Green's function approach to the neutron-inelastic-scattering determination of magnon dispersion relations for isotropic disordered magnets

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To determine the neutron inelastic coherent scattering (NIS) cross section for disordered magnets a system of equations of motion for the Green functions (GF) related to the localized-spin correlation functions $\langle S_R^+ S_{R'}^- \rangle$, $\langle S_R^- S_{R'}^- \rangle$, and $\langle S_R^z S_{R'}^- \rangle$ has been exploited. The higher-order Green functions are decoupled using a symmetric ''equal access'' (EA) form of the random-phase approximation (RPA) decoupling scheme. The quasicrystal approximation was applied to construct the space-time Fourier transformed GF $\langle G_Q^{+-}(\omega) \rangle$ related to neutron scattering. On assuming isotropy of the magnetic structure and a short range coupling between the spins (on the sphere approximation) we have found an explicit analytic form of this function. Poles of the $\langle G_Q^{+-}(\omega) \rangle$ determine the dispersion relation $\omega = \omega_Q$ for elementary excitations, such as they are seen in the NIS experiment—the positions of the NIS profile maxima in the ω-Q space. Single formula for the dispersion relations derived here covers a variety of isotropic spin structures: in particular disordered ''longitudinal'' ferromagnets ($\omega \sim Q^2$, $Q \to 0$), disordered ''transverse'' spin structures ($\omega \sim Q$, $Q \to 0$), and some intermediate cases. It should be emphasized that in particular it works for transverse antiferromagnets. For the system of spins coupled identically—the Kittel-Shore-Kac model magnet—the magnetization and the magnetic susceptibility calculated within the present EA-RPA approach do agree with the results of exact calculations. It provides an interesting insight into the nature of the RPA treatment of the localized spin dynamics in magnets.

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I. INTRODUCTION

The random phase approximation (RPA) in the Green's function (GF) theory is a theoretical framework both convenient and effective for interpretation and forecasting of various characteristics of matter. For ordered crystalline systems even with a relatively simple version of the RPA one can achieve a fairly good description. On the other hand disordered systems, very fashionable today, are more demanding—here one has to look for a more general formulation of the theory. In this work we introduce a generalization of the usual RPA procedure for crystalline magnets, which allows us to evaluate the neutron inelastic scattering cross section, and some other characteristics, for magnets in general, including disordered ones.

The RPA in the theory of spin-spin correlations, introduced by Tyablikov,[1] and quoted by Zubarev in his treatise[2] on the Green's functions method, concerned originally spins $S=1/2$ localized at the lattice sites $\boldsymbol{l}$, coupled isotropically, $J_{ll'}^{\alpha\alpha'} = \delta^{\alpha\alpha'} J_{l-l'}$ and ferromagnetically. Using this method one can determine the spin-spin correlation functions and use them to calculate such characteristics as magnetization, magnetic susceptibility, and neutron inelastic scattering (NIS) cross section. To do it one has to solve the equation of motion for the two-point (or two-spin) GF given below (in standard notation for spin operators)

$$G_{ll'}^{+-}(t-t') \equiv \langle\langle S_l^+(t), S_{l'}^-(t') \rangle\rangle = -i\theta(t-t') \langle [S_l^+(t), S_{l'}^-(t')] \rangle_T, \quad (1)$$

where $[S_l^+(t), S_{l'}^-(t')]$ is the commutator of the spin operators involved, $\langle x \rangle_T = \mathrm{tr}[x \exp(-\beta\mathcal{H})]\mathrm{tr}[\exp(-\beta\mathcal{H})]$ is the thermal average of the operator x, $\mathcal{H}$ is the Hamiltonian, t is time, $\beta = 1/k_B T$, and T is the temperature of the system. There appears in the equation a three-point GF, which is difficult to determine. The original Tyablikov's version of the RPA is given by the following decoupling scheme for this GF:

$$\langle\langle S_l^z(t) S_{l'}^+(t), S_{l''}^-(t') \rangle\rangle \cong \langle S_l^z \rangle_T \langle\langle S_{l'}^+(t), S_{l''}^-(t') \rangle\rangle. \quad (2)$$

The ferromagnet in the RPA shows the spin-wave type of the magnetic susceptibility at low temperature: $\chi(0) - \chi(T) \approx T^{3/2}$, while just below the T_C it shows the mean-field-approximation (MFA) behavior with the critical index $\beta = 1/2$. One can see that fluctuations related to the S^z operator are not included in such approximation.

There were several attempts to generalize this decoupling scheme for perfect crystals, aimed at more realistic model of crystalline ferromagnets. A general idea behind them was to create a linear combination of all two-point Green's functions one can set up from the three or four-point GF's involved, and then multiply each two-point GF by the properly weighted thermal average of the operators not included, omitted in the previous step. The Callen[3] generalization of the Tyablikov decoupling consists in introducing the decoupling factor weighting expected deviations of the S^z from the value S, and results in a more satisfactory behavior of the magnetization vs. T, than the former one. Several other ingenious methods of decoupling have been proposed, and the review of them and their motivations has been given in the paper of Kumar and Gupta.[4] Here let us explicitly mention only the decoupling procedure introduced later by Czachor and Holas,[5] which is such as the one given by the Eq. (2) but with the right-hand side (RHS) multiplied by the magnetization dependent factor $\kappa(\langle S^z \rangle_T)$. With an appropriate choice

of this factor one has the critical indices for the ferromagnetic phase transition such as the ones in the static scaling theory.

To account for weak deviations from periodicity in defected crystals, the propagator-based perturbation schemes: the ATA (average *T*-matrix approximation) and CPA (coherent potential approximation) have been invented; see the review papers of Elliot, Krumhansl, and Leath,[6] and Korenblit and Shender.[7] The NIS cross section can be calculated using them and finite width of the NIS profile appears here due to the so called multiple scattering.

Another trend of investigations concerning the NIS and the energy spectra of elementary excitations has appeared for ferromagnets far from crystalline order—for amorphous ferromagnets.[8,9] Wave vector is not ''a good quantum number'' to label elementary excitations in such nonperiodic system, but one can introduce it as the scattering vector $\boldsymbol{Q}$ of the neutron scattering experiment. One aims in such case directly at the (time and space Fourier transform of the GF involved) function $\langle G_Q^{+-}(\omega)\rangle$ appearing in the NIS formula. Also, it seems imperative to account here for departure from isotropic interspin coupling—to allow for an occurrence of some central coupling or antisymmetric coupling. The GF equation of motion for such an amorphous ferromagnet can be approximately solved in the approximation similar to the quasicrystal approximation (QCA) of Hubbard and Beeby[10] and in the average local information transfer approximation (ALITA) of Czachor.[11] It leads to magnon dispersion relations, to be seen in the neutron inelastic coherent scattering. Interestingly, the spectrum of Ising local fields is broad due to disorder, and just this spectrum, properly deformed, appears in the ALITA as the *Q*-const NIS profile for such amorphous ferromagnets.

Traditionally the discussion of elementary excitations in antiferromagnets was focused on the low-temperature excitations—the spin waves in AF crystals. Halperin and Hohenberg[12] established the form of the magnon dispersion relations for isotropic and planar magnets in the long-wave limit, using hydrodynamic arguments. Lee and Liu[13] extended the Callen's approach to evaluate the magnon energy spectrum, sublattice magnetization, and other characteristics of the two-sublattice $S=1/2$ antiferromagnet. Singh *et al.* introduced the GF technique to determine the impact of impurities on the AF magnon spectra.[14] Recently the RPA was used by Singh *et al.*[15] and by Pratap *et al.*[16] to evaluate the magnetic characteristics for highly anisotropic crystalline antiferromagnets in a broad temperature range.

In the present paper we formulate the theory of neutron inelastic scattering in the systems of localized spins $S=1/2$, in particular in disordered isotropic magnets. It should be noted that this theory works (among other cases) for *transverse antiferromagnetic structures*, although it has been formulated without the usual crystalline assumption of the existence of two spin sublattices. It is formulated in terms of the GF's involving the well-known localized-spin operators S_R^z and spin raising and lowering operators S_R^+, S_R^-, so it is directly accessible to intuition, transparent, and can be easily extended to cover a number of magnetic systems. We apply a very symmetric form of the RPA decoupling where all spin operators are treated on equal footing. In this way we achieve a rather general description of the spin-spin correlations in disordered magnets and give the form of the dispersion relations of the elementary excitations in them, such as they are seen in the NIS experiment.

As the calculation is rather cumbersome, in order to derive analytically the $\langle G_Q^{+-}(\omega)\rangle$ we seek we have introduced the following simplifying assumptions.

(a) Coupling between the spins is isotropic: $J_{RR'}^{\alpha\alpha'}=\delta^{\alpha\alpha'}J_{RR'}$, where $\boldsymbol{R},\boldsymbol{R}'$ spin-position vectors.

(b) The system is globally isotropic, i.e., the observables depend only on the length of the scattering vector: $Q=|\boldsymbol{Q}|$.

(c) Interspin coupling is of a short range—only between close neighbors at the fixed distance *W*.

However, once the derivation procedures are mastered, some of these assumptions can obviously be released, to cover more realistic situations, including possibly the ALITA theory of crystalline antiferromagnets.

