defects in the lattice breaks the translational invariance in the system. However, since we assume uniform randomly distributed defects, we can make a spatial averaging over the defects, which has the property of recovering the translational invariance of the magnon Green’s function \([54]\), which is outlined in the following.

The spatial averaging of the collection of scattering defects
\( H_{q\mathbf{q}} = cU \sum_{i\in A\cup B} \sigma_i e^{-i\mathbf{q}\cdot \mathbf{r}_i} \),
gives rise to,
\[ \tilde{H}_{q\mathbf{q}} = cU \delta_{q\mathbf{q}} \sigma_0. \] (22)
Then, the dressed Green’s function can be written as the Dyson equation \([54]\),
\[ G(\mathbf{q}, \mathbf{q}') = \delta_{q\mathbf{q}} G_0(\mathbf{q}) + G_0(\mathbf{q}, \mathbf{q}') \sum_{k\mathbf{l}} H_k e^{-i\mathbf{q}\cdot \mathbf{r}_k} G(\mathbf{k}, \mathbf{k}'). \] (23)

By retaining the first-order correction of the Green’s function, we obtain,
\[ \tilde{G}_1(\mathbf{q}, \mathbf{q}') = \delta_{q\mathbf{q}} cU G_0^2(\mathbf{q}). \] (24)

The second order correction \( \tilde{G}_2 \) provided through the averaging procedure, \( \tilde{H}_{qk} \tilde{g}_k \tilde{H}_{q\mathbf{q}} \), is given by \([54, 55]\),
\[ \tilde{G}_2(\mathbf{q}, \mathbf{q}') = c^2 U^2 (1 - 1/N) G_0(\mathbf{q}) + \Sigma(\mathbf{q}, \mathbf{q}') G_0^2(\mathbf{q}). \] (25)
where the self energy within self-consistent Born approximation is defined by,
\[ \Sigma(\mathbf{q}, \mathbf{q}') = cU^2 \sum_{i\in A\cup B} \sum_{\mathbf{q}} \sigma_i \tilde{G}(\mathbf{q}, \mathbf{q}) \sigma_i. \] (26)

Thereafter, the dressed Green’s function is self-consistently evaluated by \( \tilde{G}(\mathbf{q}, \mathbf{q}') = G_0(\mathbf{q}) - G_0(\mathbf{q}) \Sigma(\mathbf{q}, \mathbf{q}') \tilde{G}(\mathbf{q}, \mathbf{q}). \) In general, the self energy can be written as \( \Sigma(\mathbf{q}, \mathbf{q}') = 0 \) for the averaging over \( \mathbf{q} \) in the imaginary part provides a broadening of the resonant state which is proportional to the inverse of resonant lifetime \( \tau \). The summation over the sublattices yields the diagonal self energy
\[ \Sigma = cU^2 \sum_{\mathbf{q}} \begin{pmatrix} \Sigma_{AA}(\mathbf{q}) & 0 \\ 0 & \Sigma_{BB}(\mathbf{q}) \end{pmatrix} = \begin{pmatrix} \Sigma_{AA} & 0 \\ 0 & \Sigma_{BB} \end{pmatrix}, \] (27)
from which the lifetime is determined as \( 1/\tau = -2\text{ImTr} \Sigma(\mathbf{q}) \).

![FIG. 3. Integrated MLDOS for the pristine (dotted) and the perturbed (solid) isotropic AFM. Panel (a) displays the sublattice resolved and panel (b) shows the total MLDOS. Used parameters are \( J = 1, S = 1, a = 1 \text{ nm}, \) and \( U_0 = -1.8 \).](image)

IV. NUMERICAL RESULTS

Here, we proceed by analyzing the integrated MLDOS, \( n(\mathbf{q}) = n^A(\mathbf{q}) + n^B(\mathbf{q}) \), where \( n^A(\mathbf{q}) = \sum_{\mathbf{q}} n^A(\mathbf{q}, \mathbf{q}')/N \). We present our numerical findings about effects of both single and multiple randomly distributed scattering potentials.

A. Induced resonance peak

In Fig. 3, we have plotted (a) the sublattice resolved and (b) the total MLDOS for the isotropic AFM structure, as a function of energy, for both the pristine lattice (dotted lines) and the system including a single defect (solid lines). The MLDOS in the pristine lattice is not equally distributed between the two sublattices, except at \( \varepsilon = 0 \), which is shown in Fig. 3 (a), where the densities for sublattice \( A \) and \( B \) are resolved. For finite energies, both portions of the MLDOS vary linearly but while it increases in sublattice \( A \), it is reduced by the same amount in sublattice \( B \), while the overall density remains constant, see Fig. 3 (b). This effect can be understood to arise from that when magnons are created in sublattice \( A \), the spin on this sublattice gradually becomes less well-defined, until it cannot any longer be defined at all. As a consequence of the AFM exchange interaction between the two sublattices, the spin in sublattice \( B \) becomes increasingly stabilized, which is indicated by the reduced MLDOS, or, deviations of the spin from a specific direction. This aspect should be contrasted by the different outline occurring in a FM lattice [35]. Under FM interactions, the sublattices are parallel and magnon excitations on both sublattices have the equal contribution to destroy the FM order.

