Diluted quantum antiferromagnets: spin excitations and long-range order

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We have studied the static and dynamic magnetic properties of two-dimensional (2D) and quasi-two-dimensional, spin-$S$, quantum Heisenberg antiferromagnets (QHA) diluted with spinless vacancies. Using spin-wave theory and $T$-matrix approximation we have calculated the staggered magnetization, $M(x,T)$, the neutron scattering dynamical structure factor, $S(k,\omega)$, the 2D magnetic correlation length, $\xi(x,T)$, and the Néel temperature, $T_N(x)$, for the quasi-2D case. We find that in 2D the hydrodynamic description of excitations in terms of spin-waves breaks down at the wavelength larger than $\ell/a \sim e^{\pi/4x}$, $x$ being impurity concentration and $a$ the lattice spacing. We find the signatures of localization associated with the scale $\ell$ and interpret it as the localization length of magnons. The spectral function for momenta $a^{-1} \gg k \gg \ell^{-1}$ consists of two distinct parts: (i) a damped quasiparticle peak at the energy $c_0k \gtrsim \omega \gg \omega_0$ with abnormal damping $\Gamma_k \sim x c_0k$, where $\omega_0 \sim c_0 \ell^{-1}$, $c_0$ is the bare spin-wave velocity; (ii) a non-Lorentzian localization peak at $\omega \sim \omega_0$. For $k \lesssim \ell^{-1}$ these two structures merge and the spectrum becomes incoherent. The density of states acquires a constant term and exhibits an anomalous peak at $\omega \sim \omega_0$ associated with the low-energy localized excitations. These anomalies lead to a substantial enhancement of the magnetic correlation length, $\ell$, and can be lost only around $x \sim x_p$ where approximations of our approach become invalid.

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I. INTRODUCTION

The discovery of superconducting cuprates (HTC) has motivated an enormous amount of studies in low-dimensional magnetic systems during the last fifteen years \cite{1,2}. Yet, the superconducting materials now form only a subfield in the activity of low-D quantum magnetism (see Ref. \cite{3}). The hope for an insight into the physics of HTC from the study of magnetically related system has attracted much attention to the properties of diluted 2D, QHAF \cite{4,5,6}. One of such systems, $La_3Cu_1-Zn(Mg)_xO_4$ (LCO), a quasi-2D, $S=1/2$, QHAF diluted with spinless vacancies, has been a subject of great interest because of the possibility of new quantum critical points (QCP) in its phase diagram. Earlier experimental data \cite{7}, while demonstrating that LCO shows much stronger stability against doping in comparison with the mobile hole doped compound $La_{2-x}Sr_xCuO_4$, have indicated the existence of a QCP at $x = x_c \approx 0.2$, well below the classical percolation threshold. This finding was in a sharp contrast with the classical magnetic systems where dilution leads to the breaking of the magnetic bonds and long-range order (LRO) is lost only at the percolation threshold $x_p$, a characteristic value of the dilution fraction $x$ at which the last infinite cluster of connected spins disappears. For a 2D square lattice $x_p \approx 0.41$ \cite{21}. The existence of such a QCP below the percolation threshold was thought to be possible given the large amount of quantum fluctuations in the ground state of $S=1/2$ system. However, only recently the systematic experimental analysis of the diluted 2D AF has been performed in a wide range of doping \cite{22,23}. Although there are several other experimental realizations of a 2D QHAF on square lattice with $S = 1/2$ \cite{24,25} and $S = 5/2$ \cite{26,27}, the CuO-based compounds are among the few which allow a direct probe via elastic and inelastic neutron scattering. At the same time, quantum Monte Carlo (MC) studies have provided highly reliable simulations on large lattices at low temperatures \cite{28,29}. These works indicate that, in fact, no QCP point exists below $x_p$ and that at percolation threshold the phase transition is characterized by classical exponents \cite{26,27}.

Note that the theoretical studies of diluted spin systems has attracted much attention some 30 years ago in the context of magnetism in diluted magnetic alloys \cite{30,31}. Most of these studies focused on the large $S$ (classical) Heisenberg or Ising systems. Traditional view
of the effect of local disorder on the spectrum of an ordered 3D antiferromagnet is that at long wavelengths the form of the spectrum is not modified. The only effects are the reduction of hydrodynamic parameters (spin stiffness, spin-wave velocity, etc. [41]) and a weak damping. Conventional arguments for this ability of the long-wavelength spectrum to withstand perturbations on a local scale often appeal to the Goldstone theorem [37], although its applicability to systems without translational invariance requires an additional assumption that the microscopic details are virtually averaged on short distances. As a result the low-energy excitations are the weakly damped spin-waves which belong to the so called “infinite cluster” and they are well defined up to the percolation threshold [42]. This effective restoration of the translational invariance involves the spin-wave propagation on randomly directed paths with some Euclidean distance $L'$ which can be converted to a “true” distance $L$. Thus, the wave-vector preserves its meaning at long wavelengths [30]. In 3D these arguments work very well and are assumed to demonstrate a “general principle”.

There is growing evidence that in 2D, however, such a logic is not always valid. In the 2D case it was found by Harris and Kirkpatrick [39] and more recently in Ref. [37], using a perturbative (linear in $x$) approach, that the spin-wave self-energy at long wavelengths acquires a non-hydrodynamic contribution which explicitly violates the Lorentz invariance of the clean system (a feature anticipated by Chakravarty, et al. in Ref. [1]). Recently, similar results have been obtained in RPA studies of the diluted 2D Hubbard model [3]. Some of these studies have concluded that $D = 2$ is the lower critical dimension for this type of disorder [30,37], implying an instability of the long-range order to an infinitesimal doping in the Imry-Ma sense [38]. However, as we mentioned above, MC results show that the order is preserved up to $x = x_p$ in contradiction with these conclusions. We will show that the conjecture of the instability is an artifact of a perturbative expansion and is avoided when the divergent series of diagrams is summed. However, the resulting modification of the excitation spectrum is very unusual and leads to a number of observable anomalies.

Technically, our approach is similar to the one by Brenig and Kampf [15] who have studied the problem of excitations spectrum in diluted 2D QAF using spin-wave and $T$-matrix formalism. However, while the authors of Ref. [15] have noticed unusually broad peaks in the spectrum, they assumed a “normal” 3D-type of the spectrum renormalization, that is, the softening of the sound velocity and a recovery of the spectrum at long wavelength. The derivative of the spin-wave velocity with $x$, obtained numerically in Ref. [15] using this assumption, is rather large $d(c(x)/c_0)/dx \approx -3$ which has supported earlier experimental expectations of a QCP at $x < x_p$. A recent work by two of us using the non-linear $\sigma$-model allied to classical percolation theory [39] gave similar result. Another study in Ref. [14] used a generalizations of the $\sigma$-model with parameters modified according to MC data and suggested a simple renormalization of spin stiffness $\rho_s(x)$ and spin-wave velocity $c(x)$ as the only effect of impurities. We will show that these results are not correct because of the existence of localized spin excitations which are not taken into account in these works.

In this work we study the problem of impurities in 2D QHAF within the linear spin-wave theory using the $T$-matrix approach combined with configurational average over the random positions of impurities. We solve the single impurity problem exactly. The spin-wave Green’s function is evaluated by summing all multiple-scattering diagrams that involve single impurity. This approximation gives results that go beyond simple linear expansion in $x$, although not all higher order contributions in $x$ are taken into account. This approach is valid as long as single-impurity scattering is the dominant one. We recover the results of Refs. [15,37] at $k \gg \ell^{-1}$, that is, the spin-wave spectrum acquires a non-linear logarithmic contribution $\Sigma_k(\omega) \propto x \ln(\omega)$ with an abnormal damping $\Gamma_k \propto x k$. This means that an effective spin-wave velocity $c(x)$ is not well defined. However, we show that there is no instability of the system towards a disordered phase, as conjectured previously. The static properties such as staggered magnetization and Néel temperature do not possess anomalies in contrast with the dynamic properties. It is interesting to note that the spin-wave stiffness $\rho_s(x) = c(x)^2 \chi_\perp(x)$ is also well defined since the anomalous terms in the transverse susceptibility $\chi_\perp(x)$ and in $c(x)$ cancel each other.

We show that the diluted 2D AF provides an example of the system where the arguments for the spectrum to be “protected” at long wavelengths fail [11,22]. We have found that the spectrum of a 2D AF at long wavelengths is overdamped at arbitrary concentration of spinless impurities. More explicitly, the spectrum ceases to contain a quasiparticle peak of any kind beyond a certain length-scale. The actual spin excitations instead of being described as ballistic may be interpreted as diffusive spin modes. The reason for that is the influence of scattering centers on the long-wavelength excitation which is not vanishing in 2D because of the small phase space. This leads to the absence of the effective self-averaging of the system to a translationally invariant medium with the renormalized parameters as it would be in 3D. Instead, the scattering leads to a new length scale $\ell/\alpha \sim e^{\pi/4k}$ beyond which the influence of impurities on the spectrum is dominant. We associate this length scale with the localization length of spin excitations.

We show that the dynamical structure factor $S(k,\omega)$ for $a^{-1} \gg k \gg \ell^{-1}$ consists of three parts (we use units such that $\hbar = k_B = 1$): (i) a broadened quasiparticle peak at the energy $\omega \sim c_0 k (1 + 2x \ln(ka)/\pi)$, where $c_0 = 2\sqrt{2} S J a$ is the bare spin-wave velocity, $J$ is the antiferromagnetic exchange constant, with a width given by $\Gamma_k \approx x c_0 k$; (ii) a non-Lorentian localization peak at $\omega = \omega_0 \sim c_0 \ell^{-1}$, (iii) a flat background of states between $\omega = c_0 k$ and $\omega = \omega_0$. Thus, besides the lack of
the Lorentz invariance, for every \( k \)-state some weight is spread from the high energies \( \omega \sim c_0 k \) to the low energies down to \( \omega \sim \omega_0 \). For \( k \lesssim \ell^{-1} \) the quasiparticle and localization peaks in \( S(k, \omega) \) merge into a broad incoherent peak that disperses in momentum space.

The anomalies in the dynamical structure factor are reflected in the magnon density of states, \( N(\omega) \). In a clean 2D AF \( N(\omega) \propto \omega \). With the doping \( N(\omega) \) acquires a constant contribution from the localized states \( N(\omega) \propto \omega + \text{const} \cdot x \) at \( \omega \gg \omega_0 \), has a peak at \( \omega \approx \omega_0 \) of the height \( \sim 1/x \), and vanishes as \( N \propto 1/(x \ln |\omega|)^2 \) for \( \omega \ll \omega_0 \). This behavior of \( N(\omega) \) is reminiscent of the problem of localization of Dirac fermions in 2D d-wave superconductors [4] in the case of “strong” disorder (unitary scatterers). Another interesting similarity between that problem and impure 2D AF is that disorder may lead to very different physical consequences depending on its “class”. As it was noted in Ref. [27] and also in Ref. [15] in another context, one obtains drastically different results if the spin of impurity is equal to the spin of the host material and only bond strengths around impurity \((J)\) are modified. The renormalization of the spectrum in that case does not contain any anomalous terms, namely: \( \Sigma_0(\omega) \sim x c_0 k \) and \( \Gamma_0 \sim x c_0 k^2 a^2 \). According to the terminology of 2D Dirac fermions this problem falls into the class of a “weak” disorder. In the case of spinless impurities the similarity to “strong” unitary scattering centers is evident since no spin degrees of freedom exist at the impurity site.

From the density of states \( N(\omega) \) we calculate the magnetic specific heat which for a clean 2D system at low temperatures is \( C_M(0, T) \propto T^2 \). We predict a strong deviation from this behavior due to localized states. We find that specific heat acquires a quasi-linear correction \( \delta C_M(x, T) = \beta(x) T^2 / (\ln^2 |T/\omega_0| + \pi^2/4) \) which is roughly \( x T^2 \) at \( T \gg \omega_0 \), \( \beta(x) \sim 1/x \). Observation of such a behavior can provide a simple test of our theory. We remark that in our approach the contribution of the finite (decoupled) clusters is not taken into account since the whole system is considered as a single, ordered, infinite cluster. However, finite clusters of the size \( L \) have a gap in their spectrum of order \( J/L \) and thus become important in the low-\( T \) region only at \( x \) close to percolation threshold where \( L \) can be large. Another source of similar high-energy corrections is from the resonant states \((\omega_{\text{res}} \sim J)\) around impurities whose energy may go down with doping. [16]. At lower temperatures, \( T \lesssim \sqrt{J/L} \), where \( J_L \) is the inter-plane exchange constant, the crossover to a 3D behavior should be seen. Thus, for \( x \) not too close to \( x_p \) we expect a large temperature window where the predicted anomalous 2D behavior of the \( C_M \) in the infinite cluster is dominant and can be observed.

We also consider the effects of small inter-plane coupling \( \tau_{3D} = J_{L} / 2 J \) and small anisotropy gaps on our conclusions for dynamical properties of a strictly 2D isotropic AF we discussed above. It is evident that as long as these additional energy scales are small in comparison with \( J \) there will be an energy range \( 1 \gg \omega/J \gg \sqrt{T} \) (\( \tau = \tau_{eff} \) accumulating the total effect of the gaps and 3D coupling) in which the non-linearity of the spectrum and an abnormal damping of the 2D spin waves should be observable. A more delicate question is if the localization part of the spectrum and truly overdamped long-wavelength excitations can be seen in the presence of gaps or 3D coupling. The point is that the disorder induced scale \( \omega_0 \sim J_e^{-\pi/4} \) can be hindered by these additional terms which cuts off the log-singularity. Therefore a range of concentrations \( 0 < x < x^* \sim \ln^{-1}(1/\tau) \) can be found where the long-wavelength quasiparticles are still well defined deep in the 3D region of the \( k \)-space \((ka \ll \sqrt{T}) \) similar to the quasi-1D problem [15]. For the LCO materials \( \tau \sim 10^{-4} \) gives \( x^* \sim 0.1 - 0.2 \). Above the concentration \( x^* \) (and at \( x < x_p \)) localization and overdamped peaks should be observable since \( \omega_0 > \sqrt{T} \) and all the low-energy excitations become incoherent. Our order of magnitude estimation for the largest value of \( \tau \) which can allow such observation (from the condition \( x^* < x_p \)) is \( \tau \sim 0.01 \). Therefore, a rather high impurity concentration and small enough anisotropies and inter-planar coupling may be required to observe directly some of the dynamical effects we predict in this work.