It is assumed here that the system considered is stable, i.e., it is in the state of thermodynamic equilibrium. It means that we are not discussing the spin-glass-like nonergodic irreversible systems; see, e.g., Refs. 17 and 18.

II. BASIC NOTIONS FOR THE NEUTRON INELASTIC SCATTERING

In order to remind basic notions let us consider the system of *localized* vector spins $S=1/2$ characterized by the Heisenberg-type Hamiltonian

$$\mathcal{H}=-\frac{1}{2}\sum_{RR'}J_{RR'}^{\alpha\alpha'}S_R^{\alpha}S_{R'}^{\alpha'}-H\sum_R S_R^z, \tag{3}$$

where S_R^{α}, $\alpha=x,y,z$ are the components of spin operator assigned to the point $\boldsymbol{R}$ (we depart here from lattice vectors and periodic structures), $J_{RR'}^{\alpha\alpha'}$ stays for the interspin coupling, $J_{RR}^{\alpha\alpha'}=0$, and $H=\gamma H^z$ represents magnetic field with $\gamma=g\mu_B$ in the usual notation. Let us introduce the raising and lowering spin operators $S_R^{\pm}=S_R^x\pm iS_R^y$, with usual commutation relations:

$$[S_R^+,S_{R'}^-]=2S_R^z\delta_{R,R'},\quad [S_{R'}^z,S_R^{\pm}]=\pm 2S_R^{\pm}\delta_{R,R'}.$$

The neutron inelastic coherent scattering cross section (NIS) can be expressed in terms of the time (t) and position ($\boldsymbol{R}$) dependent correlation functions $\langle S_R^+(t),S_{R'}^-(t')\rangle$, $\langle S_R^-(t),S_{R'}^+(t')\rangle$, or the corresponding Green's function (GF), as[6]

$$\frac{d^2\sigma^{\mathrm{NIS}}}{d\Omega d\omega}\sim -F_Q^2[\mathrm{Im}\langle G_Q^{+-}(\omega+i\varepsilon)\rangle+\mathrm{Im}\langle G_Q^{-+}(\omega+i\varepsilon)\rangle], \tag{4}$$

where $\boldsymbol{Q}$ is the neutron scattering vector and ω is the neutron energy (frequency) change in the scattering process. Here one assumes identical coupling of the neutron probe to dif-

ferent spins, F_Q is the magnetic form factor averaged over all spins and there appears the time and space Fourier transform of the relevant GF

$$G^{+-}_{RR'}(\omega)=\int dt e^{i\omega t}G^{+-}_{RR'}(t), \tag{5}$$

$$\langle G^{+-}_{Q}(\omega)\rangle=\frac{1}{N}\sum_{RR'} e^{iQ\cdot(R-R')}G^{+-}_{RR'}(\omega), \tag{6}$$

and similar expression for $\langle G^{-+}_{Q}(\omega)\rangle$. The $G^{-+}_{RR'}(t,t')$ is in the present paper closely related to the $G^{+-}_{RR'}(t,t')$: $G^{-+}_{RR'}(\omega)=G^{+-}_{R'R}(-\omega)$, see Ref. 19, so we shall usually mention only the functions $G^{+-}_{RR'}(t,t')$ and $\langle G^{+-}_{Q}(\omega)\rangle$.

Having calculated the $\langle G^{+-}_{Q}(\omega)\rangle$ one can, to a good approximation, evaluate also the spectrum of magnetic excitations (density of states), while the poles of the $\langle G^{+-}_{Q}(\omega)\rangle$ determine the ''Q-projected'' dispersion relations for these excitations. A justification for such a procedure was given in Ref. 11.

III. GF EQUATIONS OF MOTION FOR ISOTROPIC MAGNETIC SYSTEMS

In this section we derive the equations of motion for the GF's we seek and introduce a generalized form of the RPA decoupling to be used here. In the case of isotropic coupling the hamiltonian of the system is of the form

$$\mathcal{H}=-\frac{1}{2}\sum_{RR'} J_{RR'}(S^z_R S^z_{R'}+S^+_R S^-_{R'})-H\sum_R S^z_R. \tag{7}$$

To evaluate function $G^{+-}_{RR'}(t,t')$ and related ones one has to solve the GF equations of motion derived using the standard recipe for Heisenberg operators: $i\dot{x}=[x,\mathcal{H}]$:

$$\frac{idS^+_{R_0}}{dt}=[S^+_{R_0},\mathcal{H}]=\sum_R J_{R_0R}(S^+_{R_0}S^z_R-S^z_{R_0}S^+_R)+HS^+_{R_0},$$

$$\frac{idS^-_{R_0}}{dt}=\sum_R J_{R_0R}(S^z_{R_0}S^-_R-S^-_{R_0}S^z_R)-HS^-_{R_0},$$

$$\frac{idS^z_{R_0}}{dt}=\frac{1}{2}\sum_R J_{R_0R}(S^-_{R_0}S^+_R-S^+_{R_0}S^-_R). \tag{8}$$

The (retarded) Green's functions we shall need in the present case are

$$G^{\alpha-}_{R_0R'}(t,t')\equiv\langle\langle S^\alpha_{R_0}(t),S^-_{R'}(t')\rangle\rangle=-i\theta(t-t')\times\langle[S^\alpha_{R_0}(t),S^-_{R'}(t')]\rangle_T,$$

$$\alpha=+,-,z. \tag{9}$$

The equations of motion for these functions, Fourier transformed with respect to time, have been derived from Eq. (9) in the usual way[2]

$$\omega G^{+-}_{R_0R'}(\omega)=2\langle S^z_{R_0}\rangle_T\delta_{R_0R'}+\sum_R J_{R_0R}\{\langle\langle S^+_{R_0}S^z_R,S^-_{R'}\rangle\rangle-\langle\langle S^z_{R_0}S^+_R,S^-_{R'}\rangle\rangle\}+HG^{+-}_{R_0R'}(\omega),$$

$$\omega G^{--}_{R_0R'}(\omega)=\sum_R J_{R_0R}\{\langle\langle S^z_{R_0}S^-_R,S^-_{R'}\rangle\rangle-\langle\langle S^-_{R_0}S^z_R,S^-_{R'}\rangle\rangle\}-HG^{--}_{R_0R'}(\omega), \tag{10}$$

$$\omega G^{z-}_{R_0R'}(\omega)=-\langle S^-_{R_0}\rangle_T\delta_{R_0R'}-1/2\sum_R J_{R_0R}\{\langle\langle S^+_{R_0}S^-_R,S^-_{R'}\rangle\rangle-\langle\langle S^-_{R_0}S^+_R,S^-_{R'}\rangle\rangle\}.$$

Till now the procedure is exact, but as anticipated we have arrived at the little-known three-point GF's. To be able to proceed further in this work and possibly in the following ones, let us postulate direct generalization of the original RPA decoupling

$$\langle\langle S^\alpha_{R_0}S^\beta_R,S^-_{R'}\rangle\rangle=\kappa^{\alpha\beta}_{R_0R}\langle S^\alpha_{R_0}\rangle_T G^{\beta-}_{RR'}+\kappa^{\beta\alpha}_{RR_0}\langle S^\beta_R\rangle_T G^{\alpha-}_{R_0R'}, \tag{11}$$

where the κ factors can depend on temperature and external field and are to be determined independently. It is an extension of the step introduced in the Ref. 5 for ferromagnets. There was only one such kappa-factor there and its presence permitted one to adjust the critical indices to those of the static scaling theory.

IV. EQUAL-ACCESS DECOUPLING AND THE CANONICAL SET OF THE GF EQUATIONS

Having introduced, for the sake of further developments, this very general idea of decoupling, we shall examine here its symmetric version, i.e., all $\kappa^{\alpha\alpha'}_{RR'}=1$. Both correlation functions showing here: $\langle S^\beta_R,S^-_{R'}\rangle$, $\langle S^\alpha_R,S^-_{R'}\rangle$, enter symmetrically, or have an *equal access*. We can call it the EA decoupling (EA-RPA). Introducing the local field parameters

$$h^\alpha_{R_0}=\sum_R J_{R_0R}\langle S^\alpha_R\rangle_T,\quad \alpha=+,-,z, \tag{12}$$

we obtain the nonuniform system of linear algebraic equations for the GF's we seek

$$\sum_R\{[(\omega-H-h^z_{R_0})\delta_{R_0R}+J_{R_0R}\langle S^z_{R_0}\rangle_T]G^{+-}_{RR'}+[h^+_{R_0}\delta_{R_0R}-J_{R_0R}\langle S^+_{R_0}\rangle_T]G^{z-}_{RR'}\}=2\langle S^z_{R_0}\rangle_T\delta_{R_0R'}, \tag{13a}$$

$$\sum_R\{[(\omega+H+h^z_{R_0})\delta_{R_0R}-J_{R_0R}\langle S^z_{R_0}\rangle_T]G^{--}_{RR'}+[-h^-_{R_0}\delta_{R_0R}+J_{R_0R}\langle S^-_{R_0}\rangle_T]G^{z-}_{RR'}\}=0, \tag{13b}$$

$$\sum_R \{[-h^-_{R_0}\delta_{R_0R}+J_{R_0R}\langle S^-_{R_0}\rangle_T]G^{+-}_{RR'} + [h^+_{R_0}\delta_{R_0R}-J_{R_0R}\langle S^+_{R_0}\rangle_T]G^{--}_{RR'}-2\omega\delta_{R_0R}G^{z-}_{RR'}\} = 2\langle S^-_{R_0}\rangle_T\delta_{R_0R'}. \tag{13c}$$