Upon adding a single defect, the MLDOS is substantially modified. In Fig. 3 (a), we notice that resonance peaks are induced in both \( n^A \) and \( n^B \) for an attractive defect \( U < 0 \). It should be noted that a positive scattering potential reduces MLDOS compared to the bare system, which can be interpreted as that the spin system becomes increasingly stable against magnons in the presence of a repulsive single defect. Within a small energy range, the MLDOS grows with the energy on both sublattices, while above critical energies, which are different in the two sublattices, both densities, \( n^A \) and \( n^B \),
decrease. Specifically, one should notice that the density in sublattice $B$, both has a stronger resonance and lower critical energy, compared to the density in sublattice $A$. This behavior is expected and can be traced back to the emergence of the strong impurity resonance in the $q$-resolved LDOS of sublattice $A$, see Eq. (19). The response of magnons to the perturbation in isotropic AFMs reveals that for low energy the defect on sublattice $A$ gives rise to the leakage of states into the sublattice $B$. This behavior is the same as what one observes in a honeycomb lattice, e.g., graphene and FM Dirac magnons [35] and other Dirac materials [52, 56].

The non-monotonic variations of the LDOS in each sublattice, and monotonically decreasing LDOS for energies above the critical energy, are transferred to the total LDOS. This is opposed to the pristine case, where the LDOS remains nearly constant. This different property is caused by the density redistribution caused by the impurity scattering which gives rise to the impurity resonance.

As can be seen in Fig. 3, both in the pristine as well as in the perturbed system, there is a finite LDOS at the bottom of the band, $\epsilon \to 0$, which explains the absence of a long-range order in the 2D isotropic AFM. Based on the Mermin-Wagner theorem, the existence of gapless Goldstone modes blocks the long-range order in 2D structures. Here, the non-vanishing LDOS at zero energy makes magnon available to destroy the order.

B. Induced localized peak

The plots in Fig. 4 show (a) the sublattice resolved and (b) the total LDOS for the easy-axis AFM structure, as a function of energy, for both the pristine lattice (dotted lines) and a system consisting a single defect (solid lines).

In easy-axis AFMs, the magnon gap introduced by the magnetic anisotropy, $\mathcal{K}_A$, opens up which can be seen in Fig. 4 (dotted lines). Consequently, the Goldstone modes are removed which leads to that the long-range order in the system is reestablished. Apart from the gapped LDOS, the same observations as discussed in the isotropic AFMs remain valid here. These observations are: in analogy with the isotropic case, the magnon LDOS is not equally distributed between the sublattices; introduction of a single defect in the lattice alters the resulting LDOS. By contrast to the isotropic configuration, placing a single defect induces a localized level for a strong enough scattering potential. The location of this localized level can be obtained from the correction term of density presented in Eq. (19). Similarly as in the isotropic AFM, in the gapped structure, a positive scattering potential does not induce any peak in the gap. However, a repulsive defect leads to a decreased magnon LDOS in the energy range outside the gap, showing that the presence of repulsive defects weakens the destructive effect magnons have on the long-range order in 2D AFMs.

Furthermore, in the presence of a finite easy-axis anisotropy, it can be seen that the localized peak becomes stronger in sublattice $A$, where the defect is located. This observation should be contrasted to the effect defects have on magnons in isotropic AFMs and Dirac FMs. This behaviour in easy-axis AFMs is more similar to the case of gapped Dirac materials like thin films of topological insulators [57], and can be traced back to the fact that an easy-axis anisotropy imposes a preferable direction to the spin structures and it preserves orthogonality of the magnons modes.

Impurity scattering through a repulsive defect in the easy-axis AFM, results in a non-negligible excitation around the bottom of the spectrum which may destroy the long-range order that was made possible by the gapped magnons. In order to analyze this issue in depth, we go beyond a configuration with a single defect and study the effect of multiple defects.

C. Random defects

In Fig. 5 (a), we plot the total LDOS for the easy-axis AFM with multiple defects as function of energy for different defect concentrations. Each defect gives rise a local enhancement of the magnon density. The averaged effect of each such enhancement leads to a full closing of the magnon gap for large enough defect concentrations, see Fig. 5 (a). Here, we predict that in a system with an anisotropy that is around five percents of the exchange interaction, the magnon gap is
magnonic scattering on a two-dimensional AFM lattice structure is very sensitive to defects. This observation indicates, in turn, that for a viable implementation of the magnon excitations, one should consider materials with very few defects and impurities in order to sustain reliable signals.

Experiments which address issues concerning the magnetic order and magnon lifetime in two-dimensional AFM would case more light on the questions addressed in this article.

