Finite-temperature perturbation theory for quasi-one-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnets

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We develop a finite-temperature perturbation theory for quasi-one-dimensional quantum spin systems, in the manner suggested by Schulz in Phys. Rev. Lett. **77**, 2790 (1996) and use this formalism to study their dynamical response. The corrections to the random-phase approximation formula for the dynamical magnetic susceptibility obtained with this method involve multipoint correlation functions of the one-dimensional theory on which the random-phase approximation expansion is built. This ''anisotropic'' perturbation theory takes the form of a systematic high-temperature expansion. This formalism is first applied to the estimation of the Néel temperature of $S=1/2$ anisotropic cubic lattice Heisenberg antiferromagnets. It is then applied to the compound Cs_2CuCl_4, a frustrated $S=1/2$ antiferromagnet with a Dzyaloshinskii-Moriya spin anisotropy. Using the next leading order to the random-phase approximation, we determine the improved values for the critical temperature and incommensurability. Despite the nonuniversal character of these quantities, the calculated values compare remarkably well with the experimental values for both compounds.

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I. INTRODUCTION

Quasi-one-dimensional magnets are notoriously difficult to tackle. The backbones of those compounds, namely, the spin chains, are by now very well understood, in some cases even by analytical methods. But until now no natural and efficient framework has been developed to describe their behavior when they are coupled by a weak interchain exchange $J_\perp$.

Useful results have nonetheless been obtained by combining one-dimensional exact results with a random-phase approximation (RPA) approach to cope with interchain couplings.[1–3] Recently such a method has even been applied to frustrated quasi-one-dimensional systems,[4] yielding sensible predictions.

From the RPA formalism for the dynamical susceptibility, one can deduce estimates for nonuniversal quantities, such as the Néel temperature,[2] or the possible incommensurate order developing below the transition in a frustrated antiferromagnet.[4] This is made possible by recent progress in the (exact) determination of spin chain two-point correlation functions in the low-energy regime. The RPA formalism together with those exact results are able to cope with exchange anisotropy, and/or Dzyaloshinskii-Moriya interaction.

This approach has been successful in the sense that it yields satisfactory results when compared to experimental measurement (in some cases even though the interchain ratio $J_\perp/J_\parallel$ is not small where $J_\parallel$ is the exchange coupling along the easy axis). This owes to the fact that on one hand the ratio $T_c/J_\parallel$ is small enough so that the collective one-dimensional excitations have a significant influence on the physics at the transition temperature, and on the other hand (for instance, in the case of a cubic lattice), $T_c/J_\perp$ is big enough. However, the RPA is an uncontrolled approximation.

Irkhin and Katanin have calculated corrections to RPA for spin-1/2 quasi-one-dimensional cubic lattices.[5] Their calculations owe to Moriya's empirical improvement to the RPA formula for the dynamical susceptibility[6] and it differs notably from what follows. Their work has found applications in the estimation of the Néel temperature of cubic lattice quasi-one-dimensional antiferromagnets $KCuF_3$, Sr_2CuO_3, and Ca_2CuO_3. Their estimation deviates from the RPA result by 25%.

In the following, we will develop a systematic expansion and will embed the RPA formula for the dynamical susceptibility in it as a natural leading order approximation. We will be mainly concerned with lattices made of $S=1/2$ Heisenberg spin chains. Yet the formalism equally applies to spin chains with anisotropy in spin space.[4] Such an expansion has been developed by Arrigoni[7] for the physics of Luttinger liquids. The main differences with our approach are the following. Because it is at $T=0$, he resums an infinite proper set of cumulants. On the contrary, we are at finite temperature and we will use the temperature as an additional energy scale in the disordered phase. Because of this energy scale, we need not resum all of the higher cumulants to get a sensible result. But we do have to resum temperature-dependent diagrams at the level of any cumulant (four-point correlation function for the examples given in this work), because we intend to use our expansion down to the critical temperature, where those diagrams contribute.

In Sec. II of this paper, we expose the formal steps leading to an extended perturbative expression of the dynamical susceptibility, in terms of a self-energy of the two-spin correlation function. In Sec. III, we discuss some of the results and peculiarities of this expansion. In particular we show that the expansion can be organized in terms of the number of RPA-dressed propagators indirectly related to the small parameter $J_\perp/T$. This propagator must be regularized and we hint at how it can be done. An integral representation of the first correction is given. In Sec. IV, we calculate the correction due to the leading diagram in $J_\perp/T$ and discuss its effect on the physics of cubic lattices and in particular on $KCuF_3$. In Sec. V, we investigate the effect of the same correction in

a much more involved case, a quasi-one-dimensional (or quasi-two-dimensional depending on the point of view since the interchain coupling is large) frustrated antiferromagnet with a Dzyaloshinskii-Moriya interaction: Cs_2CuCl_4.

II. GENERAL PERTURBATION THEORY FOR QUASI-ONE-DIMENSIONAL MAGNETS

We consider the general quasi-one-dimensional magnetic Hamiltonian $\mathcal{H}=\mathcal{H}_\parallel+\mathcal{H}_\perp$, where

$$\mathcal{H}_\parallel=\sum_{i,j} J_{\parallel\mu,\nu}(i,j)S_i^\mu S_j^\nu,$$

$$\mathcal{H}_\perp=\sum_{i,j} J_{\perp\mu,\nu}(i,j)S_i^\mu S_j^\nu. \quad (1)$$

The summation over the spin components is implied whereas the latin indices stand for the sites of the spins. The quasi-one-dimensional magnetic crystal can be viewed as a set of spin chains along which the exchange couplings are supposed to be dominant. $\mathcal{H}_\parallel$ is then defined as the part of $\mathcal{H}$ which connects spins on the same spin chain, whereas $\mathcal{H}_\perp$ connects by definition spins belonging to different spin chains.

We aim at giving a systematic perturbative expansion of the finite-temperature generating functional

$$Z[\vec{\psi}]=\mathrm{Tr}\left[T_\tau\exp\left(-\int_0^\beta d\tau\,\mathcal{H}-\int_0^\beta d\tau\sum_i \vec{\psi}_i\cdot\vec{S}_i\right)\right], \quad (2)$$

where $\beta=1/k_BT$. Now we define the isolated spin chain finite-temperature generating functional

$$Z_\parallel[\vec{\psi}]=\mathrm{Tr}\left[T_\tau\exp\left(-\int_0^\beta d\tau\,\mathcal{H}_\parallel-\int_0^\beta d\tau\sum_i \vec{\psi}_i\cdot\vec{S}_i\right)\right]. \quad (3)$$

If we denote $Z_\parallel=Z_\parallel[\vec{0}]$, then the average of the observable $\mathcal{O}$ with respect to this functional is

$$\langle\mathcal{O}[S_i^\mu]\rangle_\parallel=\frac{1}{Z_\parallel}\mathcal{O}\left[\frac{\delta}{\delta\psi_i^\mu}\right]Z_\parallel[\vec{\psi}]. \quad (4)$$

With those notations, we have

$$Z[\vec{\psi}]=Z_\parallel\left\langle\exp\left(-\int_0^\beta d\tau\,\mathcal{H}_\perp-\int_0^\beta d\tau\sum_i \vec{\psi}_i\cdot\vec{S}_i\right)\right\rangle_\parallel. \quad (5)$$

In a very similar fashion as was done in Ref. 8 for coupled Luttinger liquids, we now introduce a vector field $\vec{\phi}_i(\tau)$ in order to perform a Hubbard-Stratonovitch transform on $\mathcal{H}_\perp$:

$$Z[\vec{\psi}]=Z_\parallel\int\mathcal{D}\vec{\phi}\exp\left(\frac{1}{4}\int_0^\beta d\tau\sum_{i,j}[J_\perp^{-1}]_{\mu,\nu}(i,j)\phi_i^\mu\phi_j^\nu\right)\times\left\langle\exp\left(-\int_0^\beta d\tau\sum_i(\vec{\psi}_i+\vec{\phi}_i)\cdot\vec{S}_i\right)\right\rangle_\parallel. \quad (6)$$