We calculate the static magnetic properties and find a quantitative agreement with both MC simulations and experimental data. We show that at \( T = 0 \) the staggered magnetization (averaged over the magnetic sites [43]) is given by \( M(x, 0) \approx \Delta - B x \) for \( x \ll 1 \), the factor \( \Delta = \sum_k v_k^2 \approx 0.2 \) stands for the contribution of the zero-point fluctuations of the spins, \( B \approx 0.21 \) is \( S \)-independent in our approach. We find that \( T_N(x)/T_N(0) \approx 1 - A_s x \) for \( x \ll 1 \) where \( A_s = \pi - 2/\pi + B/(S-\Delta) \) is a weak function of \( S \). This linear expansion result gives \( A_{1/2} \approx 3.2 \) and \( A_{3/2} \approx 2.6 \) which work quite well up to a high value of \( x \approx 0.25 \). It is interesting that the linear expansion results point to \( x_e(1/2) \approx 0.31 \) and \( x_e(5/2) \approx 0.38 \), both below \( x_p \), which means that \( T_N(x) \) versus \( x \) should be concave, in contrast with the 2D Ising magnets for which \( T_N(x) \) is a more traditional convex curve [17]. Such an anomalous curvature of the ordering temperature has been also observed in many different magnetic systems composed of \( f \)-electron moments such as U and Ce [19].

We show that in our approach for larger values of \( x \) \( T_N(x) \) indeed bends inward and tends to saturate close to \( x_p \). We interpret this behavior as due to localization effects which tend to reduce the role of quantum fluctuations in the destruction of the long-range order.

We have calculated the 2D magnetic correlation length, \( \xi(x, T) \), to describe the paramagnetic phase of the system above the Néel temperature. We used a modified spin-wave theory formalism by Takahashi [50] and calculated \( \xi(x, T) \) numerically. Correlation length is suppressed in comparison with the pure case and also shows some deviation from the simple \( e^{2\pi p_0(x)/T} \) behavior at larger \( x \).

This paper is organized as follows: we describe the model and introduce the formalism in Section I; in Section III, we present the results for the dynamic proper-
ties; in Section IV the static properties and long range order is discussed; Section V contains our conclusions. A few Appendices are included with details of the calculations. Some of the results presented here were briefly reported in our previous paper [51].

II. FORMALISM

The systems discussed in this paper are modeled by the site-diluted quantum Heisenberg antiferromagnet:

\[ H = \sum_{\langle ij \rangle} J_{ij} p_i p_j S_i \cdot S_j - \sum_{l,\delta} J_{l,\delta} S_l \cdot S_{l+\delta} , \]

where \( p_i = 1 \) (0) if \( R_i \) site is occupied (unoccupied) by the spin \( S \). We focus on the problem of tetragonal or square lattices with in-plane, \( J \), and out-of-plane, \( J_\perp \), nearest-neighbor exchange constants, \( \langle ij \rangle \) denotes summation over bonds. In the systems of interest \( J \gg J_\perp \) (for instance, in LCO \( J \approx 1500 \) K and \( J_\perp \approx 10^{-4}J \)).

1. Spin-wave approximation.

We begin with the Hamiltonian [1] which is split into the pure host and impurity part

\[ \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{imp}} = \sum_{\langle ij \rangle} J_{ij} S_i \cdot S_j - \sum_{l,\delta} J_{l,\delta} S_l \cdot S_{l+\delta} , \]

where \( l \) runs over the impurity sites and \( \delta \) is a nearest-neighbor unity vector. Then, in the linear spin-wave approximation,

\[ S_i^z = -a_i^\dagger a_i + \sqrt{2S} b_i \]

\[ S_j^z = -S + b_j^\dagger b_j + \sqrt{2S} b_j \]

for the spins in A (i) and B (j) sublattices quadratic part of the pure host Hamiltonian \( \mathcal{H}_0 \) for the tetragonal lattice is given by:

\[ \mathcal{H}_0 = 4SJ \sum_k \left[ \hat{\gamma}_0 (a_k^\dagger a_k + b_k^\dagger b_k) + \hat{\gamma}_k (a_k^\dagger b_{-k}^\dagger + b_{-k}^\dagger a_k) \right] , \]

where we use that in-plane and out-of-plane coordination numbers are \( z = 4 \) and \( z_\perp = 2 \), respectively, and define

\[ \hat{\gamma}_k = \gamma_k + \tau \gamma_k^\perp , \]

with \( \tau = J_\perp / 2J \), \( \gamma_k = (\cos k_x + \cos k_y) / 2 \), and \( \gamma_k^\perp = \cos k_z \). From now on the in-plane and out-of-plane momenta are in units of the correspondent inverse lattice constants. Impurity part of the Hamiltonian [1] on the tetragonal lattice is:

\[ \mathcal{H}_{\text{imp}}^A = -S \sum_{l,\delta} J_{l,\delta} \left[ a_i^\dagger a_i + b_{l+\delta}^\dagger b_{l+\delta} + a_i^\dagger b_{l+\delta} + a_l b_{l+\delta} \right] , \]

\[ \mathcal{H}_{\text{imp}}^B = \mathcal{H}_{\text{imp}}^A(a \leftrightarrow b) , \]

with \( J_{l,\delta} \) for \( \delta = e_x, e_y (e_z) \). After Fourier transformation it is more convenient to write impurity Hamiltonian in the \( 2 \times 2 \) matrix notations:

\[ \mathcal{H}_{\text{imp}} = -4SJ \sum_{l,k,k'} e^{i(k-k')R_l} \hat{A}_{k,k'}^\dagger \hat{V}_{k,k'} \hat{A}_{k'} , \]

where

\[ \hat{A}_k = \left[ \begin{array}{c} a_k \\ b_{-k}^\dagger \end{array} \right] , \quad \hat{A}_k^\dagger = \left[ \begin{array}{c} a_k^\dagger \\ b_{-k} \end{array} \right] , \]

with scattering potentials for \( l \) in the sublattice A:

\[ \hat{V}_{A,k,k'}^A = \left( \begin{array}{c} \hat{\gamma}_0 \\ \hat{\gamma}_k \\ \hat{\gamma}_{k-k'} \end{array} \right) \]

and for \( l \) in the sublattice B:

\[ \hat{V}_{B,k,k'}^B = \left( \begin{array}{c} \hat{\gamma}_{k-k'} \\ \hat{\gamma}_{-k} \\ \hat{\gamma}_{k} \end{array} \right) \]

The pure host Hamiltonian [1] is diagonalized using Bogolyubov transformation:

\[ a_k = u_k a_k + v_k b_{-k}^\dagger , \]

\[ b_k^\dagger = u_k b_{-k}^\dagger + v_k a_{-k} \]

with

\[ u_k^2 - v_k^2 = 1 , \quad 2u_kv_k = -\hat{\gamma}_k / \omega_k , \]

\[ u_k = \sqrt{\frac{\hat{\gamma}_0 + \omega_k}{2\omega_k}} ; \quad v_k = -\text{sgn} \hat{\gamma}_k \sqrt{\frac{\hat{\gamma}_0 - \omega_k}{2\omega_k}} , \]

where bare spin-wave frequency is

\[ \omega_k = \sqrt{\frac{\hat{\gamma}_0^2 - \hat{\gamma}_k^2}{\tau}} . \]

The problem can be reduced to the problem in 2D square lattice by letting \( \tau \to 0 \) in Eqs. [1],[3]. In what follows all energies are expressed in the units of \( \Omega_0 = 4SJ \).

After the Bogolyubov transformation the Hamiltonian Eqs. [1],[3] is given by (in the units of \( \Omega_0 \)):

\[ \mathcal{H}_0 = \sum_k \omega_k \left( \alpha_k^\dagger \alpha_k + \beta_{k'}^\dagger \beta_{k'} \right) , \]

\[ \mathcal{H}_{\text{imp}} = - \sum_{l,k,k'} e^{i(k-k')R_l} \hat{A}_{k,k'}^\dagger \hat{V}_{k,k'} \hat{A}_{k'} , \]

where two-component vectors are:

\[ \hat{A}_k = \left[ \begin{array}{c} \alpha_k \\ \beta_{-k} \end{array} \right] , \quad \hat{A}_k^\dagger = \left[ \begin{array}{c} \alpha_k^\dagger \\ \beta_{-k}^\dagger \end{array} \right] , \]

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and $2 \times 2$ scattering potential matrices $\hat{V}_{k,k'}$ are obtained from Eqs. (1), (14) using Eq. (13). For the sake of the further use of the $T$-matrix formalism it is convenient to decompose scattering potentials into the orthogonal components according to the symmetry with respect to the scattering site. The symmetry of the tetragonal lattice is $D_{4h}$, which is a group of order 16 and has 10 irreducible representations. Since the impurity potentials Eqs. (14), (15) connect only nearest-neighbor sites, only five components of the scattering potentials in the irreducible representations of $D_{4h}$ are nonzero. They correspond to the irreducible representations $A_{1g}, B_{1g}, B_{2g}$, and $E_u$. These nonzero components are the $s$-wave, in-plane $p_x, p_y$, and $d$-waves, and out-of-plane $p_z$-wave (for details see Appendix A).

Thus, the scattering potential for the impurity in the sublattice $A$:

$$\hat{V}_{k,k'}^A = \sum_{\mu} \hat{V}_{k,k'}^{A,\mu}, \quad (17)$$

where scattering channels are $\mu = s, p_x, p_y, d, p_z$. In each channel the scattering potentials can be written as a direct product of the column and row vectors. The $s$-wave part

$$\hat{V}_{k,k'}^{A,s} = |s_k\rangle \otimes |s_{k'}\rangle + \tau |s_k^\perp\rangle \otimes |s_{k'}^\perp\rangle,$$

where $\langle s_k| = [u_k + v_k \gamma y], \quad \langle s_{k'}| = [u_{k'} + v_{k'} \gamma y]$, (18) and

$$\hat{V}_{k,k'}^{A,p_{\xi}(\xi')} = |p_k^{\xi(\xi')}\rangle \otimes |p_{k'}^{\xi(\xi')}\rangle,$$

where $\langle p_k^{\xi(\xi')}| = \sin k_{\xi(\xi')}(v_k, u_k)/\sqrt{2}$, (19)

the $d$-wave part

$$\hat{V}_{k,k'}^{A,d} = |d_k\rangle \otimes |d_{k'}\rangle,$$

where $\langle d_k| = \gamma_k^- [v_k, u_k]$, (20) and the out-of-plane $p_z$-wave contribution

$$\hat{V}_{k,k'}^{A,p_z} = \tau |p_k^z\rangle \otimes |p_{k'}^z\rangle,$$

where $\langle p_k^z| = \sin k_z[v_k, u_k]/\sqrt{2}$, (21)

For the impurity in $B$ sublattice $\hat{V}_{k,k'}^B = \hat{V}_{k,k'}^A(u \leftrightarrow v)$.

In what follows we consider the 2D ($\tau = 0$) or quasi-2D ($\tau \ll 1$) limit of the problem. It can be shown that the contribution of the out-of-plane terms in $s$-wave and $p_z$-wave scattering potentials which explicitly depend on $\tau$, as well as the one of the majority of the $\tau$-dependent terms originating from the quasi-2D form of $u_k, v_k$, and $\omega_k$ (12), (13) is negligible in the quasi-2D case ($\sim \mathcal{O}(\tau)$, see Appendix B). It allows one to simplify the scattering problem further by neglecting the $s^\perp$ and $p_z$ components in the above equations. Moreover, the solution for the 2D problem can be applied directly to the quasi-2D case since the formal expressions are identical in both cases.

The only important difference concerns the logarithmically divergent terms which in quasi-2D system acquire a low-energy cut-off provided by the implicit dependence of the scattering potentials (14), (15) on $\tau$ through $\omega_k$. This simply means that for the quasi-2D case in the limit $\tau \ll 1$ one can restrict oneself by considering purely 2D scattering including the 3-dimensionality only on the level of the spin-wave dispersion in certain terms. Thus, in the following we use

$$\hat{V}_{k,k'}^{A,s} = |s_k\rangle \otimes |s_{k'}\rangle,$$

with $\langle s_k| = \omega_k[u_k, -v_k]$. (22)

The rest of this section is devoted to the 2D limit of the problem and, unless specified otherwise, we use

$$\gamma_k = \gamma_k = (\cos k_x + \cos k_y)/2,$$

$$\gamma_0 = 1, \quad \omega_k = \sqrt{1 - \gamma_k^2}. \quad (23)$$

2. $T$-matrix. Single-impurity scattering.

We are interested in the Green’s function of the Hamiltonian (14) modified by random impurity potentials (15). The Green’s function is a $2 \times 2$ matrix defined in a standard way:

$$G_{k\mu}^{1}(t) = -i\langle T[\alpha(t)\alpha_k(0)]\rangle, \quad (24)$$

$$G_{k\mu}^{2}(t) = -i\langle T[\alpha_k(t)\beta_{-k}(0)]\rangle,$$

$$G_{k\mu}^{21}(t) = -i\langle T[\beta_{-k}(t)\alpha_k(0)]\rangle,$$

$$G_{k\mu}^{22}(t) = -i\langle T[\beta_{-k}(t)\beta_{-k}(0)]\rangle,$$

where brackets also imply a configurational average over the impurity sites.

The $T$-matrix equation for the Hamiltonian (13) is given by

$$\hat{T}_{k,k'}^{I,\mu} = -\hat{V}_{k,k'}^{I,\mu} - \sum_{q} \hat{V}_{k,q}^{I,\mu} G_{q}^{0}(\omega) \hat{T}_{q,k'}^{I,\mu}(\omega), \quad (25)$$

with $l = A(B)$, partial waves are restricted to in-plane $\mu = s, p_x, d$ harmonics according to the above discussion, and $G_{q}^{0}(\omega)$ is the $2 \times 2$ bare Green’s function:

$$G_{q,11}^{0}(\omega) = G_{q,22}^{0}(\omega) = \frac{1}{\omega - \omega_q + i\delta}, \quad (26)$$

$$G_{q,01}^{0}(\omega) = G_{q,21}^{0}(\omega) = 0.$$

The diagrammatic equivalent of the Eq. (25) is shown in Fig. 1a. The $T$-matrix equations (25) with potentials (13), (22) can be readily solved:
\[
\hat{T}^{A,\mu}_{k,\mathbf{k}'}(\omega) = \hat{\Sigma}^{A,\mu}_{k,\mathbf{k}'} \Gamma_{\mu}(\omega), \\
\hat{T}^{B,\mu}_{k,\mathbf{k}'}(\omega) = \hat{\Sigma}^{B,\mu}_{k,\mathbf{k}'} \Gamma_{\mu}(-\omega),
\]
where the frequency dependent parts are given by
\[
\Gamma_s(\omega) = \frac{1}{\omega} + \frac{(1 + \omega)\rho(\omega)}{1 - \omega(1 + \omega)\rho(\omega)} ,
\]
\[
\Gamma_p(\omega) = -\frac{2}{1 + \omega + (1 - \omega)(\omega^2 \rho(\omega) - \rho_d(\omega))} ,
\]
\[
\Gamma_d(\omega) = -\frac{1}{1 + (1 - \omega)\rho_d(\omega)} ,
\]
with
\[
\rho(\omega) = \sum_p \frac{1}{\omega^2 - \omega_p^2} , \quad \rho_d(\omega) = \sum_p \frac{(\gamma_p^-)^2}{\omega^2 - \omega_p^2} .
\]

We note here that the second term in s-wave \(\Gamma_s(\omega)\) is proportional to \(\rho(\omega)\) at \(\omega \ll 1\), where the latter appears naturally from the summation in Fig. 3(a) as a result of combination of \(G_{q11}^{11}(\omega)\) and \(c_{q22}^{11}(\omega)\) in the internal part of the diagrams. When the summation over \(p\) in Eq. (29) is restricted to 2D \(\rho(\omega)\) is a logarithmic function at low energies. In the following we show that this contribution to the s-wave scattering is solely responsible for all the anomalies in the spectrum of a 2D AF. Interestingly, similar logarithmic term in the self-energy of the 2D Dirac fermions in the problem of disorder in \(d\)-wave superconductors requires a summation of the specific subset of diagrams [12]. In our case, while one needs to sum infinite series of diagrams, no special selection or inclusion of the multiple-impurity scattering processes is necessary. Since the single-particle density of states and sensitivity of the results to the type of disorder in both problems are similar, establishing of the detailed correspondence between these two problems is an important question. Integrals in Eq. (29) can be taken analytically and, in the case of 2D, are expressed through the complete elliptic integrals [13] (see Appendix D).