Using the last equation we can eliminate $G^{z-}_{RR'}$. First, let us rewrite it in a convenient short fashion

$$G^{z-}_{RR'}=\frac{1}{\omega}\left[\left(\sum_{R''} A^-_{RR''}G^{+-}_{R''R'}-A^+_{RR''}G^{--}_{R''R'}\right)-\langle S^-_R\rangle_T\delta_{RR'}\right], \tag{14}$$

where

$$A^\alpha_{RR''}=-\frac{1}{2}[h^\alpha_R\delta_{RR''}-\langle S^\alpha_R\rangle_T J_{RR''}]. \tag{15}$$

On substituting Eq. (14) into Eqs. (13a) and (13b) one has

$$\sum_{R''}\{[\omega(\omega-H-h^z_{R_0})\delta_{R_0R''}+\omega\langle S^z_{R_0}\rangle_T J_{R_0R''}-B^{+-}_{R_0R''}]G^{+-}_{R''R'} + B^{++}_{R_0R''}G^{--}_{R''R'}\}=2\omega\langle S^z_{R_0}\rangle_T\delta_{R_0R'}-2A^+_{R_0R'}\langle S^-_{R'}\rangle_T,$$

$$\sum_{R''}\{B^{--}_{R_0R''}G^{+-}_{R''R'}+[\omega(\omega+H+h^z_{R_0})\delta_{R_0R''} - \omega\langle S^z_{R_0}\rangle_T J_{R_0R''}-B^{-+}_{R_0R''}]G^{--}_{R''R'}\} = \langle S^-_{R_0}\rangle_T[-h^-_{R_0}\delta_{R_0R'}+J_{R_0R'}\langle S^-_{R'}\rangle_T], \tag{16}$$

where

$$B^{\alpha\beta}_{R_0R''}=2\sum_R A^\alpha_{R_0R}A^\beta_{RR''}. \tag{17}$$

This set of two equations should be considered as ''canonical''—it is a prototype of the sets of equations to appear in more complete theories, including, e.g., the anisotropic coupling in the Hamiltonian (3), or some $\kappa^{\alpha\alpha'}_{RR'}\neq 1$-factors in the decoupling (11). By the appropriate specification of labels, $\boldsymbol{R}\to\boldsymbol{l},\boldsymbol{b}$ (where $\boldsymbol{l}$ is the lattice vector and **b** is the basis vector), and on introducing the lattice translational invariance $J_{RR'}\to J^{bb'}_{l-l'}$, they represent the starting point also for the theory of magnetic crystals in the generalized RPA.

V. EVALUATION OF THE NIS-RELEVANT FUNCTION $\langle G^{+-}_Q(\omega)\rangle$

As we want to determine the $\langle G^{+-}_Q(\omega)\rangle$, let us multiply both equations (16) by $\exp(i\boldsymbol{Q}\cdot(\boldsymbol{R}-\boldsymbol{R}'))$ and sum over $\boldsymbol{R},\boldsymbol{R}'$. One obtains

$$\omega(\omega-H)\langle G^{+-}_Q(\omega)\rangle-\langle(h^zG^{+-}(\omega))_Q\rangle + \omega\langle(S^zJG^{+-}(\omega))_Q\rangle-\langle(B^{+-}G^{+-}(\omega))_Q\rangle + \langle(B^{++}G^{--}(\omega))_Q\rangle=2\omega\langle S^z\rangle-2\langle(A^+S^-)_Q\rangle,$$

$$\langle(B^{--}G^{+-}(\omega))_Q\rangle+\omega(\omega+H)\langle G^{--}_Q(\omega)\rangle + \langle(h^zG^{+-}(\omega))_Q\rangle-\omega\langle(S^zJG^{--}(\omega))_Q\rangle - \langle(B^{-+}G^{--}(\omega))_Q\rangle=-\langle S^-h^-\rangle+\langle(S^-JS^-)_Q\rangle, \tag{18}$$

where the notation introduced in the definition (6) of $\langle G^{+-}_Q(\omega)\rangle$ has been used.

We have obtained in this way the equations containing not only the ''pure'' GF's we seek: $\langle G^{+-}_Q(\omega)\rangle$, $\langle G^{--}_Q(\omega)\rangle$, but also more complicated product terms composed of other factors involved in this problem. To turn these equations into a tractable form, we shall take the step introduced by Hubbard and Beeby[10] to study the liquid dynamics, and then used by Czachor[20] to calculate the NIS cross section for other disordered systems: each such term is to be decoupled in the following way:

$$\langle(XG)_Q\rangle\cong\langle(X)_Q\rangle\langle(G)_Q\rangle. \tag{19}$$

Such a step is exact in crystals, due to the lattice translational invariance, thus we call it the quasicrystal approximation (QCA). For disordered systems it is a sort of the mean field approximation. We obtain

$$[\omega(\omega-H-\langle h^z\rangle)+\omega\langle(JS^z)_Q\rangle-\langle B^{+-}_Q\rangle]\langle G^{+-}_Q(\omega)\rangle + \langle B^{++}_Q\rangle\langle G^{--}_Q(\omega)\rangle=2\omega\langle S^z\rangle-2\langle(A^+S^-)_Q\rangle,$$

$$\langle B^{--}_Q\rangle\langle G^{+-}_Q(\omega)\rangle+[\omega(\omega+H+\langle h^z\rangle) - \omega\langle(JS^z)_Q\rangle-\langle B^{-+}_Q\rangle]\langle G^{--}_Q(\omega)\rangle = -\langle h^-S^-\rangle+1/N\sum_{R_0R'}J_{R_0R'}\langle S^-_{R_0}\rangle_T\langle S^-_{R'}\rangle_T \times\exp(i\boldsymbol{Q}\cdot(\boldsymbol{R}_0-\boldsymbol{R}')), \tag{20}$$

where the following notation has been used:

$$\langle S^z\rangle\equiv 1/N\sum_R\langle S^z_R\rangle_T, \tag{21}$$

$$\langle h^z\rangle\equiv 1/N\sum_R h^z_R,$$

$$\langle h^-S^-\rangle\equiv 1/N\sum_R h^-_R\langle S^-_R\rangle_T,$$

$$\langle(A^+S^-)_Q\rangle\equiv 1/N\sum_{RR'}A^+_{RR'}\langle S^-_{R'}\rangle_T\exp(i\boldsymbol{Q}\cdot(\boldsymbol{R}-\boldsymbol{R}')),$$

$$\langle(JS^z)_Q\rangle\equiv 1/N\sum_{RR'}J_{RR'}\langle S^z_R\rangle_T\exp(i\boldsymbol{Q}\cdot(\boldsymbol{R}-\boldsymbol{R}')),$$

$$\langle G_Q^{\alpha\beta}(\omega)\rangle = \sum_{R'} G_{RR'}^{\alpha\beta} \exp(i\boldsymbol{Q}\cdot(\boldsymbol{R}-\boldsymbol{R}')),$$

$$\langle B_Q^{\alpha\beta}\rangle = 1/N \sum_{RR'} B_{RR'}^{\alpha\beta} \exp(i\boldsymbol{Q}\cdot(\boldsymbol{R}-\boldsymbol{R}')).$$

Introducing a different notation: $G_1=\langle G_Q^{+-}(\omega)\rangle$, $G_2=\langle G_Q^{--}(\omega)\rangle$, etc., we can write the equations in this self-explanatory short form

$$\begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} G_1 \\ G_2 \end{bmatrix} = \begin{bmatrix} S_1 \\ S_2 \end{bmatrix}. \tag{22}$$

The solution for $G_1=\langle G_Q^{+-}(\omega)\rangle$ is now trivial

$$G_1=(S_1M_{22}-S_2M_{12})/M, \quad M=(M_{11}M_{22}-M_{12}M_{21}). \tag{23}$$

As it follows from Eq. (4), the NIS profile is given by the $\mathrm{Im}\, G_1$. If the elementary excitation is undamped, the profile is indefinitely narrow. Zero of denominator gives then the position of the NIS peak in the (Q,ω) space. In this way the dispersion relation for the excitations can be written as

$$M(Q,\omega)=0, \tag{24}$$

while the numerator in Eq. (23) gives intensity of the NIS peaks.

VI. SPHERE-RESTRICTED COUPLING BETWEEN SPINS

To proceed analytically further and to catch the essence of the present approach we have to invent a simple model of a disordered spin system, allowing us to determine the terms involved. As the coupling between nearest neighbors is usually the strongest one, let us assume that a spin at any position $\boldsymbol{R}$ is coupled only to its n_R neighbors at a fixed distance W. We shall call it the ''*on the sphere assumption*'' (OSA). Figure 1 shows an example of a disordered two-dimensional (2D) structure of the OSA type. To have another example we can set spins at the sites of a crystal structure of regular type: fcc, bcc, sc, or even hcp, allow for the nearest-neighbor (NN) coupling, and then remove a considerable part of the spins and/or of the NN bonds in a random way.