The functional integration on $\vec{\phi}$ corresponds to an inverse Laplace transform. The second part of the integrand, which is $Z_\parallel[\vec{\psi}+\vec{\phi}]$ corresponds to a generating functional of the one-dimensional theory with current source $\vec{\psi}+\vec{\phi}$. Then $-\ln Z_\parallel[\vec{\psi}+\vec{\phi}]$ is the free energy of the sum of the individual spin chains $\ln Z_\parallel[\vec{\psi}+\vec{\phi}]=W[\vec{\phi}+\vec{\psi}]$. The summation over the spin chains is included in the functional W, which has a Ginzburg-Landau expansion

$$W[\vec{\phi}]=\frac{1}{2}\int d(1)d(2)C^{(2)}_{\mu,\nu}(1,2)\phi^\mu_{(1)}\phi^\nu_{(2)}+W_I[\vec{\phi}], \quad (7)$$

where $\phi^\alpha_{(i)}$ stands for $\phi^\alpha(\omega_i,\vec{k}_i)$. $W_I[\vec{\phi}]$ is the interaction functional

$$W_I[\vec{\phi}]=\frac{1}{4!}\int\prod_{i=1}^4 d(i)C^{(4)}_{\mu,\nu,\lambda,\kappa}(1,2,3,4)\phi^\mu_{(1)}\phi^\nu_{(2)}\phi^\lambda_{(3)}\phi^\kappa_{(4)}+O(|\vec{\phi}|^6), \quad (8)$$

where $\int d(i)=\int_0^\beta d\tau_i\int_{-\infty}^\infty dx\Sigma_m$ with m the index of the spin chain. $C^{(p)}(1,\ldots,p)$ is the time-ordered imaginary-time p-point correlation function of an isolated spin chain.

We now work in momentum space and Fourier transform the functional integrals. We therefore adopt the new convention $\int d(i)=\beta\Sigma_n\int_{-\infty}^\infty(dk_x/2\pi)\int_0^{2\pi}(dk_y/2\pi)\int_0^{2\pi}(dk_z/2\pi)$ in the case of a three-dimensional magnet. The summation indexed by n is performed over the Matsubara frequencies $\omega_n=2\pi n/\beta$. Finally let us define the field theory

$$\langle\mathcal{O}\rangle_I=\int\mathcal{D}\vec{\phi}[\exp(F[\phi])\mathcal{O}]\Big/\int\mathcal{D}\vec{\phi}\exp(F[\phi]) \quad (9)$$

with the weight

$$F[\phi]=\frac{1}{2}\int d(1)[[2J_\perp]^{-1}(1)+C^{(2)}(1)]_{\mu,\nu}\phi^\mu_{(1)}\phi^\nu_{(-1)}+W_I[\vec{\phi}]. \quad (10)$$

Rewriting Eq. (6) in terms of the theory defined by Eq. (9), we obtain

$$\frac{Z[\vec{\psi}]}{Z[\vec{0}]}=\exp\left(\frac{1}{2}\int d(1)[2J_\perp]^{-1}_{\mu,\nu}(1)\psi^\mu_{(1)}\psi^\nu_{(-1)}\right)\times\left\langle\exp\left(-\int d(1)[2J_\perp]^{-1}_{\mu,\nu}(1)\psi^\mu_{(1)}\phi^\nu_{(-1)}\right)\right\rangle_I. \quad (11)$$

Interpreting the averaged exponential in Eq. (11) as a generating functional and introducing the self-energy $\Sigma_{\mu,\nu}(\omega,\vec{k})$ for the two-point correlation function, we deduce that to second order in $\vec{\psi}$, one has [assuming for simplicity SU(2) invariance so that $C^{(2)}_{\mu,\nu}=C^{(2)}\delta_{\mu,\nu}$, $J_\perp^{\mu,\nu}=J_\perp\delta_{\mu,\nu}$, and $\Sigma_{\mu,\nu}=\Sigma\,\delta_{\mu,\nu}$]

$$\ln(Z[\vec{\psi}]/Z[\vec{0}]) = O(|\vec{\psi}|^4) + \frac{1}{2}\int d(1) \times \frac{C^{(2)}(1)+\Sigma(1)}{1+2J_\perp(1)[C^{(2)}(1)+\Sigma(1)]}\vec{\psi}_{(1)}\cdot\vec{\psi}_{(-1)}. \quad (12)$$

This form of the two-point correlation function has been suggested by Schulz in Ref. 2 in a different context.

III. CALCULATION OF THE FIRST CORRECTIONS TO THE RPA DYNAMICAL SUSCEPTIBILITY

A. RPA formula for the dynamical susceptibility

To the lowest order of approximation, one can set $\Sigma(\omega,\vec{k})=0$ in Eq. (12). We can then continue analytically (on the frequencies) the one-dimensional two-point correlation function and therefore recover the dynamical magnetic susceptibility

$$\chi_{3D}(\omega,\vec{k}) = \frac{\chi_{1D}(\omega,k_x)}{1-2\,J_\perp(\vec{k})\,\chi_{1D}(\omega,k_x)}. \quad (13)$$

As a consequence, the RPA approximation for quantum spin systems appears as the leading order of a more general expansion scheme.

B. Higher-order corrections to the RPA formula

This clearly shows that a systematic expansion can be used. The free (Euclidian) propagator of the effective theory is an RPA-dressed propagator (simply called G thereafter). Its inverse can be read off from Eq. (10):

$$[G]^{-1} = C^{(2)} + [2\,J_\perp]^{-1}. \quad (14)$$

In real space and imaginary time, it is given by

$$G(\tau,\vec{r}) = \frac{1}{\beta}\sum_n \int_{-\infty}^{\infty}\frac{dk_x}{2\pi}\int\int_0^{2\pi}\frac{dk_y}{2\pi}\frac{dk_z}{2\pi}e^{i\vec{k}\cdot\vec{r}+i\omega_n\tau} \times \frac{2J_\perp(\vec{k})}{1+2J_\perp(\vec{k})C^{(2)}(i\omega_n,\vec{k})}. \quad (15)$$

In the following, multiple integrals will be omitted and symbolised by a single one. Depending on the value of the temperature, the integration in Eq. (15) might be improper and it is then meant that the principal value of the integral is to be taken. We postpone the discussion on this issue to Sec. III D.

The vertices of the perturbation theory are given by the multiple $2n$-point correlation functions of the spin chains. In the case of the spin $S=1/2$ those are known exactly in the asymptotic limit.

The vertices of the effective field theory (10) involve separated space-time points (τ,x) and therefore always depend on (ω,k_x) when written in momentum space. On the other hand, they are pointlike vertices as far as the transverse space coordinates are concerned or, stated differently, do not depend on $\vec{k}_\perp$ in momentum space. As a consequence, all diagrams in the expansion of the self-energy $\Sigma(\omega,k_x,\vec{k}_\perp)$ are expected to depend on k_x. Yet, only those with internal RPA-dressed propagator lines which are true functions of the input transverse momentum $\vec{k}_\perp$ are to depend on it.

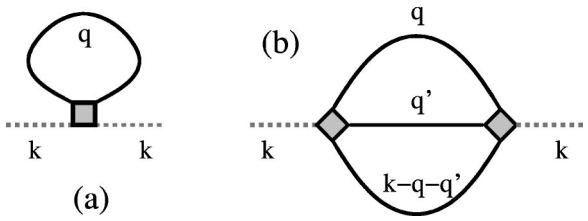

FIG. 1. Diagram (a) does not depend on $\vec{k}_\perp$ whereas diagram (b) containing RPA internal lines depending on the input $\vec{k}_\perp$ does.