The first term in the \(s\)-wave scattering Eq. (28) represents a singular zero-frequency mode which is independent of the dimension of the problem and originates from the oscillations of the fictitious spin degrees of freedom at the impurity site which are decoupled from the AF matrix.

Roughly speaking, when the spins are quantized as in Eq. (3) and \(S'\) at the impurity site is set to zero there is still \(a_{0}^{\downarrow} a_{0}^{\uparrow}\) left from \(S_{0}^{s}\). Thus, in the spin-wave approximation, it gives rise to the \(s\)-wave zero-frequency mode. This problem has been noticed since the earliest works on the diluted magnets which have used the spin-wave theory [31] and also more recently in the context of diluted AF [14,15,16,33] (for an extensive discussion see Ref. [17]). Since these states are unphysical and are unrelated to the low-energy physics of the AF they have to be projected out. One of the projection schemes involves a non-Hermitian potential which was designed to preserve the simplest factorized form of the \(s\)-wave scattering potential [33]. We use another, physically more transparent scheme which introduces a fictitious magnetic fields at the impurity sites (similar to Refs. 14,15):

\[
\Delta \mathcal{H} = H_z \sum_{l,k,k'} a_{l}^{\dagger} a_{l}
\]
\[
\Rightarrow H_z \sum_{l,k,k'} e^{i(k-k') \cdot \mathbf{R}_{l}} \hat{A}_{l}^{\dagger} \Delta \hat{V}_{l,s}^{k,k'} \hat{A}_{k'} ,
\]
where corrections to the \(s\)-wave scattering potential are:

\[
\Delta \hat{V}_{k,k'}^{s} = |\Delta s_k| \otimes |\Delta s_{k'}| ,
\]
with \(|\Delta s_k| = |u_k, v_k|\),

\[
\Delta \hat{V}_{l,s}^{k,k'} = \Delta \hat{V}_{l,s}^{k,k'} \{u \leftrightarrow v\} .
\]
Evidently, \(p\) and \(d\) waves are not affected by the projection. Within our approach after some algebra in the limit \(H_z \to \infty\) one obtains a modified \(T\)-matrix solution (for the case of an arbitrary \(H_z\) see Appendix D):

\[
\hat{T}^{A,s}_{k,k'}(\omega) = \hat{\Sigma}^{A,s}_{k,k'} \Gamma_{s}(\omega) + \Delta \hat{T}^{A,s}_{k,k'}(\omega),
\]
\[
\hat{T}^{B,s}_{k,k'}(\omega) = \hat{\Sigma}^{B,s}_{k,k'} \Gamma_{s}(-\omega) + \Delta \hat{T}^{B,s}_{k,k'}(\omega),
\]
where \(\hat{\Sigma}^{l,s}_{k,k'}\) is given, as before, by Eq. (18) and the frequency dependent part is now free from the zero-frequency pole

\[
\Gamma_{s}(\omega) = \frac{(1 + \omega)\rho(\omega)}{1 - \omega(1 + \omega)\rho(\omega)} .
\]

Comparing this expression with Eq. (28) one may note that the “physical” term is left unchanged after the projection. Additional terms in the solution (12) are also regular:

\[
\Delta \hat{T}_{k,k'}^{A,s}(\omega) = -\omega|\Delta s_k| \otimes |\Delta s_{k'}| ,
\]
\[
+ |s_k| \otimes |\Delta s_{k'}| + |\Delta s_k| \otimes |s_{k'}| ,
\]
with \(|s_k|\) from Eq. (23) and \(|\Delta s_k|\) from Eq. (11), \(\hat{T}_{k,k'}^{B,s}(\omega) = \hat{T}_{k,k'}^{A,s}(-\omega)\{u \leftrightarrow v\}\) as before. Thus, the projection (30) allows one to remove the unphysical divergence at \(\omega = 0\) which would otherwise affect the true low-energy physics of the problem.

3. Green’s function.

The averaging over random distribution of impurities readily transforms \(T\)-matrix into the spin-wave self-energies:

\[
\hat{\Sigma}_{k}(\omega) = \sum_{\mu} \hat{\Sigma}_{\mu,k}(\omega) ,
\]
with \(\mu\)-wave contributions

\[
\hat{\Sigma}_{\mu,k}(\omega) = x\delta_{k-k'} \left[ \hat{T}^{A,\mu}_{k,k'}(\omega) + \hat{T}^{B,\mu}_{k,k'}(\omega) \right] .
\]
For the 2D case the contribution of the partial waves to the self-energies are:

\[
\tilde{\Sigma}_{s, k}(\omega) = x\omega_k \left[ \left( \frac{1}{\gamma_k} \right) \frac{\Gamma_s(\omega) + \Gamma_s(-\omega)}{2} \right. \\
+ \left. \left( \frac{\omega_k}{\gamma_k} \right) \frac{\Gamma_s(\omega) - \Gamma_s(-\omega)}{2} \right]
\]

(37)

\[
\tilde{\Sigma}_{p, k}(\omega) = x\omega_k \left[ -\frac{\gamma_k}{\omega_k} \right]^2 \\
\times \left[ \left( \frac{1}{\gamma_k} \right) \frac{\Gamma_p(\omega) + \Gamma_p(-\omega)}{2} \right. \\
+ \left. \left( \frac{\omega_k}{\gamma_k} \right) \frac{\Gamma_p(\omega) - \Gamma_p(-\omega)}{2} \right]
\]

(38)

\[
\tilde{\Sigma}_{d, k}(\omega) = x\omega_k \left[ \frac{\gamma_k}{\omega_k} \right]^2 \left[ \left( \frac{1}{\gamma_k} \right) \frac{\Gamma_d(\omega) + \Gamma_d(-\omega)}{2} \right. \\
+ \left. \left( \frac{\omega_k}{\gamma_k} \right) \frac{\Gamma_d(\omega) - \Gamma_d(-\omega)}{2} \right]
\]

(39)

It is interesting to observe that “on shell” (at \( \omega = \omega_k \)) “projected” \( \tilde{T}_{k, k}(\omega) \) from Eqs. (32), (33) and “non-projected” expressions Eq. (27), (28) yield identical \( \tilde{\Sigma}_{s, k}(\omega_k) \).

FIG. 1. (a) \text{T}-matrix single-impurity scattering series, (b) Dyson-Belyaev diagram series for the diagonal, \( G^{11} \), and off-diagonal, \( G^{12} \), Green’s functions. Self-energies \( \Sigma^{11} \) (circle) and \( \Sigma^{12} \) (square) are the configurational averages of \( T^{11} \) and \( T^{12} \) components of the \( \text{T}-matrix \), respectively.

Summation of the Dyson-Belyaev diagrammatic series for the Green’s functions shown in Fig. (b) with self-energies defined in Eqs. (32)-(33) gives

\[
\hat{G}_k(\omega) = \begin{pmatrix}
-\omega - \omega_k - \Sigma^{11}_k(\omega) \\
\Sigma^{12}_k(\omega) \\
\Sigma^{21}_k(\omega) \\
\omega - \omega_k - \Sigma^{11}_k(\omega)
\end{pmatrix}
\]

(40)

\[
\frac{1}{(\omega - \omega_k - \Sigma^{11}_k(\omega))(-\omega - \omega_k - \Sigma^{22}_k(\omega)) - (\Sigma^{12}_k(\omega))^2}
\]

where \( \Sigma^{22}_k(\omega) = \Sigma^{11}_k(-\omega) \). A detailed consideration of the properties of spectral functions

\[
A^{ij}_k(\omega) = -\frac{1}{\pi} \text{Im} \hat{G}^{ij}_k(\omega)
\]

(41)

will be given in the next section.

We investigate the neutron scattering dynamical structure factor, \( S(k, \omega) \),

\[
S^{\alpha \beta}(k, \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \bar{S}_k^{\alpha}(t)S_k^{\beta}(0) \rangle
\]

(42)

which is directly related to the spin Green’s functions. The standard derivation of the single-magnon contribution to the transverse component of the dynamical structure factor \( S^+(k, \omega) \) at \( T = 0 \) gives

\[
S^+(k, \omega) = \pi S(u_k + \nu_k)^2 \times \left[ A_k^1(\omega) + A_k^{22}(\omega) + 2A_k^{12}(\omega) \right]
\]

(43)

where the kinematic (\( \omega \)-independent) form-factor \( (u_k + \nu_k)^2 = (1 - \gamma_k)/\omega_k \) is proportional to \( k \) close to the “nuclear” reciprocal lattice point \( K = 0 \) and is \( \sim 1/k \) close to the “magnetic” \( Q = (\pi, \pi) \) point. It thus enhances the signal close to the AF ordering vector and suppresses it close to the zone center. Note that the diagonal parts of the Green’s function are symmetric and off-diagonal parts are asymmetric with respect to the transformation \( k \rightarrow k + Q \) since \( G^{11} \sim \Sigma^{11} \) and \( \Sigma^{12}_{-k} = -\Sigma^{12}_k \). Therefore, the sum of the spectral functions in the bracket in Eq. (43) is, generally speaking, different in the magnetic and nuclear parts of the Brillouin zone. At \( T > 0 \) above expression (43) is modified by the factor \( [1 + n_B(\omega)] \), where \( n_B(\omega) = [e^{\omega/kT} - 1]^{-1} \) is the Bose distribution function.

The density of states associated with magnetic excitations is straightforwardly related to the magnon Green’s function (41) and is given by

\[
N(\omega) = \sum_k [A_k^{11}(\omega) + A_k^{22}(\omega)]
\]

(44)

The magnetic specific heat is then given by

\[
C_M(T) = \frac{1}{T^2} \int_0^1 d\omega N(\omega) \omega^2 \left[ n_B(\omega)^2 + n_B(\omega) \right]
\]

(45)

where \( \omega \) and \( T \) are in the units of \( \Omega_0 = 4SJ \).

The static properties of the system, such as staggered magnetization in the ordered phase, Néel temperature, and 2D correlation length in the paramagnetic phase, are calculated from the spin-wave expression of the averaged on-site magnetic moment:

\[
|\langle S_i^z \rangle| = S - \frac{1}{2} \sum_k \left( \frac{1}{\omega_k} - 1 \right) \sum_k \frac{1}{\omega_k} \left[ \langle \alpha_k^0 \alpha_k \rangle - \gamma_k \langle \alpha_k \beta_k \rangle \right]
\]

(46)
where bosonic averages can be expressed through the spectral functions \( \langle \alpha_k^\dagger \alpha_k \rangle \) as:
\[
\langle \alpha_k^\dagger \alpha_k \rangle = \int_{-\infty}^{\infty} \d\omega \, n_B(\omega) \, A_{R,k}^{\perp}(\omega) ,
\]
\[
\langle \alpha_k^\dagger \alpha_k \rangle = \int_{-\infty}^{\infty} \d\omega \, n_B(\omega) \, A_{R,k}^{\parallel}(\omega) ,
\]
which implicitly depend on impurity concentration \( x \), index \( R \) stands for retarded.

In the ordered phase these expressions \( (46), (47) \) provide us with the concentration and temperature dependence of the averaged staggered magnetization \( M(x,T) \).

The same expressions with the condition \( \langle S^z(x,T) \rangle = 0 \) define the mean-field equation on the Neél temperature as a function of \( x \). In both cases, when \( T \neq 0 \) the 3D form of the spin-wave dispersion is to be used in Eq. \( (44) \). In the paramagnetic phase \( (T > T_N) \) Eq. \( (46) \)

\[
\omega \to \gamma_k \text{ and } \omega_k \to \sqrt{1-\eta^2} \gamma_k .
\]

Then, in the framework of the modified spin-wave theory \( (50) \), equation \( <S^z>(x,T,\eta) = 0 \) is a constraint which represents a self-consistent equation on the gap \( \sqrt{1-\eta^2} \).

This, in turn, defines the 2D correlation length \( \xi_{2D} \) as a function of \( x \) and \( T \).

### III. DYNAMIC AND THERMODYNAMIC PROPERTIES

In this Section we consider in detail the structure of the spectral functions of the Green’s function Eq. \( (40) \), Fig. \( (1b) \), with self-energies given by Eqs. \( (57) - (59) \). We calculate the dynamical structure factor \( S(k,\omega) \), spin-wave density of states \( N(\omega) \), and low-\( T \) magnetic specific heat \( C_M(T) \). We consider the long-wavelength, low-energy limit of the problem and obtain analytical results for the low-energy \( S(k,\omega) \) and \( N(\omega) \) and the low-temperature \( C_M(T) \). We recall here that all wave-vectors are in units of inverse lattice spacing \( 1/a \) and all energies are in units of \( \Omega_0 = 4SJ \).