Furthermore, let us explicitly use the *isotropy* of the disordered system to carry the body angle average in the phase factors,[11] to obtain

$$\Phi_Q=\overline{\exp(i\boldsymbol{Q}\cdot\boldsymbol{W})}=\frac{\sin(p)}{p}, \quad p=QW, \tag{25}$$

where the bar in the last formula stays for the body angle average. (On taking this step we depart from the area of crystalline magnets.) In the foregoing we shall mainly use the related function

$$\Lambda_Q=(1-\Phi_Q)/2 \underset{Q\to 0}{\sim} \frac{(WQ)^2}{12}. \tag{26}$$

After these preparations we can evaluate the terms we need. Let us start with M_{12}

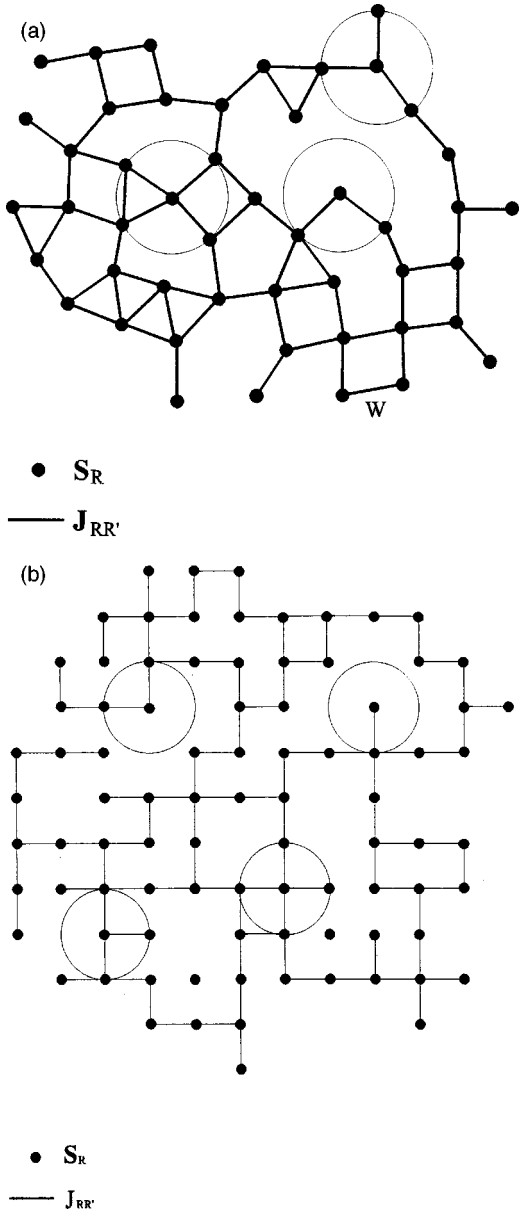


FIG. 1. Examples of 2D structures of the OSA type: (a) random network of points subject to the condition that there is no point-point distance—the interspin bond—shorter than the given one (W); (b) as above, but with the points situated at some sites of the square lattice, having up to four interacting nearest neighbors at a fixed distance. Black dots represent the spins, bars represent coupling constants $J_{RR'}\neq 0$, and missing bars: $J_{RR'}=0$. Circles show the ''spheres'' of interaction.

$$M_{12}=\langle B_Q^{++}\rangle=\frac{2}{N}\sum_{RR'R''} A_{RR''}^{+}A_{R''R'}^{+}\exp(i\boldsymbol{Q}\cdot(\boldsymbol{R}-\boldsymbol{R}'))$$

$$=\frac{1}{(2N)}(1-\Phi(Q))\sum_R (h_R^+)^2 \equiv \Lambda_Q \frac{1}{N}\sum_R (h_R^+)^2, \tag{27}$$

where number 1 in the RHS bracket appears as a consequence of the δ function in $A_{RR'}^{+}=\frac{1}{2}[h_R^+\delta_{RR'}-\langle S_R^+\rangle_T J_{RR'}]$.

Isotropy, which makes all directions in the *x-y* plane equivalent, gives that the last sum in Eq. (27) is zero, as one can see it best by returning to the S_R^x and S_R^y operators. It means that $M_{12}=0$, and similarly we can prove that $M_{21}=\langle B_Q^{--}\rangle$ is equal to zero. In general this may be not true for crystals, or in case of long-range or anisotropic coupling. In particular, these terms could not be neglected in case of the planar ferromagnet, such as discussed by Halperin and Hohenberg.[12]

Let us now exploit the isotropy and the OSA in the M_{11} term

$$M_{11}=\omega(\omega-H-\langle h^z\rangle)+\omega\langle(JS^z)_Q\rangle-\langle B_Q^{+-}\rangle. \quad (28)$$

We have

$$\langle(JS^z)_Q\rangle\equiv\frac{1}{N}\sum_{RR'}J_{RR'}\langle S_R^z\rangle_T\exp(i\boldsymbol{Q}\cdot(\boldsymbol{R}-\boldsymbol{R}'))=\Phi_Q\langle h^z\rangle, \quad (29)$$

and

$$\langle B_Q^{+-}\rangle=\frac{2}{N}\sum_{R_0RR''}A_{R_0R}^{+}A_{RR''}^{-}\exp(i\boldsymbol{Q}\cdot(\boldsymbol{R}_0-\boldsymbol{R}''))$$
$$=\Lambda_Q\langle h^+h^-\rangle, \quad (30)$$

where $\langle h^+h^-\rangle\equiv 1/N\Sigma_R h_R^+h_R^-$. The whole Q dependence is hidden in the Λ_Q and Φ_Q factors. It is useful to define at this point, as an average measure of the local fields in the system, the *configuration average of the squared local fields*

$$\frac{1}{N}\sum_R(h_R^zh_R^z+h_R^+h_R^-)=\frac{1}{N}\sum_R(h_R)^2\equiv\langle h^2\rangle \quad (31)$$

and similarly the *squared z-component of the local fields* $\langle(h^z)^2\rangle=1/N\Sigma_R h_R^zh_R^z$, so that we can write

$$\langle h^+h^-\rangle=\langle h^2\rangle-\langle(h^z)^2\rangle. \quad (32)$$

Using Eqs. (29), (30), and (32) in Eq. (28) gives

$$M_{11}=\omega[\omega-(H+2\langle h^z\rangle\Lambda_Q)]-[\langle h^2\rangle-\langle(h^z)^2\rangle]\Lambda_Q. \quad (33)$$

Similarly

$$M_{22}=\omega[\omega+(H+2\langle h^z\rangle\Lambda_Q)]-[\langle h^2\rangle-\langle(h^z)^2\rangle]\Lambda_Q. \quad (34)$$

VII. NIS-DETERMINED DISPERSION RELATIONS

Now, as long as $M_{12}=0$, we can easily calculate the GF we need

$$G_1=S_1/M_{11}. \quad (35)$$

Poles of the GF give the ''dispersion relations'' for the elementary excitations, such as seen in the NIS experiment. To be quite precise, at the GF pole position (Q,ω_Q) one has to expect the delta-function-like peak of the inelastically scattered neutrons. More practically, maxima of the NIS profiles should occur there. It follows that we have to look for roots of the determinant of the matrix M, i.e., in this case for the solutions of the equation: $M_{11}=0$. It has the following form:

$$\omega^2-\omega_L\omega-\omega_T^2=0, \quad (36)$$

where

$$\omega_{L,Q}=H+2\langle h^z\rangle\Lambda_Q,\quad \omega_{T,Q}^2=(\langle h^2\rangle-\langle(h^z)^2\rangle)\Lambda_Q. \quad (37)$$

This quadratic equation has in general two roots

$$\omega_Q^{\pm}=\frac{1}{2}(\omega_L\pm\sqrt{\omega_L^2+4\omega_T^2}). \quad (38)$$

It is the formula for *dispersion relations of elementary excitations in disordered isotropic magnetic systems*—the frequency (energy) versus the NIS scattering vector $\boldsymbol{Q}$. It has been derived assuming the EA-RPA decoupling, the QCA factorization, the short range OSA coupling and the isotropy of system investigated. The notation used will soon show its merits, when discussing special cases. It is convenient to introduce at this place an average characteristic of the amplitude of local fields: $\tilde{h}=\sqrt{\langle h^2\rangle}$, Eq. (31), to be used below.

Special cases

(1) In case of zero external field $H=0$, if $\langle h^2\rangle=\langle(h^z)^2\rangle$—all the spins are directed along the z direction—we have a *longitudinal* (ferromagnetic) configuration (*thus label L*), Fig. 2(a), and the dispersion relation for magnetic excitations takes on the form

$$\omega=\omega_{L,Q}=2\langle h^z\rangle\Lambda_Q\underset{Q\to 0}{\sim}Q^2; \quad (39)$$

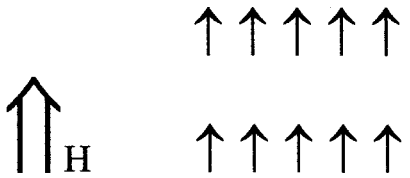
see Fig. 3, as it should be. Besides, if $\langle h^z\rangle=0$ one might think of the rather *unreal* structure of the ''longitudinal'' antiferromagnet of Fig. 2(c) characterized by $\omega=0$.