The first $\vec{k}_\perp$-dependent diagram possesses three RPA-dressed propagators and two four-point vertices as depicted on Fig. 1. What happens for the transverse momenta is reminiscent of what occurs to many-body field theories of electron gas, where the dependence on the space momenta appears only to the order of this diagram, whereas the first diagrams (Hartree-Fock) depend only on frequencies.

For diagrams which do not depend on the transverse momenta, and which are therefore merely one-dimensional, one can resort to the simplified one-dimensional RPA-dressed propagator

$$G(\tau,x) = G(\tau,x,\vec{r}_\perp=\vec{0}). \quad (16)$$

It is the propagator which has been used in Ref. 5. $\vec{r}_\perp$ denote the transverse part of the position vector.

What is the small parameter of this expansion ? In the simplest case of the cubic lattice, it is likely to be $J_\perp/T$. More precisely it is $AJ_\perp/T$ where A is a prefactor, possibly weakly dependent on the temperature. The prefactor A will be given later [Eq. (17)] in the case of $S=1/2$ Heisenberg spin chains. Indeed, each RPA line contributes by an obvious factor of $(AJ_\perp/T)^2$ in any diagram. Yet in each RPA-line expression remains a nonpolynomial dependence on $AJ_\perp/T$ corresponding to the usual RPA resummation of transverse paths. Undoing this RPA summation, the propagator can be expanded in contributions with an exact dependence in $(AJ_\perp/T)^2$, $(AJ_\perp/T)^3$, etc. For a diagram with p RPA lines in it, it is rather $(AJ_\perp/T)^{2p}$, $(AJ_\perp/T)^{2p+1}$, etc.

So whatever the subtle dependence of the RPA-dressed propagator on the temperature, this expansion can genuinely be seen as a high-temperature expansion in the parameter $(AJ_\perp/T)^2$. More formally, it is also an expansion in the number of RPA-dressed propagator lines although their dependence in the small parameter is more intricate.

As a consequence, the conditions of applicability of this perturbation theory are that $(AJ_\perp/T)^2 \ll 1$ but also $T/J_\parallel \ll 1$ in order for the field-theoretic tools to be valid (in particular in the calculations of the spin correlation functions at finite temperature). For the compounds studied here those condi-

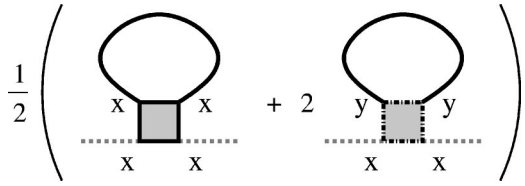

FIG. 2. Hartee-Fock diagrams with symmetry factors which are the first nontrivial terms of the self-energy $\Sigma(\omega,\vec{k})$.

tions (which have to be modified in the case of a frustrated magnet) turn out to be satisfied.

The expansion also depends on the dimensionality of the lattice. This dependence is obvious at the order of RPA, where the small parameter is there proportional to the transverse coordination number (see Ref. 5). The dependence is far less clear at higher order, where the dimensionality is encrypted in multidimensional integrals. It is nevertheless possible to take the $d\to\infty$ limit in these integrals in order to study this dependence. But this is beyond the scope of this work.

C. Details for the first correction

Let us take into account the very first correction to the dynamical susceptibility. So we consider the first nontrivial term in the perturbative expansion of the self-energy. It involves the four-point correlation functions of the spin $S=1/2$ Heisenberg spin chain. We decide to truncate the Landau-Ginzburg expansion of $W_l[\vec{\phi}]$ to the quartic term in $\vec{\psi}$ (six- and higher-point correlation function do not contribute at this order anyway). The field theory expansion formally resembles a three-component $\vec{\phi}^4$ theory. In particular the very first correction to the self-energy is given by Hartree-Fock diagrams (Fig. 2). The ''free'' propagator of this $\vec{\phi}^4$ field theory Eq. (15) is built on the usual imaginary-time two-spin correlation function of the Heisenberg chain but dressed by the RPA corrections. It is therefore a significantly enhanced propagator and the first correction to RPA in this scheme is expected not to be negligible.

The only vertices of this truncated field theory are given by the four-point spin correlation functions. The staggered four-point correlation functions at the isotropic point can be computed thanks to bosonization in addition to a renormalization group analysis that gives the logarithmic correction. The finite-T result can be deduced from the $T=0$ conformal result by a conformal mapping from the plane to the cylinder of radius $1/(\pi T)$.

We will denote by $A(\Lambda/T)$ the product of the Lukyanov-Zamolodchikov prefactor with the logarithmic correction induced by the marginally irrelevant current-current correction[9,10]

$$A\left(\frac{\Lambda}{T}\right)=\frac{2}{(2\pi)^{3/2}}\sqrt{\ln\left(\frac{\Lambda}{T}\right)+\frac{1}{2}\ln\ln\left(\frac{\Lambda}{T}\right)}. \tag{17}$$

For clarity, we decompose the imaginary-time four-point correlation function into $A(\Lambda/T)$ and the purely conformal part of the correlation functions $C^{(4)}_{xxxx}$ and $C^{(4)}_{xxyy}$:

$$T_\tau\langle S^x_{(0)}S^x_{(z_1)}S^x_{(z_2)}S^x_{(z_3)}\rangle=A^2\left(\frac{\Lambda}{T}\right)C^{(4)}_{xxxx}(z_1,z_2,z_3),$$

$$T_\tau\langle S^x_{(0)}S^x_{(z_1)}S^y_{(z_2)}S^y_{(z_3)}\rangle=A^2\left(\frac{\Lambda}{T}\right)C^{(4)}_{xxyy}(z_1,z_2,z_3), \tag{18}$$

where $C^{(4)}_{xxxx}$ as well as $C^{(4)}_{xxyy}$ are given by

$$\begin{aligned}C^{(4)}_{xxxx}(z_1,z_2,z_3)=(-1)^{x_1+x_2+x_3}&\times\left[\frac{|\Omega(z_1)\Omega(z_2-z_3)|}{|\Omega(z_2)\Omega(z_3)\Omega(z_1-z_2)\Omega(z_1-z_3)|}\right.\\&-\frac{2}{|\Omega(z_1)\Omega(z_2-z_3)|}\\&+\frac{|\Omega(z_2)\Omega(z_1-z_3)|}{|\Omega(z_1)\Omega(z_3)\Omega(z_1-z_2)\Omega(z_2-z_3)|}\\&-\frac{2}{|\Omega(z_2)\Omega(z_1-z_3)|}\\&+\frac{|\Omega(z_3)\Omega(z_1-z_2)|}{|\Omega(z_1)\Omega(z_2)\Omega(z_1-z_3)\Omega(z_2-z_3)|}\\&\left.-\frac{2}{|\Omega(z_3)\Omega(z_1-z_2)|}\right]\end{aligned} \tag{19}$$

and

$$\begin{aligned}C^{(4)}_{\mathrm{xxyy}}(z_1,z_2,z_3)&\\=(-1)^{x_1+x_2+x_3}&\frac{1}{|\Omega(z_1)\Omega(z_2-z_3)|}\\&\times\mathrm{Re}\left(\sqrt{\frac{\Omega(z_2)\Omega(\overline{z_3})\Omega(\overline{z_1}-\overline{z_2})\Omega(z_1-z_3)}{\Omega(\overline{z_2})\Omega(z_3)\Omega(z_1-z_2)\Omega(\overline{z_1}-\overline{z_3})}}-1\right),\end{aligned} \tag{20}$$

where we have denoted

$$\Omega(z=x+i\tau)=\frac{u}{\pi T}\sinh\left(\frac{\pi T}{u}(x+iu\tau)\right). \tag{21}$$

Only the staggered part of the correlation functions, which dominates, has been taken into account.