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Appendix A: Bogoliubov transformation

The eigen-modes of Hamiltonian Eq. (4) can be obtained by diagonalization through the following $2 \times 2$ unitary Bogoliubov transformation \cite{45, 46, 61} for bosonic quasiparticles where

$$
\begin{pmatrix}
\alpha_q \\
\beta_q
\end{pmatrix} = \begin{pmatrix}
u_q & -v_q \\
-v_q^* & u_q^*
\end{pmatrix} \begin{pmatrix}
\alpha_q \\
\beta_q
\end{pmatrix},
$$

in which

$$u^2_q = \frac{\varepsilon_0 + \varepsilon_q^\alpha}{2\varepsilon_q^\alpha},$$

$$v^2_q = \frac{\varepsilon_0 - \varepsilon_q^\beta}{2\varepsilon_q^\beta},$$

and they are associated with $|\nu_q|^2 - |v_q|^2 = 1$. Under this transformation, in the basis of new spinor $\begin{pmatrix}
\alpha_q \\
\beta_q
\end{pmatrix}$ the Hamiltonian Eq. (8) is obtained as

$$H^{(2)} = \sum_q \begin{pmatrix}
\alpha_q \\
\beta_q
\end{pmatrix} \begin{pmatrix}
\varepsilon_q^\alpha & 0 \\
0 & \varepsilon_q^\beta
\end{pmatrix} \begin{pmatrix}
\alpha_q \\
\beta_q
\end{pmatrix},$$

up to the quadratic terms. The density of states of AFM magnons evaluated by imaginary part of $\langle \langle \alpha_q \alpha_q^\dagger \rangle \rangle$ where

$$\alpha_q \alpha_q^\dagger = |v_q|^2 a_q a_q^\dagger + |\nu_q|^2 b_q b_q^\dagger - \nu_q^* v_q b_q^\dagger a_q - \nu_q v_q a_q b_q^\dagger,$$

reads as

$$-\frac{1}{\pi} \text{Im}(\langle \langle \alpha_q \alpha_q^\dagger \rangle \rangle) = \delta(\varepsilon - \varepsilon_q^\alpha).$$

Appendix B: On-site Green’s function

In conclusion, here we report that the magnetic order in two-dimensional AFM lattice structure is very sensitive to magnonic scattering off defects. While the absent magnetic order in the isotropic AFM lattice can be restored through an easy-axis anisotropy, scattering off local attractive impurities tends to generate localized levels in the gap below the magnon band. By considering randomly distributed scattering defects throughout the lattice, we find that even small defect concentrations lead to that the gap closes and, hence, destroy the AFM order. Moreover, in presence of scattering defects, the magnon excitations acquire an overall reduced relaxation time suggesting that also the stability of the magnons is reduced. This observation indicates, in turn, that for a viable implementation one should consider materials with very few defects and imperfectness.
Here, one can find the analytic calculation of on-site Green’s function for sublattice $A$
\[
g_0^{AA} = \frac{1}{\Omega} \int \frac{d^2q}{(2\pi)^2} \frac{\epsilon + \epsilon_0 - \epsilon_h}{(\epsilon - \epsilon_h)^2 - \epsilon_0^2 + \epsilon_h^2 + \gamma^2 q^2 |q| 2} \int \frac{q d\epsilon}{2\pi} \left[ \ln \left| \frac{1}{\Omega} \right| - \frac{\gamma^2 q^2 / 2}{(\epsilon - \epsilon_h)^2 - \gamma^2} \right] + i \pi \Theta \left( \left( \epsilon - \epsilon_h \right)^2 - \gamma^2 \right) \Theta \left( \gamma^2 q^2 / 2 - (\epsilon - \epsilon_h)^2 + \gamma^2 \right),
\]

where to solve such integral $\int_{-\infty}^{\infty} dx \frac{1}{x^{1+\eta}} f(x)$ we use Cauchy principal value as $\frac{1}{x^{1+\eta}} = P \frac{1}{x-\eta} - i\pi \delta(x)$. 

**Appendix C: Comparison with fermionic system**

In 2D Dirac fermionic structures such as graphene, there is a symmetry between positive and negative energies. Explicitly, a single defect with positive/ negative scattering potential induces a resonance peak in the density of states symmetrically at negative/positive energies. However, in magnonic systems, fluctuations with negative energy show the instability of the structure. Here, we keep our discussion within the valid regime, positive energies, for stable systems.

In Fig. (7), the MLDOS for isotropic (a,b) and easy-axis (c,d) AFM are plotted in the presence of an attractive (a,c) and repulsive (b,d) scattering potential. We observe that for a defect with a negative scattering potential the density of magnons increases for low energies. In the presence of a finite anisotropy, impact of defect on sublattice $A$ becomes much stronger in similarity with gapped Dirac materials. For the repulsive defect, a positive scattering potential annihilates magnons for both gapless and gapped structures. In these two cases as well as an isotropic AFM with an attractive defect, we have the leakage of MLDOS to the site $B$, i.e., $n^A < n^B$ for low energies. Panel (c) shows an opposite behaviour $n^A > n^B$ which comes from the existence of the gap due to the on-site easy-axis anisotropy.

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