(2) If $H\to 0$, $\langle h^z\rangle=\langle(h^z)^2\rangle=0$ and $\langle h^{\pm}\rangle=0$ (isotropy in the *x-y* plane), we have *transverse* magnetic configurations including as *a special case* the antiferromagnetic configuration shown in Fig. 2(b), and the dispersion relation is

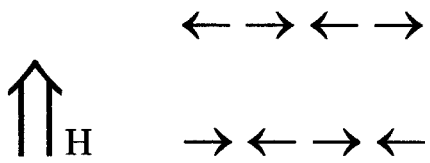
$$\omega=\omega_{T,Q}=\tilde{h}\sqrt{\Lambda_Q}\underset{Q\to 0}{\sim}Q. \quad (40)$$

(3) Note that the single dispersion relation—formula (38)—derived here covers both pure cases—longitudinal and transverse—as well as some *intermediate cases*. Interestingly, it follows that at small Q we usually have the frequency ω proportional to Q; the quadratic dependence appears under strictly longitudinal (ferromagnetic) condition $\langle h^2\rangle=\langle(h^z)^2\rangle$; see Fig. 3. Note that, for disordered magnets at $H=0$, only this longitudinal configuration characterized by $\omega\sim Q^2$ can at the long-wave limit be qualitatively distinguished with neutrons from the others: all other ones provide $\omega\sim Q$.

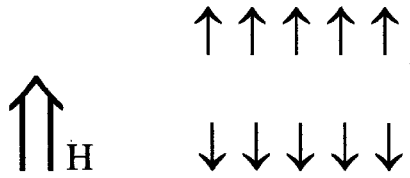
(4) *Transverse configuration in the field* deserves special attention. Having in mind the NIS scattering formula (4), we can see that one can think of the following dispersion relations:



(a) $\langle h^z\rangle \neq 0,\ \langle h^2\rangle = \langle (h^z)^2\rangle,\ \ \omega = \omega_{L,Q}$



(b) $\langle h^z\rangle = 0,\ \langle (h^z)^2\rangle = 0,\ \omega = \omega_{T,Q}$



(c) $\langle h^z\rangle = 0,\ \langle h^2\rangle = \langle (h^z)^2\rangle,\ \omega = 0$

FIG. 2. Some spins configurations with respect to the magnetic field $H\to 0$, corresponding to the dispersion relations (38), schematically: (a) Longitudinal (ferromagnetic); (b) transverse (a special case of a ''pure'' antiferromagnet); (c) longitudinal antiferromagnet (unstable). Statistical characteristics of local fields responsible for these configurations are given for each case.

$$\omega = \frac{1}{2}\left[H \pm \sqrt{H^2 + 4\omega_{T,Q}^2}\right] \underset{Q\to 0}{\sim} \begin{cases} H \\ Q^2. \end{cases} \tag{41}$$

It suggests that at some conditions we may have the gap-less dispersion relation shown in Fig. 4 also at the presence of the external field.

VIII. INTENSITY OF THE NIS PEAKS

To know about intensity of the neutron peaks we have to determine the numerator of the GF involved

$$S_1 = 2\omega\langle S^z\rangle - 2\langle (A^+ S^-)_Q\rangle$$
$$= 2\omega\langle S^z\rangle - \frac{1}{N}\sum_{RR'}\left[-h_R^+\delta_{RR'} + \langle S_R^+\rangle_T J_{RR'}\right]\langle S_{R'}^-\rangle_T$$
$$\times \exp(i\boldsymbol{Q}\cdot(\boldsymbol{R}-\boldsymbol{R}')). \tag{42}$$

The OSA gives in this case

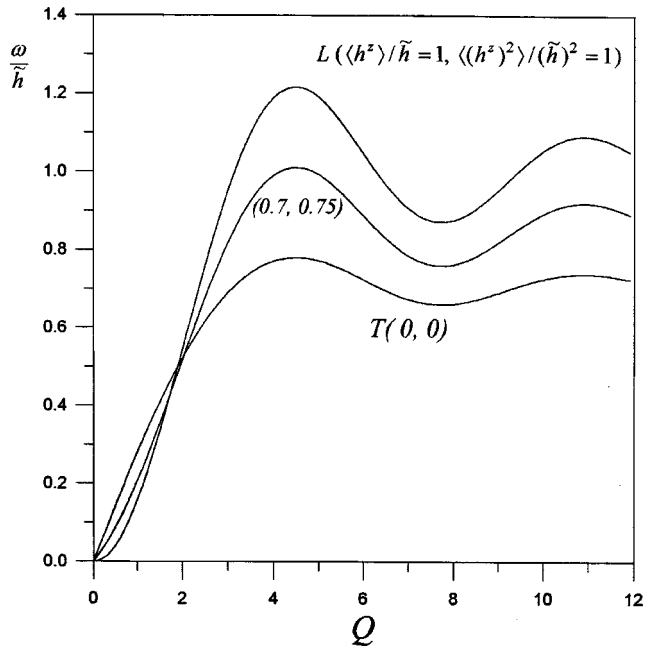


FIG. 3. Magnon dispersion relations (36) at $H\to 0$ [more precisely, the geometric place of the NIS peaks $\approx\delta(\omega-\omega_Q)$ in the (Q,ω) plane] for longitudinal (L), transverse (T), and an intermediate case. Local field characteristics are given in brackets.

$$S_1 = 2\omega\langle S^z\rangle + \frac{1}{N}\sum_R h_R^+\langle S_R^-\rangle_T - \frac{\Phi_Q}{N}\sum_{RR'}\langle S_R^+\rangle_T J_{RR'}\langle S_{R'}^-\rangle_T$$
$$= 2(\langle S^z\rangle\omega + \langle E^{+-}\rangle\Lambda_Q), \tag{43}$$

where

$$\langle E^{+-}\rangle = (N)^{-1}\sum_R h_R^+\langle S_R^-\rangle_T = (N)^{-1}\sum_{RR'}\langle S_R^+\rangle_T J_{RR'}\langle S_{R'}^-\rangle_T. \tag{44}$$

It follows that $\langle E^{+-}\rangle$ is a mean-field estimate of the thermal value of the *fluctuation term* of the Hamiltonian. Putting things together, we have

$$\langle G_Q^{+-}\rangle = \frac{2\langle S^z\rangle\omega + 2\langle E^{+-}\rangle\Lambda_Q}{(\omega-\omega_Q^+)(\omega-\omega_Q^-)}. \tag{45}$$

One can see that the NIS intensity depends crucially on the type of magnetism of the system. It can be calculated directly for purely transverse and longitudinal configurations.

In the case of a *transverse configuration* the $\langle E^{+-}\rangle$ can be estimated from the condition that at the absence of external field the magnetization of the system is to be zero: $\langle S^z\rangle = 0$. First let us decompose the $\langle G_Q^{+-}\rangle$ into its simple fraction form, using Eq. (37)

$$\langle G_Q^{+-}\rangle = \frac{\langle E^{+-}\rangle\omega_{T,Q}}{\tilde{h}^2}\left[\frac{1}{\omega-\omega_{T,Q}} - \frac{1}{\omega+\omega_{T,Q}}\right], \tag{46}$$

Now let us return to Eq. (6). On summing with respect to $\boldsymbol{Q}$, one arrives at the following general relation:

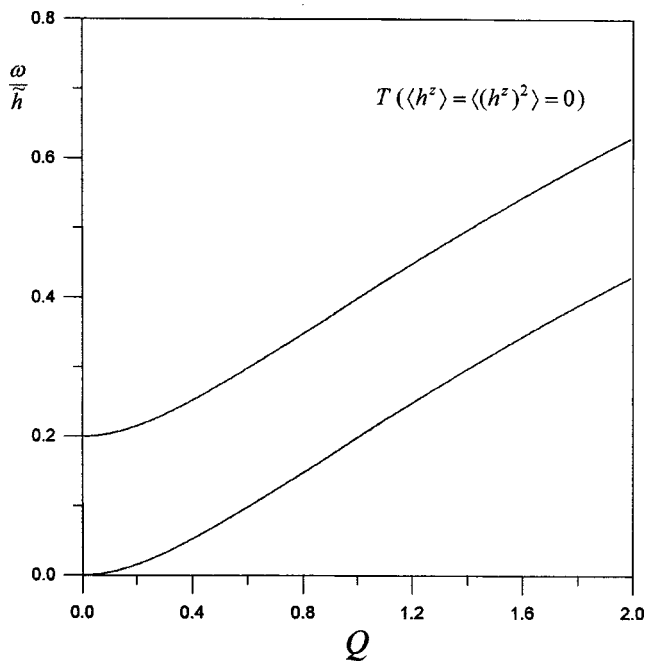


FIG. 4. Transverse dispersion relations at a finite external magnetic field $H/\tilde{h}=0.2$; see Eq. (41). Besides the well-known branch showing at $Q=0$ the field-induced frequency gap, present theory predicts also a possibility of the gapless branch.