The nonuniversal constant Λ is taken to be $\Lambda=24.27J_\parallel$ as calculated in Ref. 11. Although the values of the prefactor in $A(\Lambda/T)$, that is $2/(2\pi)^{3/2}$, and of Λ are somehow different from those extracted from numerics[12] and used in Ref. 5, there is no contradiction emerging here with the numerical estimates of the correlation functions themselves.[11] In particular, the Néel temperature estimated through RPA for $KCuF_3$ is very close. Discrepancies might nevertheless appear for a different range of temperature and when the self-energy corrections are taken into account. Finally $u=(\pi/2)J_\parallel$ is the spin-1/2 Heisenberg chain velocity given by the Bethe ansatz.

The first contribution to the self-energy is then

$$\Sigma^{(1)}(\omega,\vec{k})=\frac{1}{2}A^2\left(\frac{\Lambda}{T}\right)\int_0^\beta d\tau_1 d\tau_2 d\tau_3 \int_{-\infty}^{\infty} dx_1 dx_2 dx_3 \times e^{-ik_x x_1 - i\omega\tau_1} G(z_3-z_2)\left[\frac{1}{8}C^{(4)}_{xxxx}+\frac{1}{2}C^{(4)}_{xxyy}\right] \times(z_1,z_2,z_3), \tag{22}$$

where the integrals are performed in real space as was done in Ref. 5. We are mainly interested in the knowledge of $\Sigma(\omega,\vec{k})$ around $k_x=\pi$ because the isotropic correlation functions are most significant at this point. More precisely, most of the spectral weight remains at this point. It turns out that, for our purpose, the numerics are much more efficient when done in momentum space

$$\Sigma^{(1)}(\mathbf{k},\vec{k}_\perp)=\frac{1}{2\beta}A^2\left(\frac{\Lambda}{T}\right)\sum_n \int_{-\infty}^{\infty}\frac{dq_x}{2\pi}\left[\frac{1}{8}C^{(4)}_{xxxx}+\frac{1}{2}C^{(4)}_{xxyy}\right](\mathbf{k}, -\mathbf{k},\mathbf{q}_n,-\mathbf{q}_n)\int_0^{2\pi}\frac{d\vec{q}_\perp}{(2\pi)^2}G(\mathbf{q}_n,\vec{q}_\perp), \tag{23}$$

where $\mathbf{k}=(\omega,k_x)$ and $\mathbf{q}_n=(\omega_n,q_x)$.

Now only $C^{(2)}(\omega_n,k_x)$, which enters in $G(\mathbf{q}_n,\vec{q}_\perp)$ through Eq. (15), remains to be known. It is the spin-spin time-ordered imaginary-time (isotropic) correlation function. The large distance behavior of the finite-temperature correlation function can be determined by combining results obtained from the Bethe ansatz solution[13,14] of the Heisenberg $S=1/2$ spin chain, with field theoretic techniques[9,10,15–17]

$$C^{(2)}(\tau,x)=(-1)^x\frac{A(\Lambda/T)}{2}\frac{\pi T/u}{\left|\sinh\left[\frac{\pi T}{u}(x+iu\tau)\right]\right|}. \tag{24}$$

This result can be extended to the anisotropic spin chain as well, although Λ is known exactly only at the isotropic point. The frequency and momentum dependence is obtained by Fourier transformation and analytic continuation of the time-ordered imaginary-time staggered correlation function (24) (see Refs. 11,16,18,19):

$$\chi_{1\mathrm{D}}(\omega,\pi+k_x)=-\frac{A(\Lambda/T)}{4\,T}\frac{\Gamma\left(\frac{1}{4}-i\frac{\omega-uk_x}{4\pi T}\right)}{\Gamma\left(\frac{3}{4}-i\frac{\omega-uk_x}{4\pi T}\right)} \times\frac{\Gamma\left(\frac{1}{4}-i\frac{\omega+uk_x}{4\pi T}\right)}{\Gamma\left(\frac{3}{4}-i\frac{\omega+uk_x}{4\pi T}\right)}. \tag{25}$$

But we will mostly use this result in its Euclidian form (before analytic continuation):

$$C^{(2)}(\omega_n,k_x)=-\chi_{1\mathrm{D}}(i\omega_n,k_x). \tag{26}$$

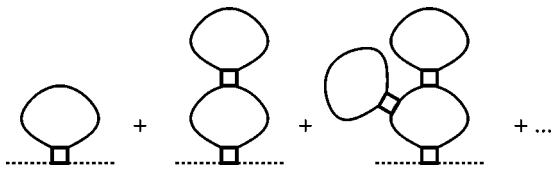

FIG. 3. Bubbles diagrams that add up to form $\mathbf{\Sigma}^{(1)}$.

Finally let us mention the fact that as claimed before, $\Sigma^{(1)}(\mathbf{k},\vec{k}_\perp)$ does not actually depend on $\vec{k}_\perp$. We also note from the above result that the obvious prefactor of $J_\perp\Sigma^{(1)}$ is expected to be $(AJ_\perp/T)^3$.

D. Prescription for the RPA-dressed propagator

The RPA-dressed propagator in momentum space (14) may, for some values of the variables $(\omega_n,\vec{k})$ and parameter (T), exhibits a singularity. In the explicit formula for the diagrams, this propagator is always integrated over and the principal values of the resulting integrals are finite. Still, the presence of this singularity has to be understood and a correct prescription for it (here taking the principal value of improper integrals) to be justified. The difficulty arising from its presence can be overcome as follows.

Let us assume that this field theory has a critical temperature T_c, which is the exact theoretical estimate of the Néel temperature. The perturbation theory is expected to be valid for high enough temperatures and only for temperatures above T_c in the disordered phase. The RPA approach provides an estimated critical temperature T_c' presumably larger (as will be verified later) than T_c. It corresponds to a pole in the dynamical susceptibility. For $T\geqslant T_c'$ no singularity is expected to appear in the RPA propagator and no problem occurs in the perturbation expansion. Whereas when $T_c\leqslant T\leqslant T_c'$, the denominator of the propagator is negative which is tantamount to realize that subdiagrams given by an RPA line just add up to infinity. Nonetheless this is an unphysical singularity which can be cured by a proper prescription as we are going to hint at.

Let us show how it is done in the case of the calculation of T_c'', the critical temperature at the next-to-leading order as was done above when calculating $\Sigma^{(1)}$. We may expect T_c'' to satisfy $T_c''\leqslant T_c'$ and hence to yield a problem. This statement is based on the fact that including the effects of the four-spin correlation functions (in addition to the two-spin correlation functions) amounts to take into account quantum fluctuations more precisely, as compared to merely restricting to the Gaussian fluctuations of the RPA approximation. As we have seen $\Sigma^{(1)}$ depends on a singular RPA-dressed propagator. Now, we will add to $\Sigma^{(1)}$ (which sum will hence be denoted $\mathbf{\Sigma}^{(1)}$) subdiagrams which would normally be appearing at higher order in the expansion. The single RPA line drawn in the diagram for $\Sigma^{(1)}$ appears now as a skeleton line in the diagram for $\mathbf{\Sigma}^{(1)}$. In this case, it stands for an RPA line plus the self-energy correction $\mathbf{\Sigma}^{(1)}$ itself. $\mathbf{\Sigma}^{(1)}$ is therefore defined as the sum of all irreducible bubble diagrams as drawn in Fig. 3.