We consider the low-energy form of the Green’s functions first. At low energies \( \omega, \omega_k \ll 1 \) self-energies \( (57) - (59) \) are given by:
\[
\Sigma_k^{11}(\omega) = x\omega_k [\rho(\omega) + 2 - \pi/2] - \omega + \mathcal{O}(\omega_k^2 \omega^2) ,
\]
\[
\Sigma_k^{12}(\omega) = x\omega_k [\rho(\omega) + \pi/2] + \mathcal{O}(\omega_k^2 \omega^2) ,
\]
with \( \rho(\omega) \simeq (2/\pi) \ln |\omega/4| - i \),

which includes contributions from 2- and 3-wave scattering, d-wave part is of higher order \( \Sigma_d \simeq \mathcal{O}(\omega_k^3), \omega_k \simeq k/\sqrt{2} \). The importance of the projection of the unphysical states can be demonstrated one more time by comparison of the above expressions with the “unprojected” \( (H_z = 0) \) form of the self-energy:
\[
\Sigma_k^{11}(\omega) = x\omega_k [\rho(\omega) - \pi/2] + \omega^2/\omega + \mathcal{O}(\omega_k^2 \omega^2) ,
\]
which possesses an \( \omega = 0 \) singularity. Noteworthy, the “physical” part of the expression containing the logarithm is not related to the unphysical states and stays intact under the projection. As it was noted before “on-shell”, \( \omega = \omega_k \), the self-energies \( (48) \) and \( (49) \) coincide \( (57) \). The off-diagonal \( \Sigma_k^{22}(\omega) \) is the same in both cases. It is also useful to note that the first-order Born approximation to the scattering problem would give a very different result
\[
\Sigma_k^{11, \text{Born}}(\omega) = -2x\omega_k , \quad \Sigma_k^{22, \text{Born}}(\omega) = 0 ,
\]
with imaginary part of the self-energy being \( \sim \mathcal{O}(xk\omega^2) \).

One can see that along with the “normal” softening and weak damping the full \( T \)-matrix consideration gives non-linear dispersion term and damping \( |\gamma_k|/\omega_k \simeq x \) which is only parametrically small with respect to the bare spectrum. A perturbative “on-shell” pole equation gives
\[
\tilde{\omega}_k + i\gamma_k = \omega_k + \Sigma_k^{11}(\omega_k) ,
\]
\[
\tilde{\omega}_k = \omega_k \left( 1 - x(\pi/2 - 1) + \frac{2x}{\pi} \ln |\omega_k/4| \right) ,
\]
\[
\gamma_k = -x\omega_k ,
\]
which already shows that the spin-wave velocity in the effective medium is not well defined since the bracket in Eq. \( (51) \) depends on \( \mathbf{k} \). Moreover, the renormalization of the real part of the spectrum is dominated by the \( \ln |\omega| \) term at low frequencies and the bracket vanishes at some wave-vector
\[
k_c^{-1} \sim \exp(\pi/2x) .
\]

Because of that one can naively suggest a vanishing of the spectrum \( (57) \) and an instability of the ground state towards some new phase. Such an instability is, of course, just a signature of the breakdown of the perturbation theory. One has to sum up all the “dangerous” terms using Belyaev-Dyson equation Fig. \( (1b) \) and Eq. \( (40) \) and analyze the spectral functions \( (41) \).

The low-energy, long-wavelength form of the Green’s functions Eq. \( (41) \) with self-energies from Eq. \( (48) \) is
\[
G_k^{11}(\omega) = G_k^{22}(\omega) \simeq \frac{\tilde{\omega} + \omega_k \left( 1 + x[\rho(\omega) + 2 - \pi/2] \right)}{\tilde{\omega} - \omega_k \left( 1 + x[2\rho(\omega) + 4 - \pi] \right)} ,
\]
\[
G_k^{12}(\omega) \simeq -\frac{x\gamma_k \omega_k \left[ \rho(\omega) + \pi/2 \right]}{\tilde{\omega} - \omega_k \left( 1 + x[2\rho(\omega) + 4 - \pi] \right)} ,
\]
where \( \tilde{\omega} = \omega(1 + x) \) and \( \rho(\omega) \) is defined in \( (48) \).

The diagonal spectral function in the same limit can be then written as:
\[
A_k^{11}(\omega) \simeq \frac{1}{\pi} \frac{\tilde{\omega} - \omega_k}{(\tilde{\omega} - \omega_k)^2 + (2x\omega_k^2)^2} ,
\]
where we make use of imaginary part of the self-energies being $\text{Im} \Sigma^{ij}_{k}(\omega) \simeq -x\omega_k$, and introduce a “stretching factor”
\[
a(\omega) = 1 + x\left(\frac{4}{\pi} \ln |\omega/4| + 4 - \pi \right).
\] (55)

The energy at which this factor vanishes defines the disorder-induced energy scale
\[
\omega_0 \sim \exp \left(\frac{\pi}{4x}\right)
\] (56)

below which the spectrum is overdamped.

A more detailed analysis of Eq. (54) gives the following picture. At the wave-vectors much larger than $\omega_0$ ($\omega_k \gg \omega_0$), that is at the wavelengths shorter than a characteristic length $\ell \sim e^{-\pi/4x}$, the spectral function has three distinct regions in $\omega$. First, it is a vicinity of a quasiparticle peak, $\omega \approx \omega_k$:
\[
A_{k}^{11}(\omega) \approx \frac{2x\omega_k^2}{\pi \left(\omega^2 - \omega_k^2\right)^2 (2x\omega_k^2)^2},
\] (57)

where the spectrum has a regular Lorentzian form with the pole at $\omega_k$ and width $\gamma_k$ given by the perturbative result Eq. (52). Second, the intermediate range of energies, $\omega_0 < \omega \ll \omega_k$, where the “stretching factor” is not too close to zero:
\[
A_{k}^{11}(\omega) \approx \frac{1}{\omega_k} \frac{1}{\omega \omega_k^2 + 4x^2} \approx \frac{1}{\omega \omega_k} \cdot \text{const},
\] (58)

one can approximate $a(\omega)$ by a constant since its dependence on $\omega$ is weak in this range. One can see that the spectral function in this region is independent of $\omega$ and corresponds to an almost flat, shallow ($\sim x$) background of states. Third, the vicinity of a “localization peak”, $\omega \approx \omega_0$:
\[
A_{k}^{11}(\omega) \approx \frac{1}{4\pi x\omega_k} \text{ at } \omega = \omega_0,
\] (59)
\[
A_{k}^{11}(\omega) \approx \frac{\pi}{16 \omega_k x \ln |\omega|} \text{ at } \omega \ll \omega_0,
\]

where the spectral function rises sharply from the shallow background states $\sim x$ to a peak of the height $\sim 1/x$ and then vanishes in a singular fashion as $\omega$ approaches zero. Note that this peak is non-Lorentzian and its position ($\omega = \omega_0$) is independent of the value of $k$.

Thus, besides the lack of the Lorentz invariance of the quasiparticle part of the spectrum Eq. (51), every $k$-mode redistributes some of its weight from the energy $\sim \omega_k$ to a flat background of states between $\omega_k$ and $\omega_0$ and to a peak at $\omega = \omega_0$. Such a behavior is similar to the other problems of linearly dispersive excitations in the presence of disorder in two dimensions and should be interpreted as the signature of localization. Then the characteristic length
\[
\ell \sim \exp \left(\frac{\pi}{4x}\right)
\] (60)
is to be understood as a localization length of the spinwaves in our problem.

The truly intriguing question is what is happening at the wavelengths of the order of $\ell$ and beyond. In our approach for $k \lesssim \ell^{-1}$ the quasiparticle and localization peaks merge into a broad incoherent peak that disperses in the momentum space. One can see that at $k \sim \omega_0 < \ell^{-1}$ factor $a(\omega)$ is negative and the “pole” in Eq. (54) becomes pure imaginary. However, since $a(\omega)$ is $\omega$ dependent this peak is non-Lorentzian and thus can not be associated with the “simple” diffusive mode. Thus, we observe an overdamped, non-Lorentzian diffuse-like excitation with a characteristic width of the order of $\omega_k$ and peak position roughly at $\omega \lesssim \omega_k$. We have to remark here that the nature of the states at the wavelength above the localization length might be beyond the ability of our approach and the proper description of them may require a different, non-perturbative type of study.

Thus, the structure of the spectral function we discuss above demonstrates an unusual, non-hydrodynamic type of behavior of the spin-excitation spectrum of a diluted 2D AF. The strong influence of disorder in the low-energy excitations in 2D results in the failure of the averaging procedure, which effectively restores translational invariance, to recover the long-wavelength excitation spectrum of this effective medium. Already at the energies much larger than the disorder-induced scale $\omega \sim k \gg \omega_0$ one finds a departure from the hydrodynamics: while the “quasiparticle” excitation can be found, it does not disperse linearly with $k$ and its damping is neither hydrodynamic nor quasiparticle-like. More importantly, above the characteristic wavelength $\ell$ no hydrodynamic description of excitations is possible. The low-frequency modes do exist in some form but they cannot be classified in terms of an effective wave-vector and thus the long-wavelength propagation is entirely diffusive.

In addition, the spectra at $k \gg \omega_0$ are not exhausted by the quasiparticle peak. They also consist of the background of localized states and a localization peak described in Eqs. (58), (59).

The spectral function $A_{k}^{11}(\omega)$ obtained from the “full” expressions for the Green’s function and self-energies without taking the low-energy limit is shown in Figs. 2-4 for a number of wave-vectors along the (1,1) direction of the Brillouin zone for a representative value of impurity concentration $x = 0.1$. The purpose of these pictures is to demonstrate the features we have discussed using the long-wavelength form of $A_{k}^{11}(\omega)$. The amplitude of each $A_{k}(\omega)$ curve is normalized to fit the picture and therefore the relative heights of the curves bear no meaning. These figures also show the bare spin-wave energy (dashed-dotted line) with arrows pointing down showing the positions of “unperturbed” delta-function peaks. Dashed line corresponds to the perturbative renormalized spin-wave dispersion, Eq. (51), while arrows pointing up show the actual positions of the peaks for selected wave-vectors. The figures show the spectral function within the different ranges of $k$ rel-
ative to $\omega_0$, $k \gg \omega_0$, $k \gtrsim \omega_0$, and $k \lesssim \omega_0$, respectively. The latter can be calculated using Eq. (50) which gives $\omega_0(x = 0.1) \sim 10^{-3}$. 

FIG. 2. The spectral function $A_{k}^{11}(\omega)$ for the wave-vectors $k = 0.1, 0.3, 0.5, 0.7$, and $1.0$, all $\gg \omega_0$ along the (1, 1) direction, $k$ is in units $1/a$. Dashed-dotted line is the bare spin-wave energy, arrows pointing down show the positions of original delta-function peaks. Dashed line is the renormalized spin-wave dispersion Eq. (51), arrows pointing up show the actual positions of the peaks for selected wave-vectors. $A_{k}^{1}(\omega)$ for each $k$ is normalized to fit the picture.

Fig. 3 shows the spectral function $A_{k}^{11}(\omega)$ for the wave-vectors $k = 0.005, 0.01$, and $0.02$ along the (1, 1) direction, $k = 0.005$ is of the order of $\omega_0$. Dashed-dotted line, dashed line, and arrows are as in Fig. 2. $A_{k}^{11}(\omega)$ for each $k$ is normalized to fit the picture.

The origin of this high-energy structure is in the presence of the high-energy resonance state $(\omega_{res} \simeq J)$ around impurity [16] which is unrelated to the low-energy physics of the system. Since our low-energy consideration does not take this high-energy feature into account the position of the lower peak in this structure deviates from the long-wavelength dispersion [15] at larger $k$. The low-energy localization peak and background are already noticeable in Fig. 2 despite the high-energy scale.

Fig. 4 shows the spectral function $A_{k}^{11}(\omega)$ for the wave-vectors $k = 0.0001, 0.0005$, and $0.001$, all $< \omega_0$, along the (1, 1) direction. Dashed-dotted line, dashed line, and arrows are as in Fig. 3. $A_{k}^{11}(\omega)$ for each $k$ is normalized to fit the picture.

Fig. 5 shows the spectral function $A_{k}^{11}(\omega)$ for the wave-vectors $k = 0.0001, 0.0005$, and $0.001$, all are smaller than $\omega_0$. As we discussed above, the quasiparticle and localization peaks merge and give a broad, overdamped, non-Lorentzian diffusive peak. In other words, one may not represent the Green’s function in this region as a sum of coherent and incoherent contributions $G_{k}^{coh}(\omega) + G_{k}^{incoh}(\omega)$, it seems that only the second part survives. The peak position deviates from the perturbative renormalized spin-wave dispersion [51] and thus indicate the region where the perturbation theory breaks down.

The off-diagonal spectral function $A_{k}^{12}(\omega)$ should pos-
sess features similar to the one of the diagonal spectral function. The low-energy, long-wavelength form of $A_k^{12}(\omega)$ is given by

$$A_k^{12}(\omega) \approx \frac{1}{\pi} \frac{x_{\gamma}}{\omega_k} \frac{1}{\omega_k^2} \frac{a(\omega)}{x^2 + 4} \quad ,$$

(61)

where $b(x) = [1 - 2x(\pi - 2)]$. Note that $A_k^{12}(\omega)$ is not a positively defined function, it changes sign as a function of $\omega$ at $\omega = \omega_k \sqrt{b(x)/(1 + x)}$. Another important difference from $A_k^{11}(\omega)$ is that $A_k^{12}(\omega)$ is odd under the transformation $k \to k + Q$ and thus has opposite sign in the first and second magnetic Brillouin zones.

A detailed analysis of $A_k^{12}(\omega)$ in different regions of $\omega_k$ and $\omega$ shows that in the vicinity of a quasiparticle peak $A_k^{12}(\omega)$ has an additional smallness of order $\omega$ in comparison with $A_k^{11}(\omega)$, but it is of the same order in the “intermediate” ($\omega < \omega_k$) and low-energy regions where it can be approximated as

$$A_k^{12}(\omega) \approx \frac{1}{\pi} \frac{x_{\gamma}}{\omega_k} \frac{1}{\omega_k^2} \frac{a(\omega)}{x^2 + 4} \quad ,$$

(62)

with the behavior above, at, and below the localization peak identical to the one of $A_k^{11}(\omega)$, Eqs. (58), (59).

![Fig. 5. The spectral function $A_k^{12}(\omega)$ for the wave-vectors $k = 0.1, 0.3, 0.5, 0.7,$ and $1.0$, all $\gg \omega_0$ along the (1,1) direction. $A_k^{12}(\omega)$ for each $k$ is normalized to fit the picture.](image)

However, the actual observation of anomalous features of the spectra can be complicated because of two reasons. First, the structure factor contains a kinematic form-factor which enhances the spectral function combination by $\approx 2/\omega_k$ close to $k = Q$ and suppresses it by $\approx \omega_k^2/2$ close to $k = 0$. Second, as we show below, the sum of the spectral functions entering $S^{+-}(k, \omega)$ is “less anomalous” close to $k = Q$ than at $k = 0$. Namely, the quasiparticle part of the spectrum is abnormally broadened and disperses nonlinearly for both $k \to 0$ and $k \to Q$, while the low-energy localization features are suppressed in the vicinity of $Q$ due to cancellation between the diagonal and off-diagonal contributions.