$$\sum_Q \langle G_Q^{+-}(\omega)\rangle = \sum_R G_{RR}^{+-}(\omega), \tag{47}$$

where, vaguely speaking, a rather uniform and dense distribution of $\boldsymbol{Q}$ points is understood, such that one can assume[20]

$$1/N \sum_Q e^{i\boldsymbol{Q}\cdot(\boldsymbol{R}-\boldsymbol{R}')} = \delta_{RR'}. \tag{48}$$

Using this relation and the spectral intensity theorem of the GF theory[2] (let us set here $k_B=1$)

$$\langle A,B\rangle = \int \frac{d\omega}{2\pi} \frac{1}{\exp(\omega/T)-1}[-2\,\mathrm{Im}\,G^{BA}(\omega+i\varepsilon)],$$

we obtain the configurational average of the $\langle S_R^- S_R^+\rangle_T$ correlation functions we seek. It can be given in terms of the above GF

$$\begin{aligned}\langle S^- S^+\rangle &\equiv \frac{1}{N}\sum_R \langle S_R^- S_R^+\rangle_T \\ &= \frac{1}{2\pi}\int d\omega \frac{1}{e^{\omega/T}-1}\left(-2\,\mathrm{Im}\frac{1}{N}\sum_R G_{RR}^{+-}(\omega+i\varepsilon)\right) \\ &= \frac{1}{2\pi}\frac{1}{N}\sum_Q \int d\omega \frac{1}{e^{\omega/T}-1} \\ &\quad \times(-2\,\mathrm{Im}\langle G_Q^{+-}(\omega+i\varepsilon)\rangle).\end{aligned} \tag{49}$$

The $d\omega$ integration can be done immediately using Eq. (46) and the usual trick: $\mathrm{Im}(1/(X+i\varepsilon)) = -\pi\delta(X)$. For $S=1/2$ we have $S_R^z = 1/2 - S_R^- S_R^+$, therefore the average magnetization $\langle S^z\rangle$ can be expressed in terms of the correlation function $\langle S^- S^+\rangle$. Finally, as the magnetization for the *transverse* configuration of spins at $H=0$ is $\langle S^z\rangle = 0$, we arrive at the following result for $\langle E^{+-}\rangle$:

$$\langle E^{+-}\rangle = \frac{\tilde{h}^2}{2}\left[\frac{1}{N}\sum_Q \omega_{T,Q}\coth\left(\frac{\omega_{T,Q}}{2T}\right)\right]^{-1}. \tag{50}$$

The scaling factor $\tilde{h}$ entering here depends on temperature in a complicated way via the thermal averages $\langle S_R^+\rangle_T, \langle S_R^-\rangle_T$ in the definition of the local fields, Eq. (12),

$$\tilde{h}^2 \equiv \langle h^2\rangle \equiv \frac{1}{N}\sum_R h_R^+ h_R^- = \frac{1}{N}\sum_{RR'} (\boldsymbol{J}^2)_{RR'}\langle S_R^+\rangle\langle S_{R'}^-\rangle, \tag{51}$$

where $(\boldsymbol{J}^2)_{RR'} = \Sigma_{R''} J_{RR''} J_{R''R'}$.

The $\boldsymbol{Q}$ summation (or integration) in Eq. (50) is in fact a rather delicate problem in itself. Till now we treated the $\boldsymbol{Q}$ vectors as the scattering vectors appearing in the process of neutron scattering. From now on in the sums of the above type we have to treat them as ordinary variables. To arrive at meaningful results one has to confine oneself to a finite number of $\boldsymbol{Q}$ points. In case of a crystal it is the number N of lattice sites, i.e., the number of vectors $\boldsymbol{Q}$ distributed uniformly in the first Brillouin zone. In this paper the N, being a number of localized spins, is also assumed to be the number of $\boldsymbol{Q}$ vectors involved, without knowing a much about the distribution of the corresponding $\boldsymbol{Q}$ points. To give a *rough* representation of the $\langle E^{+-}\rangle$ versus temperature T we assume a flat dispersion relation, $\Lambda_Q = 1/2$. The $\boldsymbol{Q}$ summation in Eq. (50) can be done immediately, and we have $\langle E^{+-}\rangle = \tilde{h}/\sqrt{2}\,\tanh(\tilde{h}/(2\sqrt{2}T))$. The plot, neglecting the temperature dependence of $\tilde{h}$, is shown in Fig. 5. It would be interesting to extract the true $\tilde{h}$ vs T dependence from experimental data on the temperature dependence of the NIS peaks.

Let us note, that one can avoid discussing the meaning of the $\boldsymbol{Q}$ vectors by introducing the ''virtual T spectrum'' of Ref. 5

$$\Delta_T(\omega) = 1/N \sum_Q \delta(\omega - \omega_{T,Q}).$$

Using it, the above formula for $\langle E^{+-}\rangle$ takes on the form

$$\langle E^{+-}\rangle = \frac{\tilde{h}^2}{2}\left[\int d\omega \Delta_T(\omega)\omega\coth\left(\frac{\omega}{2T}\right)\right]^{-1}. \tag{50'}$$

Such a formulation offers a perspective of studying models characterized by various virtual spectra without any explicit reference to dispersion relations of magnetic excitations or to dimensionality of systems investigated

In the same way, for the purely longitudinal spin configuration we have $\langle h^2\rangle = \langle (h^z)^2\rangle$, $\langle E^{+-}\rangle = 0$, and one arrives at the magnetization formula

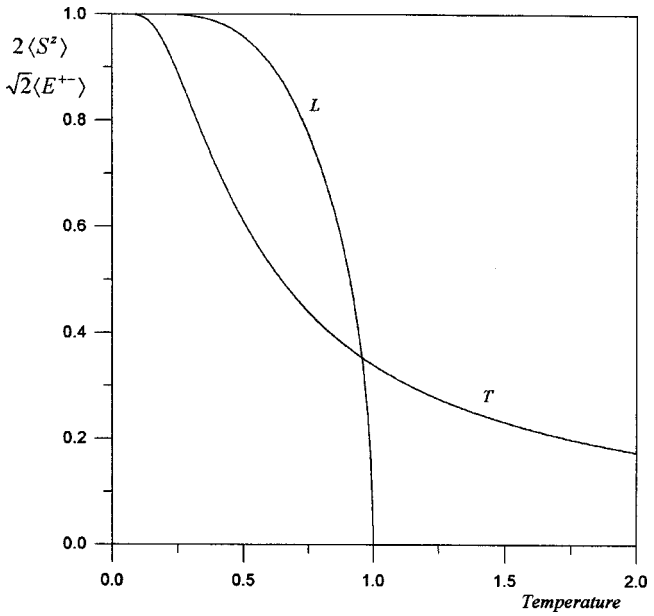


FIG. 5. Neutron inelastic scattering (NIS) intensity factors vs temperature (schematically): $2\langle S^z\rangle$ for longitudinal (ferromagnetic) configuration (L), temperature in the units of $T_C=nJ/4$; $\sqrt{2}\langle E^{+-}\rangle$ for transverse (antiferromagnetic) configuration (T), temperature in the units $\tilde{h}/(2\sqrt{2})$.

$$\langle S^z\rangle=\frac{1}{2}\left[\frac{1}{N}\sum_Q \coth\left(\frac{H+\omega_{L,Q}}{2T}\right)\right]^{-1}$$
$$=\frac{1}{2}\left[\int d\omega\Delta_L(\omega)\coth\left(\frac{H+\omega}{2T}\right)\right]^{-1}, \qquad (52)$$

where this time the virtual L-spectrum has the form $\Delta_L(\omega)=1/N\Sigma_Q\delta(\omega-\omega_{L,Q})$.

The form essentially the same as in the case of the original RPA for ferromagnets,[1,2] involving just a single GF via the decoupling (2). (One should mention that the original formula concerns the crystalline case with arbitrary range of interspin coupling and the $\boldsymbol{Q}$ summation there is carried there over the Brillouin zone.) Having in mind the system of three interdependent GF equations (13a)–(13c) appearing in the present approach—i.e., a mutual dependence of three correlation functions: $\langle S_R^+S_{R'}^-\rangle_T,\langle S_R^-S_{R'}^-\rangle_T,\langle S_R^zS_{R'}^-\rangle_T$—this fact, joyfully acceptable, is not trivial.

Note that in case of the flat dispersion relation, e.g., $2\Lambda_Q=1$, we get from Eq. (52) the result

$$\langle S^z\rangle=\frac{1}{2}\tanh\left(\frac{\langle h^z\rangle+H}{2T}\right). \qquad (53)$$

If the spin coupling to its n nearest neighbors is J, from Eq. (12) one finds $\langle h^z\rangle=nJ\langle S^z\rangle$ and Eq. (53) turns into the usual MFA equation for the magnetization, thus into the NIS-peak intensity factor such as for ferromagnets, via the GF formula (45).