It satisfies a self-consistency Dyson equation given by the expression (23) but where $G(\mathbf{q}_n,\vec{q}_\perp)$ is now replaced by $\mathbf{G}(\mathbf{q}_n,\vec{q}_\perp)$ defined by an enhanced version of Eq. (14)

$$[\mathbf{G}]^{-1}=C^{(2)}+[2\,J_\perp]^{-1}+\mathbf{\Sigma}^{(1)}. \tag{27}$$

By construction, the singularity is now avoided, the pole of $\mathbf{G}$ being displaced to a boundary of the integration domain. At this boundary the singularity is genuinely integrable provided the lattice is at least three dimensional (which is fully consistent with the Mermin-Wagner theorem). Hence subdiagrams have ultimately canceled the singularity encountered above. Yet our method is a systematic one and does not rely on a self-consistent approach. But we can now extract from this construction the part of $\mathbf{\Sigma}^{(1)}$ which corresponds to the regularized $\Sigma^{(1)}$ we have to calculate in our scheme. In order to do so, we decompose the integral $\int_0^{2\pi}[d\vec{q}_\perp/(2\pi)^2]\mathbf{G}(\mathbf{q}_n,\vec{q}_\perp)$ appearing in the expression of $\mathbf{\Sigma}^{(1)}$

$$\begin{aligned}\int_0^{2\pi}\frac{d\vec{q}_\perp}{(2\pi)^2}\mathbf{G}(\mathbf{q}_n,\vec{q}_\perp)&=\int_0^{2\pi}\frac{d\vec{q}_\perp}{(2\pi)^2}\frac{2J_\perp}{1+2J_\perp(C^{(2)}+\mathbf{\Sigma}^{(1)})}\\&=\int_0^{2\pi}\frac{d\vec{q}_\perp}{(2\pi)^2}\left[\frac{2J_\perp}{1+2J_\perp C^{(2)}}-\frac{(2J_\perp)^2\mathbf{\Sigma}^{(1)}}{[1+2J_\perp(C^{(2)}+\mathbf{\Sigma}^{(1)})](1+2J_\perp C^{(2)})}\right]\\&=P\int_0^{2\pi}\frac{d\vec{q}_\perp}{(2\pi)^2}\frac{2J_\perp}{1+2J_\perp C^{(2)}}-P\int_0^{2\pi}\frac{d\vec{q}_\perp}{(2\pi)^2}\frac{(2J_\perp)^2\mathbf{\Sigma}^{(1)}}{[1+2J_\perp(C^{(2)}+\mathbf{\Sigma}^{(1)})](1+2J_\perp C^{(2)})}.\end{aligned} \tag{28}$$

The first term of the last right-hand side is the regularised expression for the RPA-dressed propagator we use in $\Sigma^{(1)}$ whereas the second term (which also ought to be regularized) is a correction to it at a higher order in $A\,J_\perp/T$. The prescription scheme consists therefore (at least in this case) in taking the principal value of the integral (symbolized by P) which turns out to be finite.

IV. APPLICATION TO CUBIC $S=1/2$ ANTIFERROMAGNETS

Corrections to RPA in the framework of cubic $S=1/2$ antiferromagnets was the subject of Ref. 5. In particular, the authors have derived the integral expression for the diagrams of Fig. 2. However, their correction does not correspond to the first self-energy correction but rather to a subset of diagrams. The self-energy correction derived here includes the resummation of the one-particle reducible diagrams made of chains of their contribution.

Let us apply our formalism, using the $\Sigma^{(1)}$ correction to the self-energy to the compound $KCuF_3$. The experimental value is $T_c=39$ K.[21] The RPA Néel temperature is estimated to be $T_c=52.3$ K. Values for the RPA result were given in Refs. 2,5. Differently, the result obtained here makes use of the analytical value of $A(\Lambda/T)$.

Taking into account their correction, Irkhyn and Katanin then deduced $T_c=36.7$ K, which correction is of order 30%. The singularity of the RPA-dressed propagator is removed by using a semiempirical approximation due to Moriya.[6] But its nontrivial dependence on the temperature and the couplings constant $J_\perp$ disappears as well.

From their calculation, one can deduce the value of some intermediate integrals to be calculated. Making use of the values of these integrals, and therefore resorting to Moriya's approximation, but within the self-energy correction approach on obtains the value $T_c=31.2$ K (that is, at this order, resumming the reducible diagrams). This correction of order 40% is significantly stronger.

To determine the critical temperature with the method developed here is somewhat more complicated. Indeed, the self-energy is also T dependent in a nonsimple way. We have therefore to solve the problem by iteration on the value of the estimated critical temperature. The formal calculations detailed above can be applied with the transverse lattice structure factor

$$J_\perp(\vec{k}_\perp)=J_\perp[\cos(k_y)+\cos(k_z)] \tag{29}$$

of three-dimensional cubic lattices. From Eq. (12) and after analytic continuation, we obtain the three-dimensional dynamical magnetic susceptibility

$$\chi^{xx}_{3D}(\mathbf{k},\vec{k}_\perp)=\frac{\chi^{xx}_{1D}(\mathbf{k})+\Sigma^{xx}(\mathbf{k},\vec{k}_\perp)}{1-2\,J_\perp(\vec{k}_\perp)[\chi^{xx}_{1D}(\mathbf{k})+\Sigma^{xx}(\mathbf{k},\vec{k}_\perp)]}. \tag{30}$$

The instability condition which can only be satisfied at zero frequency is therefore

$$2\,J_\perp(\vec{k})X(0,\vec{k})=1, \tag{31}$$

where $X(\mathbf{k})=\chi^{xx}_{1D}(\mathbf{k})+\Sigma^{xx}_{(1)}(\mathbf{k})$. Because at this order $\Sigma^{xx}(\mathbf{k},\vec{k}_\perp)$ does not depend on $\vec{k}_\perp$ and because it does not *a priori* change the monotony of $\chi^{xx}_{1D}(\mathbf{k})$ with respect to k_x, one can first maximize the left-hand side on $\vec{k}$. It leads to Néel order in the main direction $k_x=\pi$. If the couplings in the transverse directions are ferromagnetic as it is the case for $KCuF_3$ then $k_y=k_z=0$. So that the instability condition is reduced to $4\,J_\perp X(0,\vec{0})+1=0$, where $J_\perp=J_y=J_z$.

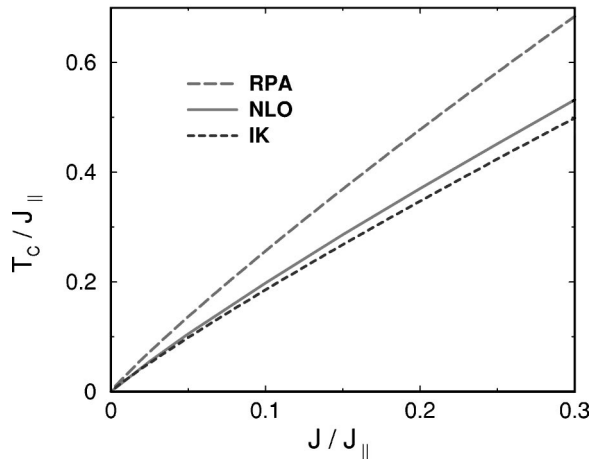

FIG. 4. RPA, next-to-leading order and Irkhin and Katanin's estimations of the critical temperature T_c of cubic lattices in units of $J_\parallel$ as a function of the interchain exchange $J=J_\perp=J_y=J_z$ in units of $J_\parallel$.

For $KCuF_3$, the exchange values are $J_\parallel=406$ K and $J_\perp=-19.1$ K (5% of the main coupling).[21] The small parameter close to the transition is $AJ_\perp/T\simeq 0.3$. The numerical result of this calculation is $T_c=40.3$ K, fairly close to the experimental value. Finally let us mention that not taking into account the log-log correction would have led us to $T_c=37.7$ K. So the subtle log-log correction would presumably be more significant than the second order correction to the self-energy $\Sigma^{(2)}(\mathbf{k},\vec{k}_\perp)$.