One can show explicitly using the low-energy, long-wavelength limit of the sum of spectral functions $[A_k^{11}(\omega) + A_k^{22}(\omega) + 2A_k^{12}(\omega)]$ given by

$$A_k^{\alpha}(\omega) = \sum_{\alpha = 1, 2} A_k^{\alpha}(\omega) \approx \frac{2x_{\gamma}}{\pi} \frac{\omega_k^2(1 - \gamma_k)}{\omega_k^2(1 + \gamma_k) - 2x_{\gamma}\omega_k^2(\pi - 2)} \quad ,$$

(63)

that aside from the kinematic form-factor the dynamical structure factor should be different in the first ($k \to 0$)
and the second \((k \to Q)\) magnetic Brillouin zones

\[
A_k^\Sigma(\omega) \approx \frac{1}{\pi} \left( \omega^2 - \omega_k^2 a(\omega) \right)^2 + \left( 2x \omega_k \right)^2, \tag{64}
\]

due to the asymmetry of \(A_k^{12}(\omega)\) to \(k \to k + Q\). One can see that around the quasiparticle peak \(\omega \approx \omega_k\) these expressions are identical and are simply equal to the diagonal spectral function Eq. (57), but at lower energies for \(k \sim Q\) the localization features are suppressed by the factor of \(\omega^2\).

This asymmetry is demonstrated in Fig. 7 which shows the intensity map of \(S^{+\Sigma}(k, \omega) \cdot \omega_k/(1 - \gamma_k) = \pi S A_k^\Sigma(\omega)\), that is the structure factor divided by the kinematic form-factor, in the \(k - \omega\) plane across the Brillouin zone in the \((1, 1)\) direction from \(k = 0\) to \(k = (\pi, \pi)\), for \(x = 0.25\). The higher intensity corresponds to the higher value of the function. One can clearly see all the features of the spectrum described in this Section: the resonance and its splitting from the dispersive mode at high energies, the low-energy damped spin-wave mode in both the center and the corner of the Brillouin zone, and the asymmetric background of localized states with the low-energy peak at the bottom. The nonlinearity of the quasiparticle mode also seem to be quite visible though the actual detection of it or of the abnormal \(k\)-dependence of the damping can be a challenging experimental problem.

Evidently, the low-energy localized states should strongly affect \(N(\omega)\) and one readily finds the anomalous corrections already on the level of perturbative analysis of the Green’s function. If one uses the full \(T\)-matrix form of the self-energy but expands the Green’s function in \(x\):

\[
G_k^{11}(\omega) \approx G_k^{0,11}(\omega) + G_k^{11}(\omega) \Sigma_k^{11}(\omega) G_k^{0,11}(\omega), \tag{67}
\]

one immediately gets a constant correction

\[
N(\omega) = \frac{2}{\pi} \omega + xC + \mathcal{O}(x \omega \ln |\omega|), \tag{68}
\]

which also implies a finite density of states at \(\omega = 0\). A more sensible result can be obtained without using \(x\)-expansion from the long-wavelength expression for the spectral function \(A_k^{11}(\omega)\) (64):

\[
N(\omega) = \frac{2}{\pi} \omega + xC_1/[a(\omega)^2 + 4x^2] + \mathcal{O}(x \omega \ln |\omega|), \tag{69}
\]

where \(a(\omega)\) is the same “stretching factor” Eq. (53) we used in Eqs. (54), (55), (57)-(59). At \(\omega \gg \omega_0\) \(a(\omega) \approx const\) and we are back to the previous result given by \(x\)-expansion perturbation theory (68). At \(\omega \approx \omega_0\) density of states has a peak of the height \(\sim 1/x\) whose origin is evident: the low-energy non-dispersive localized states altogether contribute to it. At \(\omega \ll \omega_0\) the density of states vanishes as \(N \propto 1/(x \ln |\omega|)^2\). Such a strong dependence of the result on the degree of approximation is reminiscent to the dispute over \(N(\omega)\) for the certain types of disorder in 2D systems with linear excitation spectrum (43, 44) where different approaches result in drastically different answers for the low-energy part of the density of states.

**FIG. 7.** The intensity map of \(\pi S A_k^\Sigma(\omega)\) in the \(k - \omega\) plane for \(k\) from \((0, 0)\) to \((\pi, \pi)\) in the \((1, 1)\) direction and from \(\omega = 0\) to \(\omega = 1\) for \(x = 0.25\).

The density of states of spin-excitations can be easily calculated using Eqs. (43) and (44). We recall that for the pure 2D system with linear spectrum of excitations low-energy density of states is a linear function of \(\omega\) and in our case

\[
N(\omega) = \frac{2}{\pi} \omega. \tag{66}
\]

**FIG. 8.** Density of states \(N(\omega)\) v.s. \(\omega\) for \(x = 0\) (pure system, dashed curve), \(x = 0.1\), and \(x = 0.2\) (dotted and solid curves). Dotted curves are the long-wavelength result Eq. (44) with \(C_1 = 4/\pi^{3/2}\). Solid curves are the result of numerical integration using the full Green’s function (44).
Our Fig. 8 shows the results for the density of states for \( x = 0 \) (pure system, dashed curve), \( x = 0.1 \), and \( x = 0.2 \). The dotted curves show \( N(\omega) \) given by Eq. (69) with \( C_1 = 4/\pi^{3/2} \), which is obtained from a long-wavelength expression for the spectral function (44). The solid curves are the result of numerical integration using the “full” Green’s function (49). While the overall agreement of these curves is very good, there is a significant discrepancy at low energies which has the following origin. In the long-wavelength limit we regarded the localization peak at \( \omega = \omega_0 \) as non-dispersive, whereas at larger \( k \), close to the magnetic Brillouin zone boundary, it does disperse down to \( \omega \sim \omega_0^2 \sim e^{-\pi/2x} \ll \omega_0 \). This can be noticed in our Fig. 8 as well. As a result of such a dispersion the peak in the density of states at \( \omega_0 \) is spread to lower energies. Technically, there is a term in the denominator of the Green’s function \( \sim x^2 \rho(\omega)^2 \omega_k \), negligible at low \( k \), which leads to such a behavior. Since this term is of the order of \( x^2 \) and our approach does not take into account all such terms we have no certainty on whether it is a spurious feature or not. As we show below this discrepancy does not affect any of our conclusions.

In this context it is interesting to note that the constant term in the density of states, which is a prominent feature of all three “full”, long-wavelength, and perturbative results, is directly related to the flat background of states below the quasiparticle peak in the spectral function. The localization-peak feature of the spectral function is responsible for the peak in \( N(\omega) \) at low \( \omega \).

The calculation of magnetic contribution to the spectral function (54) is given by the expression for the spectral function (54). The solid curves are the results from the long-wavelength expression for \( N(\omega) \), solid curves are from numerical integration using Eqs. (40) and (45). One can see that the results are very close and point to the same behavior. The dashed sector shows the temperature region \( T \lesssim \sqrt{T/J} \), which is the crossover to the 3D behavior (which provides higher powers of \( T \) to \( C_M \)) should occur. We use the value \( J_\perp = 10^{-4}J \) characteristic for the cuprates.

Our Fig. 9 shows the results for the magnetic specific heat of the spin-1/2 system \( (\Omega_0 = 2J) \) v.s. \( T \) for \( x = 0 \) (dashed curve), \( x = 0.1 \), and \( x = 0.2 \). Dotted curves are the results from the long-wavelength expression for \( N(\omega) \), solid curves are from numerical integration using Eqs. (40) and (45). One can see that the results are very close and point to the same behavior. The dashed sector shows the temperature region \( T \lesssim \sqrt{T/J} \), which is the crossover to the 3D behavior (which provides higher powers of \( T \) to \( C_M \)) should occur. We use the value \( J_\perp = 10^{-4}J \) characteristic for the cuprates.

The finite value of the inter-plane coupling together with the small anisotropy gaps leads to the finite value of the ordering temperature \( T_N \) whose dependence on impurity concentration is considered in the next Session. The effect of the 3D coupling in the dynamic properties, briefly mentioned above in the context of the specific heat, is the following. The energy scale introduced by the inter-plane coupling \( \tau = J_\perp/2J \) is \( \omega_{3D} = \sqrt{4\tau} \) as seen from Eqs. (3), (13) and therefore is rather small for the realistic systems of interest (for LCO \( \omega_{3D} \approx 0.01 \) in the units of the magnon bandwidth). We show in Appendix (3) that the 3D corrections to the 2D scattering are given by \( O(\tau \ln \tau) \) which is truly negligible (\( \sim 10^{-4} \) for LCO).

Therefore, the only appreciable correction to the dynamic wavelength expression for the density of states we obtain for such a correction:

\[
\delta C_M(T) \approx \frac{A(x)}{x \ln^2 |T/\omega_0| + \pi^2/4},
\]

where \( A(x) \) is a weak function of \( x \). At \( T \gg \omega_0 \) (it is also in units of \( \Omega_0 \)) this gives

\[
\delta C_M(T) \approx xT \cdot \text{const}.
\]
properties from 3D coupling is the low-energy cut-off of the logarithmic terms in the self-energy at \( \omega = \omega_{3D} \). As we describe in Appendix 3

\[
\rho_{3D}(\omega) \simeq \frac{1}{\pi} \ln \left| \frac{\tau}{16} \right| - i \frac{\omega}{\pi \sqrt{\tau}} \quad \text{at} \quad \omega \ll \omega_{3D} , \tag{72}
\]

that is, below the 3D energy scale the real part is a constant and imaginary part has an extra power of \( \omega \) in comparison with the pure 2D form of \( \rho(\omega) \). \( \rho(\omega) \) remains essentially two-dimensional at \( \omega > \omega_{3D} \). Evidently, this proves that the 3D coupling has little or no effect on the properties of the spectral functions, dynamical structure factor, or density of states at \( \omega > \omega_{3D} \).

However, the 3D coupling does affect some of the localization features in the following way. Below the 3D energy scale the “stretching factor” (55) saturates at the value \( a(\omega_{3D}) \) and the imaginary part of the self-energy acquires an extra power of \( \omega \). In other words, it should be understood as the competition of disorder-induced and 3D energy scales. Therefore, there are two regions of \( x \).

First, when \( x \) is small enough \( 0 < x \lesssim x^* \sim 1/\ln \tau^{-1} \) so that \( a(\omega_{3D}) > 0 \). In this region the well-defined spin waves can be found deep in the low-\( k \), low-\( \omega \) region \((k, \omega \ll \omega_{3D})\), similar to the quasi-1D problem [7]. Concentration \( x^* \) is defined from the equality of the energy scales \( e^{-\pi/4x} = \sqrt{\tau} \) which gives \( x^* \sim 1/\ln \tau^{-1} \). The localization peak in the spectral function at \( \omega \sim \omega_1 \sim J e^{-\pi/4x} \) in the low-\( \omega \), \( k \gg \omega \) region will be replaced by

\[
A_{11}^{3D} (\omega) \simeq \frac{1}{\pi} \frac{x \omega}{\omega_k} \frac{1}{a(\omega_{3D})^2} \quad \text{at} \quad \omega \ll \omega_{3D} , \tag{73}
\]

which smoothly vanishes as \( \omega \) goes to zero instead of showing a peak. However, the nonlinearity of the spectrum, abnormal damping of the quasiparticles, and the flat background of the localized states below \( \omega_k \) are all in the 2D-region of \( k - \omega \) space (\( \omega > \omega_{3D} \)) and will remain intact.

Second region is \( x \gtrsim x^* \) where \( a(\omega_{3D}) < 0 \). In this region the pole at low-\( k \) and low-\( \omega \) becomes pure imaginary as in 2D case and the localization peak for low-\( \omega \), \( k \gg \omega \) reappear above the 3D scale. Above the concentration \( x^* \) all the low-energy excitations are incoherent because the 2D disorder-induced energy scale \( \omega_0 \) (localization length \( \ell \)) is larger (shorter) than the 3D energy scale \( \omega_{3D} \) (length scale \( 1/\sqrt{\tau} \)) so the spin waves lose their coherence before they can propagate in 3D. A self-consistent calculation is required to determine accurately the value of \( x^* \) and the details of the 3D to 2D crossover. Our estimation gives \( x^* \sim 0.1 - 0.2 \) for \( \tau \sim 10^{-4} \).

Thus, we find that the 3D coupling for the realistic materials will modify the 2D density of states, structure factor, and specific heat only at the energies (temperatures) \( \omega < \omega_{3D} \simeq 0.01 \) and at impurity concentrations \( x < x^* \simeq 0.1 - 0.2 \). The estimated value of the 3D coupling \( \tau_c \) which would make \( x^* \) larger than the percolation threshold is \( \tau_c \sim 0.01 \).

The consideration given above also applies to the case of small anisotropies introducing gaps in the spectrum with a modified \( \tau = \tau_{eff} \) accumulating the total effect of the gaps and 3D coupling. It should be noted that the incoherence comes from the averaging procedure which converts the dissipation of momentum into the dissipation of the energy. Therefore, the overdamped excitations should be understood as diffusive. It is interesting that it requires 2D and “strong” disorder to restrict the number of Euclidean paths for spin waves and to break down the description of the problem in terms of an effective medium.

### IV. STATIC PROPERTIES

The static properties such as average staggered magnetization \( M(x, T) \), Néel temperature \( T_N(x) \), and 2D correlation length \( \xi(T, x) \) are considered in this Section.

The average on-site magnetic moment Eq. (16) for randomly diluted AF with the averaging over magnetic sites \( M(x) = \sum_i |S_i^z|/N_m \), see [3], can be expressed through the integral of the spectral functions (11) as:

\[
M(x, T) = S - \Delta - \delta M(x, T) , \tag{74}
\]

\[
\delta M(x, T) = \sum_k \int_{-\infty}^{\infty} \frac{n_B(\omega)}{\omega_k} \left[ A_{11}^{i, k}(\omega) - \gamma_k A_{12}^{i, k}(\omega) \right] , \tag{75}
\]

where \( \Delta = \sum_k \nu_k^2 \simeq 0.1966 \) is the zero-point spin deviation, \( n_B(\omega) = |e^{\omega/T} - 1|^{-1} \) is the Bose distribution function, subscript \( R \) denotes retarded. Note that one should not expect this formula to be valid at large doping level, \( x \) close to \( x_p \), since our approach neglects decoupled clusters and interactions of impurities. However, at not too large \( x \) these effects should be negligible and one expects Eq. (74) to be adequate. We would also like to note here that our definition of \( M(x, T) \) is physically equivalent to the “quantum-mechanical factor” of the averaged staggered magnetization, the definition used in the recent Monte Carlo study [20]. In other words, the “classical” (“geometrical”) effect of dilution on magnetization, which simply accounts for the decrease of the magnetic substance, is multiplicative to the quantum effects and is not taken into account in Eq. (74).