IX. GF-METHOD CALCULATIONS VERSUS EXACT RESULTS FOR THE KITTEL-SHORE-KAC MODEL

For the ensemble of N spins $S=1/2$ coupled identically, $J_{RR'}=J/N(1-\delta_{RR'})$, one can *exactly* calculate thermodynamic functions in the thermodynamic limit, both for Ising spins (Kac[21]) and for vector spins (Kittel and Shore[22]); see Ref. 23. Magnetic properties of this *Kittel-Shore-Kac* (KSK) model magnet are of the mean field type. In case of real magnets the interspin coupling is obviously more complicated and one has to apply approximate methods to determine their physical characteristics. The GF method, often used and successful, is in general an approximate method, due to the approximations introduced by assumed decoupling schemes. We find it interesting to apply the method based on the symmetric EA-RPA decoupling (11) developed here to this KSK model, in order to compare the results so obtained with the exact ones.

With the symmetric RPA decoupling (11) and the QCA factorization (19) of the GF in question we can easily evaluate functions (21). Assuming the external field $H\to 0$, in the limit $N\to\infty$ one obtains

$$\langle h^z\rangle=J\langle S^z\rangle,$$

$$A^\alpha_{RR'}=-J/2[\langle S^\alpha\rangle\delta_{RR'}+N^{-1}\langle S^\alpha_R\rangle], \quad \alpha=+,-,z,$$

$$\langle B_Q^{\alpha\beta}\rangle\equiv 2/N\sum_{RR'R''}A^\alpha_{RR'}A^\beta_{R'R''}=0,$$

$$\langle (JS^z)_Q\rangle=J\langle S^z\rangle\delta_{Q,0},$$

$$\langle (A^+S^-)_Q\rangle=J/2(\langle S_Q^+\rangle\langle S_Q^-\rangle-\langle S_0^+\rangle\langle S_0^-\rangle),$$

$$\langle S^\alpha_Q\rangle=N^{-1}\sum_R\langle S^\alpha_R\rangle_T\exp(i\boldsymbol{Q}\cdot\boldsymbol{R}). \qquad (54)$$

In the plane (x,y) perpendicular to the magnetic field there is isotropy, i.e., $\langle S^\alpha_Q\rangle=0$ for $\alpha=+,-$ and so $\langle (A^+S^-)_Q\rangle=0$. It follows that $M_{12}=0$, $M_{11}=\omega[\omega-H-J\langle S^z\rangle(1-\delta_{Q,0})]$, and from Eqs. (20) one finds the GF of the oscillator type

$$\langle G_Q^{+-}(\omega)\rangle=\frac{2\langle S^z\rangle}{\omega-\omega_Q}. \qquad (55)$$

The dispersion relation is flat—practically, there is only one oscillator frequency

$$\omega_Q=H+J\langle S^z\rangle(1-\delta_{Q,0}). \qquad (56)$$

Using the formula (49) one arrives immediately at the MFA result for the magnetization [just put $n=N$, $J\to J/N$ in Eq. (53)]

$$\langle S^z\rangle=\frac{1}{2}\tanh\left(\frac{\langle S^z\rangle J+H}{2T}\right), \qquad (57)$$

which for the KSK model is the exact one. Let us discuss shortly the features of the oscillator model involved.

In case of ferromagnet for $T<T_C=J/4$ and $H=0$ one has a finite oscillator frequency and the usual MFA magnetiza-

tion $\langle S^z\rangle > 0$ and specific heat $C_V > 0$. For $T > T_C$ and $H = 0$ there is $\omega_Q = J\langle S^z\rangle_T = 0$. One has to read it as an indication, *that above T_C the oscillator simply does not exist*, there is no mechanism capable of absorbing energy, thus $C_V = 0$. This is true for a ferromagnet in the paramagnetic region of temperature and for the KSK antiferromagnet at all temperatures. [Note that just taking the mathematical limit $\omega_Q \to 0$ would lead to opposite result: $C_V \to$ const at any temperature (the Dulong-Petit law), because oscillator has infinite number of energy levels and can absorb energy at any temperature.] With $H \to 0$ and $J < 0$ in Eq. (53) one arrives at the paramagnetic type of the susceptibility at all temperatures, such as it is for the KSK model.[23]

Summing up, for the KSK model the GF-RPA-QCA procedure provides correct results for magnetization and specific heat vs T. At $T < T_C$ the mathematical formalism provides these results automatically. At $T > T_C$ and $H = 0$ the oscillator frequency is zero and the argument for zero specific heat is a logical one—there is no oscillator to absorb energy. With $H > 0$ the oscillator reappears, one has the field-induced magnetization proportional to the field and the usual MFA magnetic susceptibility—see Ref. 23.

X. EXPERIMENTAL SITUATION

''The existence of spin waves in amorphous ferromagnets is now firmly established''—this phrase of Coey[24] is valid also now. Neutron inelastic scattering (NIS) experiments have confirmed the theoretically predicted $\omega \sim Q^2$ form of the dispersion relation for ferromagnets at small scattering vectors **Q**. At larger **Q** values the NIS profiles are usually very broad, so one has to think of heavily damped spin waves of short wavelengths.

The theory of neutron inelastic scattering (NIS) for amorphous ferromagnets has been developed long ago, starting from the RPA (see Ref. 11 for earlier references). The novelty of the present work is not related to its ferromagnetic version, which is just a typical MFA description—it is its ability to cover the NIS for a wide class of disordered magnets, in particular for systems with dominant contribution of antiferromagnetic (AF) interspin coupling. It is so due to the ''equal access'' extension of the RPA, which includes wider class of spin-spin correlations, than it had been in the original formulation of the RPA (Refs. 1 and 2) aimed at ferromagnets. Three local field characteristics introduced here—$\langle h^z\rangle, \langle h^2\rangle, \langle (h^z)^2\rangle$—allow one to foresee the dispersion relations also for the AF-type elementary excitations, such as they are seen via NIS for disordered spin systems with interspin coupling of short range (OSA). Conversely, having the NIS determined dispersion curves one could estimate the above local field characteristics. In formulating our predictions we implicitly assume that in spite of the possible contribution of the AF interspin coupling the system considered has a rather uniquely determined ground-state configuration of spins—that its behavior is not dominated by spin-glass-like effects.

There are several papers on the structure, magnetization and related properties of nonferromagnetic amorphous magnets—antiferromagnets, speromagnets and asperomagnets. Some general features of such materials have been emphasized.[24] For example, it is intuitively obvious, that the notion of a magnetic domain may lose its meaning in amorphous antiferromagnets. As far as elementary excitations are concerned it has been even argued that long range amorphous antiferromagnetism cannot appear at all—rather, such an order can establish itself only over a few interatomic distances.[25]

As far as they do exist, the elementary excitations in nonferromagnetic amorphous systems are expected to be heavily damped, so it can be difficult to determine the corresponding dispersion relations even in the limit $Q \to 0$. And indeed, due to these difficulties till now there are no reliable data on magnetic elementary excitations in nonferromagnetic amorphous systems. Therefore, let us only mention magnetic systems of such a type investigated till now—they may be good targets for the future NIS attempts to observe such excitations.

As it has been shown by Burke and Rainford,[26] some FeCr alloys evolve towards antiferromagnetic properties close to a critical concentration.

A search for high energy excitations in the $Mn_{73}Ni_{27}$ alloy, which is an itinerant antiferromagnet, has been undertaken,[27] till now without decisive results.

According to Hasegava,[28] the Mn-base glassy alloys should display AF properties. The AF properties of the Pd_3Mn seem to support such a suggestion.[29]

The properties of amorphous invar $Fe_{70}Ni_{20}Zn_{10}$ are rather complex, but some AF features can be seen in them.[30]

Let us also assess the range of applicability of the approximations used.

The random phase approximation (RPA) of Tyablikov,[1] Eq. (2), is explicitly aimed at ferromagnets and leads directly to the mean field results. The equal-access random-phase approximation (EA-RPA) introduced in this paper,

$$\langle\langle S_R^\alpha(t) S_{R'}^\beta(t), S_{R''}^-(t')\rangle\rangle = \langle S_R^\alpha\rangle_T \langle\langle S_{R'}^\beta(t), S_{R''}^-(t')\rangle\rangle + \langle S_{R'}^\beta\rangle_T \langle\langle S_R^\alpha(t), S_{R''}^-(t')\rangle\rangle,$$

is a natural extension of the RPA, conserving more information on the spin-spin correlation, than the original RPA. In case of ferromagnetic coupling it leads directly to the RPA description. It covers a multitude of spin systems including antiferromagnets, but its basic physics and range is of the MFA type. It can probably be improved to adjust its critical indices to the indices of the static scaling theory, using the method developed earlier by Czachor and Holas[5] for the RPA.

The quasicrystal approximation (QCA) introduces a certain uniformization of the spin-spin correlations in space by the substitution in Eq. (19): $\Sigma_{R'} G_{RR'} \exp[iQ(R-R') = \langle G_Q\rangle$; we can see that the site dependent quantity of the LHS is approximated here by a site-independent ''typical'' quantity $\langle G_Q\rangle$. It means that the QCA can break for evidently nonuniform systems.

The ''on the sphere approximation'' (OSA) of Sec. VI imposes a short-range interspin coupling, which is improper whenever the physical coupling is of the long-range type.

Still, the difference should mainly show up in the high-energy wiggles in the dispersion relations measured at large scattering vectors $\boldsymbol{Q}$. It can easily be omitted, at the price of having a less explicit ω vs Q dependence.