On Fig. 4, we have drawn the general curve of the estimated critical temperature T_c of cubic lattices as a function of the interchain exchange $J=J_\perp=J_y=J_z$. The upper curve (RPA) corresponds to the RPA estimation of the critical temperature. The lower curve (IK) is deduced from the estimation of Irkhin and Katanin. It can be deduced from their main result[5] reformulated with our notations and from the use of the exact correlation function prefactor

$$T_c=kJ_\perp A\left(\frac{\Lambda}{T_c}\right)\left[\frac{\Gamma(1/4)}{\Gamma(3/4)}\right]^2, \tag{32}$$

where $k\simeq 0.70$. The intermediate curve (NLO) corresponds to our next-to-leading order estimation of the critical temperature. It is significantly lower than the RPA one as expected (about 25%).

The critical temperature of spatially isotropic $S=1/2$ cubic lattices ($J_\perp=J_\parallel$) has been computed with great accuracy using quantum Monte Carlo (QMC) simulations:[20] $T_c/J_\parallel=0.946\pm 0.001$. Unfortunately, the case $J_\perp=J_\parallel$ is *a priori* beyond the scope of our approach. Indeed the condition $T/J_\parallel\ll 1$ is clearly violated, whereas $(AJ_\perp/T)^2\ll 1$ still holds close to the transition predicted by QMC simulations. The RPA value of T_c is $T_c=1.96J_\parallel$. In the calculation of the next-to-leading order, no fixed point can successfully be reached for T_c, the value of T_c wandering between $1.1<T_c/J_\parallel<1.5$ with no satisfying convergence. This is not surprising since the functionnal dependence of the Hartree-Fock corrections in T_c being presumably meaningless when $T/J_\parallel\ll 1$ is unsatisfied.

The graph Fig. 4 has been plotted in the safer range $J_\perp/J_\parallel<0.3$. It would be very interesting to have QMC simulations to determine the critical temperature in this range. That would be a precise test of the perturbation theory for anisotropic cubic $S=1/2$ lattices.

V. APPLICATION TO FRUSTRATED $S=1/2$ ANTIFERROMAGNETS

A. RPA approach for the dynamical susceptibility in the disordered phase of Cs_2CuCl_4

Cs_2CuCl_4 is a spin-1/2 frustrated antiferromagnet. At a temperature of $T_c=0.62$ K, it shows a transition to an ordered phase. The order is cycloidal. Its parameter is incommensurate and measured to be $k_0=0.186$. Remarkably, in this phase as well as in the disordered phase, the excitations spectrum is incoherent.[22–25]

Its magnetic Hamiltonian has been recently experimentally determined with great accuracy.[26] It can be decomposed as

$$\mathcal{H}=\sum_k \mathcal{H}^{(k)}_{\text{plane}}+\mathcal{H}^{(k,k+1)}_{\text{interplane}}+\mathcal{H}_{\text{DM}},$$

$$\mathcal{H}^{(k)}_{\text{plane}}=J_\parallel\sum_{i,j}\vec{S}_{i,j,k}\cdot\vec{S}_{i+1,j,k}+J_\perp\sum_{i,j}\vec{S}_{i,j,k}\cdot[\vec{S}_{i,j+1,k}+\vec{S}_{i-1,j+1,k}],$$

$$\mathcal{H}^{(k,k+1)}_{\text{interplane}}=J_z\sum_{i,j}\vec{S}_{i,j,k}\cdot\vec{S}_{i,j,k+1},$$

$$\mathcal{H}_{\text{DM}}=\sum_{i,j,k}\vec{D}\cdot[\vec{S}_{i,j,k}\times\vec{S}_{i+1,j,k}]. \tag{33}$$

In particular a Dzyaloshinskii-Moriya interaction ($\mathcal{H}_{\text{DM}}$) has been proven to exist on the interchain exchange paths, revealed by its anisotropic nature. Experimental estimates for the exchange couplings in Cs_2CuCl_4 are $J_\parallel=4.34$ K, $J_\perp=1.48$ K (about one third of the main coupling), $J_z=0.20$ K and finally $|\vec{D}|=0.23$ K (about 5% of the main coupling).[22,26]

So it appears that this compound is essentially two-dimensional. One of the two-dimensional spin lattices is represented in Fig. 5. Although the interchain coupling $J_\perp/J_\parallel$ is considerable, the smallness of the ratio of transition temperature to bandwidth $T_c/\pi J_\parallel\approx 0.05$ indicates that the quasi-one-dimensional approach we are advocating might be tried on Cs_2CuCl_4.

An RPA approach has been proven to reproduce qualitative features of the compound (incommensurability, asymmetry of the dynamical structure factor around $k_x=\pi$, as

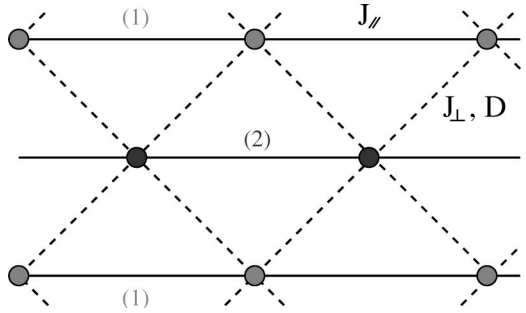

FIG. 5. Exchange paths within the planes: solid lines denote the strong exchange $J_{\parallel}$, dashed lines the weaker, frustrated exchange $J_{\perp}$. Dzyaloshinskii-Moriya exchange of magnitude D also stands on the interchain paths. Two types of sites among the four in an elementary cell of the lattice are distinguished.

well as by construction, the incoherent spectra).[4] It also gives very reasonable estimates for the critical temperature and the incommensurability.

Given the latest experimental data, and also taking into account the subleading correction in the logarithmic dependence of the spin correlation functions (which was intentionally neglected in Ref. 4), RPA gives $k_0=0.197$ and $T_c=0.85$ K. Those numbers are off by less than 25% compared to the experimental values, which is fairly good given the complexity of the physics displayed by Cs_2CuCl_4. It was shown that some qualitative features of Cs_2CuCl_4 were without doubt reproduced by the approach advocated in Ref. 4. Knowing the corrections to the RPA result would hopefully decide whether such a perturbative approach can be used on this compound for determining quantitative results.

We now briefly reproduce the calculation leading to an RPA formula for the dynamical susceptibility as the calculation of the subleading order makes use of it. The elementary cell of the Cs_2CuCl_4 crystal has four Copper ions. In addition, the vector of the Dzyaloshinskii-Moriya (DM) interaction which lies on the interchain bounds, points in the third direction (denoted Oz here). The orientation of the DM vector is staggered from one plane to another: $\vec{D}=\pm D\,\vec{e}_z$.

Hence the magnetic Hamiltonian is now spin anisotropic. Those complications make the RPA-dressed propagator possess a matrix-form which can ultimately (in the complex representation $(+-)$ of the quantum spins) be reduced to a 4 by 4 matrix. Eq. (14) is still valid under its matrix form

$$[\mathbb{G}^{+-}]^{-1}=\mathbb{G}^{(2)}_{+-}+[\mathbb{J}^{+-}_{\perp}]^{-1}. \tag{34}$$

The four components of the vectorial space in which it is defined correspond to the $-$ component of the four distinct spins in an elementary cell on the right (resp. $+$ component of the spins on the left).