First we address the question of the presence of explicit divergences in the integral Eq. (74) which would point to the instability of the long-range order discussed in Refs. [30,37]. At \( T = 0 \) \( n_B(\omega) = -\theta(\omega) \) and the impurity-induced quantum reduction of the magnetization, which can be interpreted as a result of the “condensation of magnons”, is given by

\[
\delta M(x) = - \sum_k \int_{-1}^{0} \frac{d\omega}{\omega_k} \left[ A_{11}^{i, k}(\omega) - \gamma_k A_{12}^{i, k}(\omega) \right] , \tag{75}
\]

where we use that the spectral functions are zero outside of the magnon band \( \omega > 1 \). Since the perturbative
result Eq. (51) suggests the instability at small wave-vectors the long-wavelength expressions for the spectral functions can be used for an analysis. From the form of the spectral functions in Eqs. (53), (54) one can readily see that the integral over \( \omega \) is always finite. The integration over \( k \) is two-dimensional but has a factor of \( 1/\omega_k \) in the integrand. From our expression of the spectral functions in the intermediate and localization peak energy ranges Eqs. (58), (61), (62) one may suggest that the convergence of the integral is restored. To show that more explicitly one can use the \( x \)-expanded form of the Green’s function Eq. (77) for \( A_{R,k}^{11}(\omega) \) and an equivalent expression for \( A_{R,k}^{12}(\omega) \)

\[
G_{k}^{12}(\omega) \simeq G_{k}^{0,22}(\omega) \Sigma_{k}^{12}(\omega) G_{k}^{0,11}(\omega).
\]

Since all \( \Sigma \)’s are linear in \( x \) this provides an expression for the linear in \( x \) term in the staggered magnetization:

\[
\delta M(x) \simeq x B = - \sum_{k} \int_{-1}^{0} d\omega \left[ \frac{\text{Im} \Sigma_{R,k}^{11}(\omega)}{\omega - \omega_k^2} + \frac{\gamma_k \text{Im} \Sigma_{R,k}^{12}(\omega)}{\omega^2 - \omega_k^2} \right] + \sum_{k} \frac{\gamma_k \text{Re} \Sigma_{R,k}^{12}(\omega)}{2\omega_k^2}.
\]

In the long-wavelength limit this gives

\[
\delta M(x) \simeq x B = \frac{1}{\pi} \sum_{k} \int_{0}^{1} d\omega \left[ \frac{1}{(\omega + \omega_k)^2} + \frac{1}{\omega^2 - \omega_k^2} \right] + \frac{x}{\pi} \sum_{k} \frac{1}{\omega_k} \left[ \ln \frac{\omega_k}{4} - \pi^2/4 \right],
\]

where the strongest divergence of the integrand is \( \ln k d k \) and all integrals are convergent.

Numerical integration of the expression in Eq. (74) without the long-wavelength approximation gives the suppression rate of the staggered magnetization \( M(x) \simeq M(0) - B x \) with \( B = 0.209(8) \). For \( S = 1/2 \) it gives the slope of the normalized staggered magnetization \( M(x)/M(0) \approx 1 - B x/(S - \Delta) \approx 1 - 0.691(5) \cdot x \). It is interesting to note that the second Born approximation to the impurity scattering gives three times smaller rate \( B_{\text{Born}} = 0.0725 \) showing the necessity of the full T-matrix treatment of the problem. The estimation of \( B \), given in the previous study Ref. [77] using \( 1/x \) approximation for the expression similar to our Eq. (77), provides even smaller \( B_{1/x} \approx 1/x^2 = 0.0625 \) showing yet another inadequacy of that work.

We have also performed a numerical integration in Eq. (73) for the impurity-induced reduction of the staggered magnetization without \( x \)-expansion. This yields the results presented in Fig. 10 for \( S = 1/2 \) (solid line). Monte Carlo data from Ref. [25] (filled circles), and NQR data (open circles) from Ref. [56] are also shown. Note that the original Monte Carlo data of Ref. [25] are normalized by the total number of sites while both NQR and our results are averaged over the magnetic sites only. In order to extract the same quantity from the Monte Carlo data we divided them by the classical probability to find a spin-occupied site within the infinite cluster [8]. A recent Monte Carlo study Ref. [26] provided an analytical expression for the fit of the “quantum-mechanical factor” in the magnetization (see the comment after Eq. (74)) which we plot in Fig. 10 as well (dashed line). One can see a very good agreement of our results with numerical data up to high concentrations. The oxidation of the crystals can be the reason of a faster decrease of \( M(x) \) in NQR data.

The absolute value of impurity-induced quantum fluctuations \( \delta M(x) \) is independent of \( S \) in the linear spin-wave approximation similar to the quantum reduction of \( S \) by zero-point fluctuations \( \Delta \). We plot our results for \( \delta M(x) \) in Fig. 11 in order to emphasize the agreement with the MC data for \( S = 1/2 \) (circles) and \( S = 1 \) (squares), which show only weak \( S \)-dependence.

It is worth mentioning here that the discrete static quantities, zero-point spin deviations at the neighboring sites around impurities in an AF, were studied using spin-wave theory and Green’s functions methods since sixties [57] with most recent results obtained in Refs. [6], [58]. Quite remarkably, these results [53] were found to be in a very good agreement with the recent Monte Carlo studies of 2D \( S = 1/2 \) Heisenberg model with impurities, Ref. [9]. Note that while Refs. [53], [58] were focused on the discrete quantities our results concern the averaged ones.
At $T > 0$ Eq. (74) for the staggered magnetic moment can be rewritten separating the quantum, $T = 0$, and thermal, $T$-dependent, parts

$$M(x, T) = S - \Delta - \delta M(x) - \delta M_T(x, T) ,$$

$$\delta M_T(x, T) = \sum_k \int_0^1 \frac{n_B(\omega)}{\omega_k} \left[ A_1^k(\omega) + A_2^k(\omega) \right] \left( -2\gamma_k A_0^k(\omega) \right) ,$$

where $\delta M(x)$ is the zero-temperature part given in Eq. (73) and we used evident symmetries of the spectral functions with respect to $\omega \to -\omega$ and that $n_B(\omega) = -1 - n_B(-\omega)$.

For the true 2D system at $x = 0$ and $T > 0$ thermal fluctuation destroy the LRO which manifests itself as a log-divergency of the thermal correction to the magnetization

$$\delta M_T(0, T) = \sum_k \int_0^1 \frac{n_B(\omega)}{\omega_k} \delta(\omega - \omega_k) \approx 2 \frac{\pi}{T} \int_0^T \frac{T d\omega}{\omega} ,$$

where we use that $n_B(\omega) \approx T/\omega$ at $T \ll \omega$. The 3D coupling provides a cut-off to this divergence in a quasi-2D problem which yields the finite value of the thermal correction

$$\delta M_T(0, T) \approx 2 \frac{\pi}{T} \int_0^T n_B(\omega) d\omega \approx 2 \frac{T}{T} \ln \left| \frac{T}{\sqrt{4\pi}} \right| ,$$

and the finite value of the Néel temperature whose mean-field value can be found from the condition $M(0, T) = 0 = S - \Delta - \delta M_T(0, T)$ which gives

$$T_N^{MF} \approx \frac{\pi(S - \Delta)}{\ln \tau} \ll 1 ,$$

in units of $4SJ$. $T_N$ vanishes when $\tau \to 0$.

One would expect that the thermal part of the staggered magnetization for the diluted system may possess other divergences, stronger than the simple log-$\omega$ for the pure system. In fact, this suggestion is quite natural since the spectrum is not linear and, therefore, the non-linear corrections must show themselves up. Indeed, since the correction to the spectrum is $\delta \omega_k \sim 2\omega_k \ln|\omega|$ [71], one immediately suggests that the thermal part of the magnetization should acquire a term

$$\sim xT \int \frac{\ln |\omega| d\omega}{\omega} \sim xT \ln^2 |\omega| .$$

However, we show that such anomalous terms from diagonal and off-diagonal spectral functions cancel each other. As a result, there is no signature of any new divergency in this quantity caused by the anomalies of the spectrum.

Using the $x$-expanded form for the Green’s functions [73], [76] in the long-wavelength approximation one finds the diagonal

$$\delta M_\delta(x, T) = \sum_k \frac{1}{\omega_k} \langle a_k^\dagger a_k \rangle T \approx \sum_k \int_0^1 \frac{n_B(\omega)}{\pi \omega_k} \left( -2\gamma_k \right)$$

$$\times \left\{ \pi \delta(\omega - \omega_k) \left| 1 - \frac{\partial \Re \Sigma_k(\omega_k)}{\partial \omega_k} \right| - \frac{2\gamma_k}{\omega_k^2} \right\}$$

$$\approx \frac{2}{\pi} \int_0^1 n_B(\omega) d\omega \left[ 1 - x \left( 2\rho(\omega) - \frac{\pi}{2} + 1 - \frac{2}{\pi} \right) \right] ,$$

and off-diagonal

$$\delta M_{\text{off}}(x, T) = -\sum_k \frac{\gamma_k}{\omega_k} \langle a_k^\dagger a_k \rangle T \approx \sum_k \int_0^1 \frac{n_B(\omega)}{\pi \omega_k} \left( \rho(\omega_k) + \frac{\pi}{2} + \frac{2\omega_k}{\omega^2 - \omega_k^2} \right)$$

$$\approx \frac{2}{\pi} \int_0^1 n_B(\omega) d\omega \left[ 2\rho(\omega) + \frac{\pi}{2} \right] ,$$

parts of the temperature dependent $\delta M_T(x, T)$, where we kept only $O(\ln |\omega|)$ and $O(1)$ terms in the integrand, $\rho'(\omega) \equiv \Re \rho'(\omega)$, integration by parts was used in $\delta M_\delta$, superscript $T$ in the averages means the thermal part.

The total result is

$$\delta M(x, T) \approx \left[ 1 + x \left( \pi - \frac{2}{\pi} \right) \right] \delta M(0, T) ,$$

which shows that the thermal correction is enhanced by impurities but there is no new divergency associated with them in this quantity. Suppression rate of the Néel temperature can be readily obtained from the condition $M(x, T) = 0 = S - \Delta - \delta M(x) - \delta M_T(x, T)$ using Eq. (83) which gives:

$$\frac{T_N(x)}{T_N(0)} \approx 1 - A x = 1 - x \left( \pi - \frac{2}{\pi} + \frac{B}{S - \Delta} \right) .$$
For $S = 1/2$ this gives $A_{1/2} = 3.196(5)$ and for $S = 5/2$ it is $A_{5/2} = 2.600(4)$. It is important to note that these suppression rates point to $x_p((1/2) \approx 0.31$ and $x_p((5/2) \approx 0.38$, both below $x_p$, so that one may suggest that in order to have the phase transition at the classical percolation threshold the $T_N(x)/T_N(0)$ curves should have a rather unusual concave form.

It is interesting to compare our result for the decline rate of $T_N(x)$ to the answers of different approaches to the same problem and to the results for similar models. A naive mean-field treatment of the impurity effects as simple renormalization of magnetic coupling gives $T_N(x)/T_N(0) = 1 - x$. Application of our formalism to the Ising limit of the 2D problem gives $T_N(x)/T_N(0) = 1 - A^I x$ with $A^I \approx 1.37$ (see Appendix F) which is very close to the RPA answer $A^I_{RPA} = 1.33$ and below the exact answer $A^I_{exact} \approx 1.57$ [55].

For the 2D Ising magnets $T_N(x)$ vs. $x$ has a more traditional convex form [17]. Previous result on the suppression rate of $T_N$ for the 2D Heisenberg model [22] is $T_N(x)/T_N(0) = 1 - x x$ which is obtained using Green’s function technique and spin-wave theory in approximations very similar to ours. However, Ref. [59] misses $-2/\pi$ and neglects $1/S$ terms.

We have also performed a numerical integration in Eq. (87) and solved an implicit equation $M(x, T_N) = 0$ on $T_N(x)$ numerically. This procedure requires the finite 3D coupling and the use of quasi-2D form of the spectral functions. Since the integration involves an additional dimension and the 3D region is quite narrow the convergence of the result as a function of number of $k, \omega$-points at small $x$ can be an issue. We plot our numerical results for $T_N(x)/T_N(0)$ for the case of $S = 1/2$ in Fig. 12 together with the analytical slope Eq. (87) with $A_{1/2} = 3.2$ and experimental data. Experimental data are obtained by $\mu$SR [21] and magnetic susceptibility measurements [19] of LCO systems and by ESR [22] of Zn-doped copper formate tetrahydrate, a layered quasi-2D AF. One can see that our linear-$x$ results agree very well with the experimental data up to a rather high doping level $x \approx 0.25$. There is a slight disagreement between our own numerical and linear-$x$ analytical results already at small $x$ which may be connected not only to the numerical accuracy but to the corrections of the order $\sim x T_N/J \sim x/\ln^{-1}$. Note that the linear-$x$ result is free from such corrections since it is obtained in the $\tau \to 0$ limit.

As it is discussed extensively in Ref. [60] the spin-wave theory for layered materials is not really adequate at $T \sim T_N$ because of the lack of the kinematic constraints. When it is applied to the mean-field equation $M(x, T_N) = 0$ it tends to overestimate the absolute value of the Néel temperature and has some other artifacts such as $M(T) \sim T_N - T$ at $T \sim T_N$. This may also provide an additional $x$-dependence in our numerical values of $T_N(x)/T_N(0)$.

We plot our numerical results for $T_N(x)/T_N(0)$ vs. $x$ for $S = 5/2$. Analytical linear-$x$ results (1 $- A_{5/2} x$) Eq. (87) (solid line), and (circles) $\mu$SR (diamonds) [21] data for Zn-doped LCO, and ESR (squares) [22] of Zn-doped copper formate tetrahydrate $\text{Cu}_{1-x} \text{Zn(Mg,Cd)}_x (\text{HCO}_2)_22(\text{NH}_2)_2\text{CO}$.

FIG. 13. $T_N(x)/T_N(0)$ v.s. $x$ for $S = 5/2$. Analytical linear-$x$ results (1 $- A_{5/2} x$) Eq. (87) (solid line), and (circles) $\mu$SR magnetic susceptibility, specific heat data for $\text{Mn}_{1-x} \text{Zn(Mg,Cd)}_x (\text{HCO}_2)_22(\text{NH}_2)_2\text{CO}$. One can see that while the scattering of experimental points seems to be smaller than in $S = 1/2$ case the linear-$x$ result fits them very closely up to $x = 0.2$. The older $T_N(x)/T_N(0)$ data for the more traditional $S = 5/2$ material $\text{K}_2\text{Mn}_{1-x} \text{Mg}_x \text{F}_3$ [29] show a big scattering of the data which allows almost any reasonable fit [17].