It seems, both the experimental and, to some extent, the conceptual problems with elementary excitations in nonferromagnetic amorphous systems have in recent years damped experimental efforts in this field. Hopefully, the present paper, with its average-local-field description of the neutron inelastic scattering in such systems, will encourage future experimental attempts to observe magnetic excitation spectra in these materials.

XI. SUMMARY AND DISCUSSION

To solve the problem of neutron scattering in a disordered magnet—in general a disordered set of localized spins coupled randomly—one has to take into account a greater variety of spin-spin correlations than in case of ferromagnets. To do so, we have first introduced a generalized RPA decoupling (11) of the three-spin correlation functions (Green's functions) involved. We claim that in doing so we have entered a reasonable and promising way towards improving the GF method for the solid state calculations, the way more systematic than those quoted in the Introduction. On assuming then an equivalent and symmetric role of two different two-spin correlation functions pertinent to the problem one has the symmetric ''equal access'' form of the RPA decoupling (EA-RPA). At this step one obtains the ''canonical'' set (16) of two equations of motion for the 2 two-spin GF's, $\langle G_Q^{+-}(\omega)\rangle$, $\langle G_{RR'}^{--}\rangle$, we seek. To solve it analytically for the NIS-relevant Fourier-transform of the GF's involved—the $\langle G_Q^{+-}(\omega)\rangle$ and $\langle G_Q^{--}(\omega)\rangle$ (where Q is the length of the neutron scattering vector and ω represents the energy change in scattering)—we have adapted the quasicrystal factorization (QCA) of the Q transforms [such as in Eq. (19)] of the products of terms involved in the equations into the products of the Q-transformed terms, and assumed an overall isotropy of the system. Finally, in the case of the nearest-neighbor on-the-sphere interspin coupling (OSA) one succeeds in the factorization of terms involved into the Q-dependent and ω-dependent factors, Eqs. (27)–(30), and an explicit expression (35) for the GF has been found. On looking at the roots of its denominator one finds the formula (36) for the dispersion relations ω_Q of magnetic excitations of the system, such as they can be seen in neutron scattering. Here a quadratic equation for the ω_Q function does appear, its parameters being dependent on the configuration averages $\langle h^2\rangle$, $\langle h^z\rangle$, and $\langle (h^z)^2\rangle$ of the local fields h_R^α in the system and on the external magnetic field. We would like to emphasize that this *single equation* takes on the form of dispersion relation valid for a number of spin configurations, including as *special cases* longitudinal ferromagnetic and transverse antiferromagnetic ones, and intermediate configurations as well, depending on the values of the above mentioned fields. It should also be emphasized that in our approach we do not have to introduce the concept of different sublattices for different spin orientations in order to arrive at the dispersion curves $\Omega \approx Q$ in the small Q limit, such as for crystalline antiferromagnet—this characteristic depends entirely on the interplay between the above mentioned local field averages. It is a conceptually important feature. One should add, however, that the antiferromagnetic spin configuration is just one of many *transverse* configurations, all of them being characterized by such a dispersion in the long wave limit.

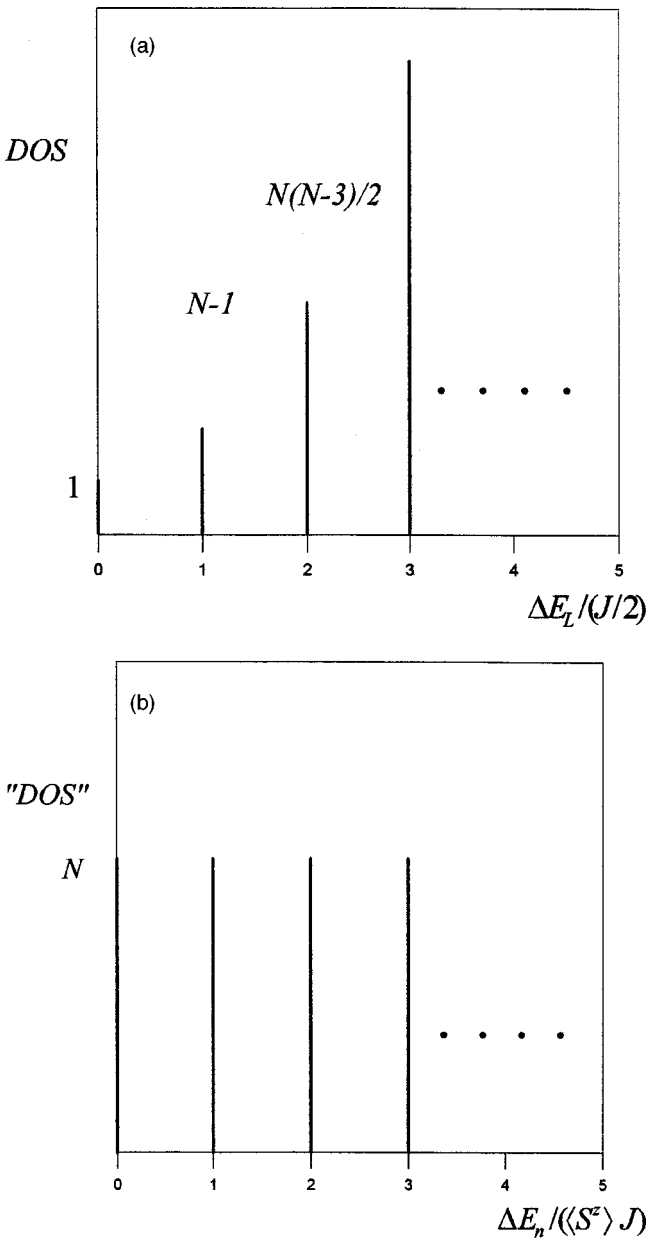


FIG. 6. Density of states, schematically, for the KSK model of N spins $S=1/2$ interacting identically, $J_{RR'}=J/N(1-\delta_{RR'})$, and ferromagnetically, $J>0$. (a) Exact solution (Ref. 23): $\Delta E=E_L-E_0=1/2JL[1+(L-1)/N]$; degeneracy: $d_L=\binom{N}{L}-\binom{N}{L-1}$, $L=0,1,2,\ldots$. (b) Quasi-DOS of the harmonic oscillator type, appearing in the GF-RPA-QCA procedure of this work. $\Delta E=E_n-E_0=n\omega_Q$, $n=0,1,2,\ldots,d_n=N$, where the oscillator frequency ω_Q is given by Eq. (56). Distance between the energy levels is here temperature-dependent—it is proportional to the magnetization $\langle S^z\rangle$ of the Eq. (57).

The NIS profiles predicted here are of the $\delta(\omega-\omega_Q)$-

function type. To calculate their intensities (50) and (52), we had to extend the idea of the scattering vector Q so that it could be treated as the usual summation or integration variable. The NIS peak intensity vs. temperature was found to be proportional to the mean-field-approximation magnetization for longitudinal ferromagnets, while in case of transverse spin structures the temperature decline of the peak intensity is a problem in itself and has only roughly been assessed till now.

We have carried out our GF calculations also for the KSK system of spins interacting identically with each other and found that, as far as the thermodynamic functions are concerned, the results are such as the exact ones.[23] It is an intriguing situation: the GF method, which is in principle approximate due to the decoupling (11) and substitutes the actual KSK system by a system of harmonic oscillators, leads nevertheless to correct results for observables. The corresponding densities of states (DOS) for both procedures are known and they are basically different; see Fig. 6. One should ask the following question: how can this coincidence of results happen?

The answer lies in temperature dependence of the GF-introduced frequency ω_Q, Eq. (56), which represents the separation between energy levels of the oscillators. It essentially means that the *oscillator density of states obtained in the GF method is not a true DOS for the KSK system*. It is an auxiliary function, self-tailored by the GF method itself so, that the oscillator system with T-dependent frequency provides correct macroscopic characteristics.

This example throws an interesting light on the way the GF method can adjust and ''upgrade'' itself to build up a fair representation of macroscopic physical characteristics of systems investigated. Besides, the accord of the GF calculations with the exact ones for the KSK model shows that in the GF method it makes some sense to use the $\boldsymbol{Q}$ vectors as the summation (or integration) variables to calculate thermodynamic functions, although they were originally introduced merely as scattering vectors for the NIS experiment. However, this point requires further attention.

The agreement of the RPA-evaluated magnetic susceptibility with the exact result in the case of the KSK interspin coupling may suggest that the RPA becomes exact in case of long range interactions. There is no ground for such a general claim, though. For example, in case of coulomb interacting electron gas (which is obviously the longest-range physical interaction in three dimensions we have) Langerth and Perdow[31] have obtained the agreement of some RPA-calculated characteristics with the exact results, but only at long wavelength limit (wave vector $k \to 0$).

Experience of this work suggests that it is worthy and feasible to use the generalized RPA-decoupling introduced here to set up a description of magnetism in disordered systems more profound than given here, such as an extension of the ALITA (Ref. 11) to link broad NIS profiles to some distributions of local fields, or, following Czachor and Holas,[5] a refined version of the theory of neutron scattering in crystalline antiferromagnets including the static scaling indices, and others. Some work along these lines is underway.

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