We have $\mathbb{G}^{(2)}_{+-}=C^{(2)}_{+-}\mathbb{I}_4$ and

$$\mathbb{J}^{+-}_{\perp}=\begin{bmatrix} 0 & \mathsf{J}+\mathsf{K} & \mathsf{I} & 0 \\ \mathsf{J}+\mathsf{K} & 0 & 0 & \mathsf{I} \\ \mathsf{I} & 0 & 0 & \mathsf{J}-\mathsf{K} \\ 0 & \mathsf{I} & \mathsf{J}-\mathsf{K} & 0 \end{bmatrix}, \tag{35}$$

where

$$\mathsf{J}(\vec{k})=J_{\perp}[\cos(k_y)+\cos(k_x-k_y)],$$

$$\mathsf{K}(\vec{k})=D[\sin(k_y)+\sin(k_x-k_y)],$$

$$\mathsf{I}(\vec{k})=J_z\cos(k_z). \tag{36}$$

The transverse RPA-dressed propagator of the effective field theory is related to the transverse RPA imaginary-time correlation function $\mathbb{G}^{+-}_{\mathrm{RPA}}(k_x,\omega)$ [itself related to the transverse RPA dynamical susceptibility $\chi^{+-}_{3\mathrm{D}}(k_x,\omega)$ by analytic continuation] by

$$\frac{\mathbb{G}^{+-}}{\mathbb{J}^{+-}_{\perp}}+\mathbb{J}^{+-}_{\perp}\mathbb{G}^{+-}_{\mathrm{RPA}}=\mathbb{I}_4. \tag{37}$$

Note that from Eq. (34), $\mathbb{G}^{+-}$ and $\mathbb{J}^{+-}$ are commuting 4 $\times$4 matrices. The transverse time-ordered imaginary-time two-point correlation function of spins is obtained by adding the contributions from the various sublattice correlators, i.e., by taking, e.g.,

$$\sum_{i,j}\langle S^{+}_{(i)}(\omega,\vec{k})S^{-}_{(j)}(-\omega,-\vec{k})\rangle, \tag{38}$$

where the summation is over the four types of sites. After analytic continuation on the frequencies, we obtain the following RPA expression for the transverse dynamical susceptibility:

$$\chi^{+-}_{3\mathrm{D}}(\mathbf{k},\vec{k}_{\perp})=\frac{\chi^{+-}(\mathbf{k})[1+\mathsf{N}_1(\vec{k})\chi^{+-}(\mathbf{k})]}{\{1-2\mathsf{J}(\vec{k})\chi^{+-}(\mathbf{k})+\mathsf{N}_2(\vec{k})[\chi^{+-}(\mathbf{k})]^2\}}, \tag{39}$$

where $\mathbf{k}=(\omega,k_x)$ and

$$\mathsf{N}_1(\vec{k})=\mathsf{I}(\vec{k})-\mathsf{J}(\vec{k}),$$

$$\mathsf{N}_2(\vec{k})=\mathsf{J}^2(\vec{k})-\mathsf{K}^2(\vec{k})-\mathsf{I}^2(\vec{k}). \tag{40}$$

The RPA critical temperature as well as the incommensurability are then determined through the instability condition obtained by annihilating the denominator of Eq. (39)

$$[\mathsf{J}(\vec{k})\pm\sqrt{\mathsf{K}^2(\vec{k})+\mathsf{I}^2(\vec{k})}]\chi^{+-}(0,k_x)=1. \tag{41}$$

The relevant instability corresponds to the higher possible temperature. In order to solve Eq. (41) for it, one can maximize the left-hand side of Eq. (41) over $\vec{k}$. Then one deduces that the instability occurs along the chains direction $k_y=k_x/2$ and that $k_z=\pi$ (Néel order in the third direction). Then k_x and T_c have to be determined numerically.

We have assumed that the main instability is given by transverse excitations. So we need not calculate the longitudinal RPA propagator to calculate the RPA instability condition. However, it participates to the next-to-leading order correction and we shall need it later. Eq. (14) is still valid under its matrix form

$$[\mathbb{G}^{zz}]^{-1}=\mathbb{C}^{(2)}_{zz}+[2\,\mathbb{J}^{zz}_{\perp}]^{-1}. \tag{42}$$

The four components of the vectorial space in which it is defined correspond to the z component of the four distinct spins in an elementary cell. We have $\mathbb{C}^{(2)}_{zz}=C^{(2)}_{zz}\mathbb{I}_4$ and

$$\mathbb{J}^{zz}_{\perp}=\begin{bmatrix} 0 & \mathsf{J} & \mathsf{I} & 0 \\ \mathsf{J} & 0 & 0 & \mathsf{I} \\ \mathsf{I} & 0 & 0 & \mathsf{J} \\ 0 & \mathsf{I} & \mathsf{J} & 0 \end{bmatrix}. \tag{43}$$

B. First correction to RPA

In the complex spin representation which is more convenient in the case of Cs_2CuCl_4, the (matrix) dynamical magnetic susceptibilities are after Eq. (11):

$$\chi^{+-}_{3D}(\mathbf{k},\vec{k}_{\perp})=\frac{\chi^{+-}_{1D}(\mathbf{k})+\Sigma^{+-}(\mathbf{k},\vec{k}_{\perp})}{1-\mathbb{J}^{+-}_{\perp}(\vec{k})[\chi^{+-}_{1D}(\mathbf{k})+\Sigma^{+-}(\mathbf{k},\vec{k}_{\perp})]},$$

$$\chi^{zz}_{3D}(\mathbf{k},\vec{k}_{\perp})=\frac{\chi^{zz}_{1D}(\mathbf{k})+\Sigma^{zz}(\mathbf{k},\vec{k}_{\perp})}{1-2\,\mathbb{J}^{zz}_{\perp}(\vec{k})[\chi^{zz}_{1D}(\mathbf{k})+\Sigma^{zz}(\mathbf{k},\vec{k}_{\perp})]}. \tag{44}$$

Because of the staggering of the DM vector from one plane to another, there is no chirality on the three-dimensional spin correlation functions and $\chi^{+-}_{3D}(\mathbf{k},\vec{k}_{\perp})=\chi^{-+}_{3D}(\mathbf{k},\vec{k}_{\perp})$.

In the particular case of the first correction (Hartree-Fock-like correction), the matrix $\Sigma^{+-}_{(1)}$ appears to be diagonal. Indeed, it is made up of a single four-point correlation function which involves four spins belonging to one type of sites (among four). This does not hold at higher order. As a consequence, we may see $\Sigma^{+-}_{(1)}$ as a number which is given by

$$\begin{aligned}\Sigma^{+-}_{(1)}(\mathbf{k},\vec{k}_{\perp})=\frac{A^2}{\beta}\sum_n\int_{-\infty}^{\infty}\frac{dq_x}{2\pi}\Bigg[\left(\frac{1}{8}C^{(4)}_{xxxx}+\frac{1}{4}C^{(4)}_{xxyy}\right)(\mathbf{k},\\ -\mathbf{k},\mathbf{q}_n,-\mathbf{q}_n)\times\int_0^{2\pi}\frac{d\vec{q}_{\perp}}{(2\pi)^2}[2\,G^{+-}](\mathbf{q}_n,\vec{q}_{\perp})\Bigg]\\ +\frac{A^2}{\beta}\sum_n\int_{-\infty}^{\infty}\frac{dq_x}{2\pi}\Bigg[\frac{1}{4}C^{(4)}_{xxyy}(\mathbf{k},-\mathbf{k},\mathbf{q}_n,-\mathbf{q}_n)\\ \times\int_0^{2\pi}\frac{d\vec{q}_{\perp}}{(2\pi)^2}G^{zz}(\mathbf{q}_n,\vec{q}_{\perp})\Bigg].\end{aligned} \tag{45}$$

The three terms in $\Sigma^{+-}_{(1)}(\mathbf{k},\vec{k}_{\perp})$ are derived from the diagrams in Fig. 6. The integrals over k_y and k_z are performed over an extended Brillouin zone (from $(k_y,k_z)\in[0,\pi]^2$ to $(k_y,k_z)\in[0,2\pi]^2$) and the propagators expressions below take this extended scheme into account. A similar expression can be obtained for $\Sigma^{zz}_{(1)}$ but is useless for our purpose.