It is worth mentioning that the numerical results of our approach for $T_N(x)$ bends inward at larger values of $x$ and show the above mentioned concave form, which
has been recently observed experimentally for LCO compounds [18] and has been anticipated in other works [24]. While our approach is certainly not adequate at such high impurity concentrations and tends to overestimate the value of $T_N(x)$ in comparison with experiments, it nevertheless points to the same physics. We interpret this behavior as due to localization effects which tend to reduce the role of quantum and thermal fluctuations in the destruction of the long-range order.

In the paramagnetic phase above the Néel ordering temperature the 3D coupling is irrelevant and the spin fluctuations in the layered AF system are characterized by the in-plane correlation length $\xi_{2D}$ which is exponentially diverging with $T$ as $T \to 0$. The correlation length is uniquely determined by the $T = 0$ properties of the system such as spin stiffness constant $\rho_s$.

The correlation length can be derived from the modified spin-wave theory, as was suggested in Ref. [50], by introducing a chemical potential for magnons which produces a gap in the spin-wave dispersion and then by resolving a constraint $\langle S_i^z \rangle = 0$ which defines the correlation length self-consistently. The result of such calculations at $x = 0$ is [50]

$$\xi(T) \simeq \frac{c}{2T} \exp \left( \frac{2\pi \rho_s}{T} \right). \quad (88)$$

One should bear in mind, however, that while this approach gives the correct exponential behavior of $\xi_{2D}(T)$ it provides a prefactor equivalent to the one-loop renormalization-group result [61]. This prefactor must be modified according to the higher order renormalization-group treatment [21] which gives [62]

$$\xi(T) \simeq \frac{c c}{2\pi \rho_s + T} \exp \left( \frac{2\pi \rho_s}{T} \right). \quad (89)$$

This expression shows excellent agreement with experiments and Monte Carlo data [12][13][14]. This discrepancy between the results of modified spin-wave theory and result of more exact, non-perturbative approach is of the same origin as the overestimation of the $T_N$ by the mean-field solution of $\langle S_i^z \rangle = 0$ equation [60].

We generalize the approach of Ref. [50] for the case of an AF with impurities and obtain for the constraint:

$$S - \frac{1}{2} \sum_k \left( \frac{1}{\omega_k(\eta)} - 1 \right) = \sum_k \frac{1}{\omega_k(\eta)} \left[ \langle \alpha_k^\dagger \alpha_k \rangle - \gamma_k \langle \alpha_k^\dagger \beta_k^\dagger \rangle \right]$$

where $\omega_k(\eta) = \sqrt{1 - \eta^2 \omega_k^2}$ and magnon averages are given by the integrals of the spectral functions $A_k^{11}(\omega)$, $A_k^{12}(\omega)$ from Eqs. [41], [42] in which the gapped form of the spin-wave spectrum is used.

We have performed a numerical integration in Eq. [40] and calculated the correlation length $\xi_{2D}(x,T) = \eta^2 / \sqrt{8(1 - \eta^2)}$ as a function of $T$ for several values of $x$. We fit the results of such a numerical procedure in a wide temperature range almost exactly with the help of original Takahashi formula, Eq. [88], with spin-stiffness $\rho_s(x)$ being a free parameter. These fitting values of $\rho_s(x)/\rho_s(0)$ v.s. $x$ follow closely our result for $T_N(x)/T_N(0)$ dependence, Fig. [13]. Such a result can be anticipated from the mean-field picture of the ordering in layered systems. The transition occurs when the inter-plane coupling is strong enough to stabilize the LRO in comparison with the thermal fluctuations: $J_{12} M^2(x) \xi^2(x,T_N(x)) \approx T_N$. If the correlation length preserves its exponential form the dominant part of the left-hand side comes from $e^{2\pi \rho_s(x)/T_N(x)}$ and one immediately arrives to

$$\frac{\rho_s(x)}{\rho_s(0)} = \frac{T_N(x)}{T_N(0)} + \mathcal{O}(x/ \ln \tau^{-1}). \quad (91)$$

Therefore, the important conclusion one can make from our analysis is that (i) the correlation length should follow the $x = 0$ type of behavior Eq. (89) with $x$-dependent $\rho_s$, at least for not too low $T$ and not too high $x$, (ii) $\rho_s(x)/\rho_s(0) \approx T_N(x)/T_N(0)$.

Our Fig. 14 shows a semi-log plot of $\xi(x,T)$ given by formula in Eq. [88] with $\rho_s(x) = \rho_s(0)(1 - A_{1/2})$, $A_{1/2}$ is from Eq. [77], v.s. $J/T$ for $x = 0$ (dashed line), $x = 0.1$, $x = 0.2$, and $x = 0.3$ (solid lines). An important observation can be made here. At small $x$ $2\pi \rho_s$ is of the order of $J$ and at all reasonable temperatures the dominant behavior is exponential in $J/T$ (straight line in the semi-log scale). When the spin stiffness becomes small ($\rho_s \ll J$) there is an additional temperature range $J \gg T \gg \rho_s$ where the exponential behavior is not seen yet while the prefactor gives a $\log(J/T)$ behavior of the log($\xi$) clearly seen for $x = 0.3$. The experimentally observed deviation from the simple exponential behavior of the correlation length $\xi(T,x)$ v.s. $1/T$ [18] can be related to this effect.
At larger doping level close to the percolation threshold one expects a new length-scale to appear. This length-scale is associated with the crossover from translational invariance to the self-similarity in the percolative systems. Below \( x_p \) the “geometrical length”, \( \xi_G \propto |x - x_p|^{-\nu} \), separates the regions of Euclidean and fractal geometry. Above \( x_p \), where no infinite clusters left, \( \xi_G \) is the characteristic size of the finite clusters. Earlier experimental studies of the 2D and 3D Ising (Rb\(_2\)Co\(_1-x\)Mg\(_1-x\)F\(_4 \) and Fe\(_{1-x}\)Zn\(_x\)F\(_2 \)) \([16,19]\) and near-Heisenberg (Rb\(_2\)Mn\(_1-x\)Mg\(_1-x\)F\(_4 \) and Mn\(_{1-x}\)Zn\(_x\)F\(_2 \)) \([17,68]\) systems close to \( x_p \) have demonstrated that the static structure factor \( S(q) \) contains contributions from both “thermal” and “geometrical” lengths in agreement with the theoretical studies \([12,63]\). The experimental data suggest that these lengths combine in the simplest possible form \( \xi^{-1} = \xi^{-1}(T) + \xi_G^{-1}(x) \) and that the Lorentzian form of the structure factor near ordering vector is preserved. Yet another interesting result of the proximity to the percolation is that at \( T = 0 \) the elastic Bragg peak should be accompanied by the Lorentzian whose width at \( T = 0 \) is solely defined by the inverse “geometrical length” \( \xi_G^{-1} \). One would expect similar effects to be observed in newly available LCO systems close to \( x_p \) \([15]\).

It is not clear, however, whether the localization effects in the infinite cluster, which we discuss in this work, can manifest themselves in the static structure factor or correlation length. Such contributions, if they exist, may lead to a new behavior of correlation length, different from the simple renormalization of spin stiffness. However, in our approach the potential sources of such anomalous terms appear in the higher order in \( x \sim x^2 \) and, most certainly, do not affect the results for the experimentally reachable domain of lengths \( \xi \lesssim 200a \) above which the ordering occurs. At larger concentrations \( x \), such contributions can become important for shorter correlation lengths but in reality they might be screened by the similar effects from the decoupled clusters.

Theoretically, it is very intriguing if such localization effects of the infinite cluster can really affect the behavior of correlation length. We reserve this subject for the further study.

**V. CONCLUSIONS**

We have studied the problem of diluted 2D and quasi-2D quantum Heisenberg antiferromagnets in a tetragonal lattice making use of linear spin-wave theory and \( T \)-matrix approach. We have shown, contrary to the earlier findings, that the 2D is not the lower critical dimension for this kind of disorder and that at \( T = 0 \) long-range order persists up to concentrations close to the classical percolation threshold. These results are consistent with Monte Carlo simulations in large lattices \([23]\). In agreement with earlier works on this subject, which studied the problem in the leading order of the dilution fraction \( x \) \([30,37]\), we found that the spin-wave spectrum is strongly modified by disorder. However, contrary to these works we have shown that this result does not imply an instability of the system to a paramagnetic phase. It rather indicates magnon localization on a length scale \( \ell \), exponentially large in \( 1/x \). We have shown that this new length-scale appears explicitly in the dynamic properties such as the dynamical structure factor \( S(k, \omega) \), Eqs. \((67)\)\-(\(68)\), which can be measured directly in neutron scattering experiments, and the magnon density of states \( N(\omega) \), Eqs. \((69)\)\-(\(70)\), which is directly related to the magnetic specific heat Eqs. \((71)\)\-(\(72)\). The measurement of such quantities will provide a direct test of our theory. Furthermore, we show that the static properties such as the zero-temperature staggered magnetization \( M(x) \), Eq. \((73)\) and Néel temperature \( T_N(x) \), (in the quasi-2D case) do not show any anomaly associated with the spectrum and are finite up to the concentration close to the classical percolation threshold. These results are in a quantitative agreement with the NQR \([54]\), \( \mu \)SR \([20]\), ESR \([22]\), and magnetic susceptibility \([14]\) measurements in different compounds as well as with the Monte Carlo data \([23]\).

We have shown that the effect of dilution of an AF with non-magnetic impurities is quite strong because dilution removes completely spin degrees of freedom from the impurity site and, therefore, the spin waves are strongly scattered. Moreover, the low dimensionality of the system constraints significantly the phase space for scattering leading to the localization effects. We have shown that the hydrodynamic description of the problem breaks down for length-scales larger than \( \ell \) and the spin excitations become diffusive instead of ballistic. The conventional averaging procedure which is used to treat disorder does not lead to an effective medium with renormalized parameters. Therefore, one needs to use a different approach for length-scales larger than \( \ell \), the problem which is beyond the scope of this paper.

In fact, the physics of localization described in our work has similarities to the Anderson localization for non-interacting electrons in disordered lattices where the statistics of the excitations does not matter \([71]\). Note that our problem should be close to the problem of localization of relativistic bosons (with chemical potential \( \mu = 0 \)) in a random potential. On the other hand, that problem is related to the problem of disorder in Bose-Hubbard model where non-relativistic bosons with kinetic energy \( J \) interact through the local Coulomb term \( U \) \([71]\). In the latter model the Bose glass phase appears for small \( J \) at zero chemical potential, and transition into a superfluid state is possible when \( J \) is large enough. In our case superfluidity is not possible but we may conjecture that our localized phase is somewhat similar to the Bose glass phase and magnons are trapped in the regions which are more ordered than in average. It is not clear, however, if the relativistic nature of the bosons is important for the nature of localization.

Furthermore, we find the close similarity of our prob-
lem to the problem of disorder in 2D \(d\)-wave superconductors [13,23]. The large enhancement of the density of states at low frequencies in our case, which comes about because of the redistribution of spectral weight over the entire Brillouin zone, is reminiscent of that problem. In \(d\)-wave superconductors the elementary excitations are nodal quasiparticles, or relativistic (Dirac) fermions. It is known that for these excitations localization occurs on nodal quasiparticles, or relativistic (Dirac) fermions. It is known that for these excitations localization occurs on a length scale \(\ell_L\) (localization length) which is an exponential function of the conductance \(\sigma: \ell_L \propto e^{\sigma/\pi \sigma_0} \) [24] where \(\sigma_0 = e^2/h\). Since in the dilute limit one expects the conductance to diverge with \(x\) (that is, \(\sigma \propto 1/x\)) the localization length has the same type of non-analytic dependence on \(x\) as in our case. However, it is not clear how (if possible) the two problems map onto each other. A further investigation, beyond the scope of this paper, can clarify the connection of the diluted antiferromagnet with other similar problems of disorder in low-dimensional systems.

In summary, we have presented a comprehensive study of diluted quantum Heisenberg antiferromagnets in 2D and quasi-2D. We have shown that while the dynamic properties possess anomalies associated with magnon localization the static properties are free from such anomalies. Thus, in low-dimensional systems with disorder the connection between static and dynamic quantities is not straightforward. We have compared our results to the numerical simulations and experimental data with a very good agreement. We have also proposed other experiments which can further test the results of our theory. Altogether this provides a self-consistent picture of the effects of disorder in low-dimensional quantum antiferromagnets.

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APPENDIX A: TETРАГОНAL LATTICE GROUP THEORY

We first resolve the scattering potential \(\hat{V}\) [1], [10] in \(r\)-space by inserting the closure relations [23,24]:

\[
\hat{V}_{k_1,k_2} = \int dr_1 \int dr_2 \phi^*_k(r_1) \hat{V}_{r_1,r_2} \phi_k(r_2),
\]

where \(U_i\) is any symmetric operator in the group of tetragonal symmetry, and \(\phi_k(r)\) is a plane wave function, \(\phi_k(r) = (2\pi)^{3/2} e^{ikr}\), which can be decomposed by projection operators:

\[
\phi_k(r) = \sum_{p} \phi_k(r)_n\),
\]

where

\[
\phi_k(r)_n = \sum_{p} \phi_k(r)_n U_i \phi(r),
\]

where the set of functions, \(\{\phi_k(r)_n\}_{n=1,...,l_p}\), form a basis of the \(n\)th irreducible representation, and \(l_p\) is the dimension of the \(n\)th irreducible representation; \(D^{(p)}(U_{in})\) is the diagonal matrix elements of the \(n\)th irreducible representation for the symmetric operator \(U_i\) in point group \(D_{4h}\) whose order is \(g\) (16). We readily project the potential into irreducible representations as \(\hat{V}_{k_1,k_2} = \sum_p \hat{V}_{k_1,k_2}^{(p)}\), where

\[
\hat{V}_{k_1,k_2}^{(p)} = \sum_{n=1}^{l_p} \sum_{j=1}^{g} \frac{l^2}{g} D^{(p)}(U_{in}) D^{(p)}(U_{jn}) \int dk_3 \int dk_4 A_{k_1,k_3}^i A_{k_4,k_2}^j,
\]

where

\[
A_{k_1,k_2}^i = \int dr \phi^*_{k_1(r)} U_i \phi_k(r).
\]

Using the tetragonal symmetry group one notices that each \(A_{k_1,k_2}^i\) is a \(\delta\)-function. Thus, the scattering potential \(\hat{V}_{k_1,k_2}^{A}\), Eq. [8], can be decomposed into channels of irreducible representations. The non-zero orthogonal channels are (before the Bogolyubov transformation):

- \(A_{1g}\) (s-wave):
  \[
  \hat{V}_{k_1,k_2}^{A,s} = |s_{k_1}\rangle \otimes |s_{k_2}\rangle + |s_{k_2}\rangle \otimes |s_{k_1}\rangle,
  \]

- \(E_u\) (in-plane p-waves):
  \[
  \hat{V}_{k_1,k_2}^{A,p\{u\}} = |p_{k_1}\rangle \otimes |p_{k_2}\rangle\]

- \(B_{1g}\) (d-wave):
  \[
  \hat{V}_{k_1,k_2}^{A,d} = |d_{k_1}\rangle \otimes |d_{k_2}\rangle,
  \]

- \(A_{2u}\) (p_z-wave):
  \[
  \hat{V}_{k_1,k_2}^{A,p_z} = |d_{k_1}\rangle \otimes |d_{k_2}\rangle,
  \]
\[
\tilde{V}_{k_1,k_2}^{A,p} = |\tilde{p}_{k_1}\rangle \otimes |\tilde{p}_{k_2}\rangle, \quad (A9)
\]
where \( |\tilde{p}_{k}\rangle = [1, \gamma_{\tilde{p}}] \), \( |\tilde{p}_{k}^{(0)}\rangle = [0, 1] \sin k_{x}\gamma_{\tilde{p}}/\sqrt{2} \), \( \langle \tilde{p}_{k}\rangle = [0, 1] \gamma_{\tilde{p}} \) and \( |\tilde{p}_{k}\rangle = \sqrt{\tau} \sin k_{x}[0, 1]/\sqrt{2} \). Bogoliubov transformation yields Eqs. ([18]-[21]).