The RPA-dressed propagators $G^{+-}(\mathbf{q}_n,\vec{q}_{\perp})$ and $G^{zz}(\mathbf{q}_n,\vec{q}_{\perp})$ can be derived from Eqs. (34) and (42):

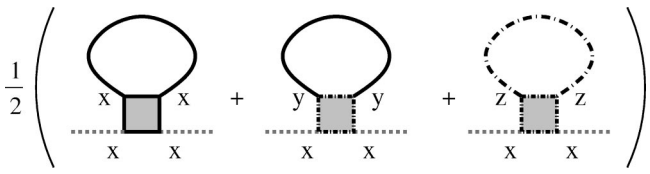

FIG. 6. Hartee-Fock diagrams with symmetry factors which are the first non-trivial terms of the self-energy $\Sigma^{+-}(\omega,\vec{k})$. The full line propagator is associated with G^{+-}, whereas the dashed-dotted line corresponds to G^{zz}. The full line box is associated with $C^{(4)}_{xxxx}$ whereas the dashed-dotted line box corresponds to $C^{(4)}_{xxyy}$.

$$G^{+-}=\frac{\mathsf{J}+(\mathsf{J}^2-\mathsf{K}^2-\mathsf{I}^2)C^{+-}_{(2)}}{1+2\,\mathsf{J}\,C^{+-}_{(2)}+(\mathsf{J}^2-\mathsf{K}^2-\mathsf{I}^2)[C^{+-}_{(2)}]^2},$$

$$G^{zz}=\frac{2(\mathsf{J}+\mathsf{I})}{1+2(\mathsf{J}+\mathsf{I})C^{zz}_{(2)}}, \tag{46}$$

where $C^{zz}_{(2)}=C^{+-}_{(2)}/2$ is the time-ordered imaginary-time spin-spin correlation function of the isolated Heisenberg chains. When the temperature approaches the theoretical critical temperature, we expect the second contribution to the self-energy correction $\Sigma^{+-}_{(1)}$ (which depends on G^{zz}) to be quantitatively much smaller than the first contribution depending on G^{+-}. Indeed the RPA propagator G^{zz} has an RPA critical temperature (its pole in T) much higher than the one for G^{+-}. It is therefore much less singular that the latter in the temperature range of interest. This has been checked numerically.

In the case of such a frustrated system, it is less clear what the small expansion parameter is. However, we can get a rough idea on inspecting the next-to-leading order correction. First of all there is a prefactor $(A/T)^2$, given by each RPA line. In addition there is a dimensionful contribution coming from the transverse lattice structure factor which depends on the interchain exchange couplings. But contrary to cubic lattices, it cannot be meaningfully extracted from the integral. The RPA-dressed propagator G^{+-} appearing in the integral is more singular at $(T_c,\vec{k}_0)$ estimated thanks to RPA. The integral value will therefore be dominated by the value of the integrands when $\vec{k}\simeq\vec{k}_0$, when T is close to T_c. So, at least when T is close to T_c, the expansion parameter is of the order of $[A\,J_{\perp}(\vec{k}_0)/T]^2$. As a consequence, in the case of frustrated quasi-one-dimensional magnet leading at the transition to an incommensurate order, $A\,J_{\perp}/T$ does not necessarily have to be small provided $A\,J_{\perp}(\vec{k}_0)/T$ is. Note that the small parameter in the RPA formula is genuinely $A\,J_{\perp}(\vec{k}_0)/T$.

After analytic continuation, we obtain the following expression for the transverse dynamical susceptibility:

$$\chi^{+-}_{3D}(\mathbf{k},\vec{k}_{\perp})=\frac{\chi^{+-}_{1D}(\mathbf{k})[1+\mathsf{N}_1(\vec{k})X(\mathbf{k})]}{\{1-2\mathsf{J}(\vec{k})X(\mathbf{k})+\mathsf{N}_2(\vec{k})[X(\mathbf{k})]^2\}}, \tag{47}$$

with $X(\mathbf{k})=\chi^{+-}_{1D}(\mathbf{k})+\Sigma^{+-}_{(1)}(\mathbf{k})$. The instability condition at this order is therefore

$$[\mathsf{J}(\vec{k}) \pm \sqrt{\mathsf{K}^2(\vec{k}) + \mathsf{I}^2(\vec{k})}]X(0,k_x) = 1. \quad (48)$$

Because at this order $\Sigma(\mathbf{k},\vec{k}_\perp)$ does not depend on $\vec{k}_\perp$, it is as easy as in the RPA case to maximize the left-hand side on $\vec{k}_\perp$. It leads again to a longitudinal instability and a Néel order from one plane to another.

C. Numerical results

The numerical computations performed to evaluate the critical temperature T_c as well as the incommensurability, are more involved than in the cubic lattice case, where it is obvious that a Néel order prevails below T_c. The instability condition has to be solved with respect to T_c and k_0. The self-energy correction itself, once the obvious dimensionful prefactor has been put aside, depends on the temperature T through the RPA propagator and depends on the ratio k_0/T through the four-point correlation function. An iterative algorithm on (T_c, k_0) can nevertheless be used. The small parameter of the expansion close to the transition is $(-\mathsf{J} + \sqrt{\mathsf{K}^2+\mathsf{I}^2})(\pi + k_0) \times A/T \simeq 0.4$.

Our findings are the following. The critical temperature is estimated to be $T_c = 0.66$ K to be compared to the experimental result $T_c = 0.62$ K. The incommensurability is estimated to be $k_0 = 0.182$ to be compared to the experimental result $k_0 = 0.186$. Therefore those values compare quite remarkably with the experimental ones.

This in return validates the rougher estimates from RPA (Ref. 4) which were already quite satisfying. It makes it improbable for the success of RPA applied to quasi-one-dimensional magnets to be merely due to chance.

VI. SUMMARY AND CONCLUSIONS

We have shown that recent one-dimensional exact results from integrable models and quantum field theory can be applied to quasi-one-dimensional spin-1/2 antiferromagnets to compute quantities such as critical Néel temperatures. Their computation can be made systematic in perturbation theory. On rough grounds, it can be seen as a high-temperature expansion in $J_\perp/T$. To the next-to-leading order, the leading order being the random-phase approximation, the errors committed differ by less than 10% from the experimental values at least in the two cases investigated above. Although those observables are nonuniversal, the calculation only depends on the magnetic Hamiltonian, i.e., exclusively on the knowledge of the exchange couplings. Even incommensurate order parameter can be accurately determined this way. At least this has be shown on the case of the frustrated compound Cs_2CuCl_4.

The perturbation theory allows more generally to give a perturbative estimation of the three-dimensional dynamical susceptibility. But it could as well be used to calculate corrections to multispin three-dimensional correlation functions starting from the one-dimensional functions.

A test of this perturbation theory could be provided by quantum Monte Carlo simulations for $S = 1/2$ cubic lattices for a reasonably weak value of the ratio $J_\perp/J_\parallel$. It is somehow hazardous to go beyond the next-to-leading order mainly used in this work. Although the numerical calculations for higher-order corrections are achievable, the resulting corrections are likely to be within the field theory approximation error range. The spin two-point correlation functions are indeed only asymptotically exact. Being more precise would require to go beyond the knowledge of the (mathematical) equivalent of the correlations at large distances. For example, one could include the space-dependent renormalization group corrections.[10,27]

Finally, the perturbation theory could be applied to determine other quantities of interest. For example, it might be useful to determine the lifetime of the theoretically predicted[3] and experimentally observed[28] longitudinal mode in the ordered phase of $KCuF_3$. Indeed the next-to-leading order correction to RPA is expected to yield an imaginary part in the self-energy and hence a damping of the mode.

ACKNOWLEDGMENTS

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