APPENDIX B: 3D T-MATRIX

In this Appendix we provide the solution of the s-wave T-matrix equation in the tetragonal lattice for the arbitrary relative value of the inter-plane and in-plane exchange integrals \( \tau = J_{1}/2J \). With this solution we demonstrate the smallness of the 3D corrections to the 2D result in quasi-2D case \((\tau \ll 1)\). After some algebra one can solve the T-matrix equation ([24]) with the s-wave scattering potential from Eq. ([13]) (sublattice \( A \), \( u_{k}, u_{k} \), and \( \omega_{k} \) from Eqs. ([12], [13]) and obtain:

\[
\Gamma_{k,k'}(\omega) = |s_{k}\rangle \otimes |s_{k'}\rangle \cdot \Gamma_{1}(\omega) + |s_{k}\rangle \otimes |s_{k'}^{\perp}\rangle \cdot \Gamma_{2}(\omega) + |s_{k}\rangle \otimes |s_{k'}^{\parallel}| + |s_{k}^{\perp}\rangle \otimes |s_{k'}^{\perp}| \cdot \Gamma_{3}(\omega), \quad (B1)
\]

where the \( \omega \)-dependence of the in-plane scattering (first term) is given by expression which is formally similar to the pure 2D result Eq. ([B3]):

\[
\Gamma_{1}(\omega) = \frac{1}{\omega} + \frac{1}{\omega} \rho(\omega) + \tau R_{1}(\omega), \quad (B2)
\]

with \( \rho(\omega) \) given by Eq. ([29]). Note that the integration over \( p \) in this case is three-dimensional. The inter-plane scattering is:

\[
\Gamma_{2}(\omega) = -\tau + \frac{\tau^{2}}{\omega} - \frac{\tau^{2} R_{2}(\omega)}{1 - \omega(1 + \omega)\rho(\omega) + \tau D(\omega)}, \quad (B3)
\]

The \( \omega \)-dependence of the cross-term is given by:

\[
\Gamma_{3}(\omega) = \frac{\tau}{\omega} \frac{R_{3}(\omega)}{1 - \omega(1 + \omega)\rho(\omega) + \tau D(\omega)}. \quad (B4)
\]

All three parts of the scattering matrix possess the same “unphysical” \( 1/\omega \) contribution discussed in the text. Application of the projection procedure Eqs. ([30], [31]) to this problem is out of the scope of this Appendix.

The auxiliary functions \( D \) and \( R_{i} \) are given by rather cumbersome combinations of \( \omega, \rho(\omega) \) and two additional integrals:

\[
\alpha(\omega) = \sum_{p} \frac{(\gamma_{p}^{+})^{2}}{\omega^{2} - \omega_{p}^{2}}, \quad \beta(\omega) = \sum_{p} \frac{\gamma_{p}^{+}}{\omega^{2} - \omega_{p}^{2}}, \quad (B5)
\]

with \( \gamma_{p}, \gamma_{p}^{\perp}, \omega_{p} \) from Eqs. ([1], [13]). Note that at \( \tau \to 0 \), \( \alpha(\omega) \to \rho(\omega)/2 \) and \( \beta(\omega) \to 0 \).

The expressions for \( D \) and \( R_{i} \) are:

\[
D = P - \omega P_{2}, \quad (B6)
\]

\[
R_{1} = \rho - \alpha + P_{2}, \quad R_{2} = \rho - (\omega - \tau)P_{2}, \quad R_{3} = (\rho - \alpha - P_{2})/2 + \tau(\rho - \alpha)/2 + P_{2}, \quad (B7)
\]

where the following shorthand notations are used:

\[
P = \frac{\gamma_{0}(\rho + \alpha)}{2}, \quad P_{2} = \frac{\gamma_{0}^{2} \rho^{2}}{2} + \omega^{2} \rho \alpha. \quad (B8)
\]

Recall that in 2D \( \Gamma_{1}(\omega) \approx \rho \) and \( \Gamma_{2}(\omega) = \Gamma_{3}(\omega) \equiv 0 \). Since \( \text{Re} \rho \sim \ln |\omega| \) at \( \omega \gg \sqrt{\tau} \) and \( \text{Re} \rho \sim \ln |\tau| \) at \( \omega \leq \sqrt{4\tau} \), the largest relative correction to the 2D terms in the scattering matrix is \( \mathcal{O}(\tau \ln(\omega)) \). The same statement can be proved for all higher powers of \( \omega \) in Eq. ([22]) without making \( \omega \ll 1 \) assumption.

The conclusion is, once again, that at \( \tau \ll 1 \) one can safely drop all terms explicitly proportional to \( \tau \) in Eqs. ([22]-[24]) and thus arrive to the purely 2D expression for the scattering matrix given in Eq. ([23]). The only modification in quasi-2D case versus 2D case is the change of the behavior of \( \rho(\omega) \) at low \( \omega \), whose real part saturates at \( \omega \leq \sqrt{4\tau} \) and imaginary part acquires an extra power in \( \omega \) (see Appendix [E]).

APPENDIX C: ELLIPTIC INTEGRALS

The energy-dependent part of the T-matrix Eqs. ([27], [28]) is expressed through the integrals of the Green’s functions Eqn. ([29]). These integrals can be evaluated in the case of 2D and are given by combinations of complete elliptic integrals of the first and second kind:

\[
\rho(\omega) = \sum_{p} \frac{1}{\omega^{2} - \omega_{p}^{2}} = -\frac{2}{\pi \omega'} \left[ K(\omega') + iK(\omega) \right], \quad (C1)
\]

\[
\rho_{d}(\omega) = \sum_{p} \frac{(\gamma_{p}^{2})^{-2}}{\omega^{2} - \omega_{p}^{2}} = 1 + \frac{2}{\pi \omega'} \left[ \omega^{2} K(\omega') - 2E(\omega') \right]
\]

\[+ i \left( (\omega^{2} - 2)K(\omega) + E(\omega) \right) \],
where $\omega' = \sqrt{1 - \omega^2}$, $K$ and $E$ are the complete elliptic integrals of the first and second kind, respectively \cite{24}.

In the low-energy limit:

\[
\rho(\omega) = \frac{2}{\pi} \ln |\omega/4| - i ,
\]

\[
\rho_d(\omega) = 1 - \frac{4}{\pi} .
\]

**APPENDIX D: PROJECTION OF UNPHYSICAL STATES**

After introduction of the fictitious magnetic field to project out the unphysical on-site mode the $s$-wave scattering potential (sublattice $A$) is given by the sum of two terms from Eqs. (22), (31):

\[
\hat{V}_{k,k'}^{s,s,\text{total}} = -|s_k| \otimes |s_{k'}| + H_z |\Delta s_k| \otimes |\Delta s_{k'}| ,
\]

with $|s_k| = \omega_k |u_k, -v_k|$, $|\Delta s_k| = |u_k, v_k|$.

One immediately suggest the form of the solution of the $T$-matrix equation:

\[
\hat{T}_{k,k'}^{A,s}(\omega) = |s_k| \otimes |s_{k'}| \cdot \Gamma_1(\omega) + |\Delta s_k| \otimes |\Delta s_{k'}| \cdot \Gamma_2(\omega) + \langle |\Delta s_k| \otimes |s_{k'}| + |s_k| \otimes |\Delta s_{k'}| \rangle \cdot \Gamma_3(\omega) ,
\]

and, after some algebra, one finds:

\[
\Gamma_1(\omega) = \frac{H_z (1 + \omega) \rho(\omega) + 1}{1 - \omega (1 + \omega) \rho(\omega) (H_z - \omega)} ,
\]

\[
\Gamma_2(\omega) = -\frac{\omega H_z}{H_z - \omega} ,
\]

\[
\Gamma_3(\omega) = \frac{H_z}{H_z - \omega} ,
\]

which yield the answer given in Eqs. (32)-(34) in the limit $H_z \to \infty$.

**APPENDIX E: 3D $\rho(\omega)$**

The key ingredient of the low-energy $T$-matrix scattering is given by the integral of the Green’s function over $k$, $\rho(\omega)$ \cite{23}. Appendix E gives an analytical expression of $\rho(\omega)$ in the 2D case. In the quasi-2D case the interplane coupling provides a cut-off in the logarithm and gives an extra power of $\omega$ in the imaginary part of the integral in the 3D energy range. This can be obtained explicitly using 3D form of the spin-wave dispersion Eq. \cite{4}, $\omega_k = \sqrt{\frac{\pi}{2\tau}} - \frac{\omega}{\sqrt{\tau}}$.

In the limit $\sqrt{\tau} = \sqrt{J_z/2J} \ll 1$, and $\omega \ll 1$ (for arbitrary $\omega/\sqrt{\tau}$) one obtains for the real part of $\rho(\omega)$:

\[
\text{Re}(\omega) = \frac{2}{\pi} \ln \frac{\sqrt{\tau}}{4} + O(\tau, \omega^2) , \quad \text{for } \omega \leq \sqrt{4\tau} ,
\]

\[
\text{Re}(\omega) = \frac{2}{\pi} \ln \frac{\omega + \sqrt{\omega^2 - 4\tau}}{8} + O(\tau, \omega^2) , \quad \text{for } \omega \geq \sqrt{4\tau} ,
\]

at $\omega \gg \sqrt{4\tau}$ the 3D energy scale is irrelevant and $\text{Re}(\omega) = \frac{2}{\pi} \ln |\omega/4|$ is back to its 2D form. Imaginary part of $\rho(\omega)$ is

\[
\text{Im}(\omega) = -\frac{1}{\pi} \arccos \left( \frac{(1 + \tau)^2 - \omega^2 - 1}{\tau} \right) + O(\omega^2) ,
\]

\[
\text{Im}(\omega) = -\frac{1}{\pi} \arccos \left( 1 - \frac{\omega^2}{2\tau} \right) + O(\tau^2, \omega^2) , \quad \text{for } \omega \leq \sqrt{4\tau} ,
\]

at small $\omega \ll \sqrt{4\tau}$ deep into the 3D range of energies $\text{Im}(\omega) = -\frac{1}{\pi \sqrt{\tau}}$ is linear in $\omega$.

**APPENDIX F: $T_N(x)$ FOR THE ISING PROBLEM**

In this Appendix we apply the formalism of our work to the problem of $T_N(x)$ v.s. $x$ dependence for the Ising $S = 1/2$ case. While the spin-wave approximation is much less adequate in the Ising limit than for the pure Heisenberg model it is nevertheless a very instructive exercise which gives a quantitatively correct answer.

Quadratic part of the 2D $S = 1/2$ Ising model in the spin-wave approximation reads as

\[
\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{imp}}
\]

\[
= \sum_k a^\dagger_k a_k - \sum_{l,k,k'} e^{i(k-k')l} V_{k,k'} a^\dagger_k a_{k'} ,
\]

where we omit from the beginning the “unphysical” term which will result in $\omega = 0$ mode. $T$-matrix gives the total result for all scattering channels:

\[
\hat{T}_{k,k'}^{\text{tr}}(\omega) = -\gamma_{k-k'} \frac{\omega - 1}{\omega - 3/4} ,
\]

where we used the property

\[
\sum_p \gamma_{k-p} \gamma_{p-k'} \equiv \gamma_{k-k'}/4 ,
\]

The self-energy is then given by:
\[ \Sigma(\omega) = -x \frac{\omega - 1}{\omega - 3/4}. \]  
\hspace{1cm} (F5)

The Green’s function has two poles now:

\[ G(\omega) = \frac{1}{\omega - 1} \frac{\omega - 3/4}{\omega - 3/4 + x}, \]  
\hspace{1cm} (F6)

and the spectral function is given by two \( \delta \)-peaks:

\[ A(\omega) = \frac{1}{1 + 4x} \left[ \delta(\omega - 1) + 4x\delta(\omega - 3/4 + x) \right]. \]  
\hspace{1cm} (F7)

Néel temperature is defined from the condition:

\[ \langle S^z \rangle(T_N, x) = \frac{1}{2} - \int_{-\infty}^{\infty} d\omega \ n_B(\omega) A(\omega) = 0, \]  
\hspace{1cm} (F8)

which transforms to

\[ \frac{1 + 4x}{2} = n_B(1) + 4x n_B(3/4 - x). \]  
\hspace{1cm} (F9)

In a pure system \( T_N(0)/2J = 1/\ln 3 \). At small \( x \)
\( T_N(x) \approx T_N(0)(1 - A^I x) \) and, after some algebra, one obtains an analytical expression for \( A^I \)

\[ A^I = 4 \left[ \frac{2}{3} \ln 3 \left( \frac{2}{3^{3/4} - 1} - 1 \right) \right] \approx 1.025 \frac{4}{3} \approx 1.37, \]  
\hspace{1cm} (F10)

which should be compared with the RPA answer \( A_{RPA}^I = 4/3 \) and an exact answer \( A_{exact}^I \approx 1.57 \). One can see that in spite of the roughness of the approximation of the Ising spin degrees of freedom by bosons our approach gives a good quantitative agreement with other approaches and an exact result.

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We use $M(x) = \sum_i |S_i|^2/N_m$, where $N_m$ is the number of magnetic sites. Another physically meaningful normalization is by the number of magnetic sites inside the infinite clusters $N_m$. These definitions are connected $M(x) = M_{\text{tot}}(x)P(x)/(1-x)$ and at $x=0$ they are equivalent $M(x) \approx M_{\text{tot}}(x)$ since the probability to find a magnetic site in the infinite cluster $P(x) \approx 1 - x - \pi x^2$. Sometimes magnetization is normalized by the total number of sites $N_{\text{tot}}$, like in MC study [25]. Evidently, $M_{\text{tot}}(x) = M(x) (1-x)$.

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