Inelastic Neutron Scattering Signal from Deconfined Spinons in a Fractionalized Antiferromagnet

C. Lannert[1] and Matthew P. A. Fisher[2]
[1] *Department of Physics, University of California, Santa Barbara, CA 93106*
[2] *Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106–4030*
(August 26, 2005)

We calculate the contribution of deconfined spinons to inelastic neutron scattering (INS) in the fractionalized antiferromagnet (AF^*), introduced elsewhere. We find that the presence of free spin-1/2 charge-less excitations leads to a continuum INS signal above the Néel gap. This signal is found above and in addition to the usual spin-1 magnon signal, which to lowest order is the same as in the more conventional confined antiferromagnet. We calculate the relative weights of these two signals and find that the spinons contribute to the longitudinal response, where the magnon signal is absent to lowest order. Possible higher-order effects of interactions between magnons and spinons in the AF^* phase are also discussed.

I. INTRODUCTION

Theories of spin-charge separation in the high-T_c cuprates have been hotly debated almost since the original discovery of these materials [1]. Finding a theory of electrons in more than one spatial dimension which exhibits zero-temperature spin-charge separation has proved to be as theoretically challenging as it is phenomenologically appealing [2]. It can be argued that all such theories will admit, in the low-energy limit, a formulation in terms of a Z_2 gauge theory [3]. Recent papers have addressed the problem of finding microscopic models of electrons which become fractionalized in some range of their parameters [4]. It remains an important task to enumerate concrete, experimentally- measurable consequences of these exciting theoretical ideas. Previously, we have explored the consequences of two-dimensional fractionalization on the spectral function, as probed by angle-resolved photo-emission spectroscopy [5]. In this paper, we calculate the inelastic neutron scattering signal from spinons in a fractionalized antiferromagnet (AF^*). We find that these spin-1/2, charge-less excitations lead to a continuum of excitations above a gap. Because we are interested in the parent insulators of cuprate superconductors, we have taken a phenomenological model for the spinons which gives them both a Néel gap arising from antiferromagnetic ordering and a d-wave pairing gap which becomes the pseudogap at moderate doping and the superconducting gap in the superconducting phase. We contrast this signal with the signal from excitations in a conventional antiferromagnet and calculate the strength of the spinon signal compared to the magnon signal (which is also present). This comparison estimates the feasibility of measuring this anomalous signal in the parent insulators. We also discuss higher-order effects stemming from interactions between spinons and magnons.

II. THE MODEL

The AF^* phase has been discussed elsewhere [6–8] and here we use the same phenomenological model introduced and justified [5,6] previously. We assume that the steps of: (1) deriving a lattice Hamiltonian containing all important effective interactions between electrons and (2) splitting the electron into chargon and spinon fields ($c_{i\alpha} = b_i f_{i\alpha}$) and deriving the appropriate Z_2 gauge theory have been performed and we have arrived at the following effective low-energy Hamiltonian for the system in 2-dimensional fractionalized phases:

$$H = \sum_{<ij>} [-t_s \hat{f}^\dagger_{i\alpha}\hat{f}_{j\alpha} + \Delta_{ij}\hat{f}_{i\uparrow}\hat{f}_{j\downarrow} - t_c \hat{b}^\dagger_i \hat{b}_j + H.c.] + U\sum_i [\hat{b}^\dagger_i \hat{b}_i - (1-x)]^2 + H_g, \tag{1}$$

$$H_g = g \sum_{<i,j>} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j, \tag{2}$$

where the spinon pairing Δ_{ij} is taken to be d-wave:

$$\Delta_{ij} = \begin{cases} +\Delta & \text{along } \hat{x}, \\ -\Delta & \text{along } \hat{y}, \end{cases} \tag{3}$$

and the spin operator is $\hat{\mathbf{S}}_i = \frac{1}{2}\hat{f}^\dagger_i \boldsymbol{\sigma} \hat{f}_i$. Here, $<i,j>$ are nearest neighbors on a 2d square lattice. The U term is a Hubbard-like interaction for $(1-x)$ chargons per unit cell.

We now briefly justify this model for the underdoped cuprate materials on phenomenological grounds. For sufficiently small doping and low temperatures such that the Z_2 theory exhibits fractionalization, the Hamiltonian is as written in Eq.(1). At temperatures below the energy scale Δ, the spinons are effectively paired into d-wave singlets and there is a d-wave gap to spin-1/2 excitations. For large enough g (and an additional minuscule 3d spin coupling) the system develops long-range antiferromagnetic order. At half-filling, the chargons are gapped into an insulating phase and we obtain a fractionalized insulator with long-range Néel order and an additional d-wave gap to spin-1/2 excitations, previously dubbed AF^* [6]. Moving away from half-filling, the antiferromagnetic order will be quickly suppressed, while for $t_c \ll U$ and with an additional long-range Coulomb interaction, one still expects the chargons to be insulating. We then have a fractionalized insulating phase with a d-wave gap to spin-1/2 excitations. Within a spin-charge separation scenario, this phase is identified with the pseudogap regime in the cuprates. For chargon hopping, t_c, sufficiently large, the chargons Bose condense, giving a d-wave superconductor. At large dopings, we expect the system to recover Fermi liquid properties, as occurs when the vortex excitations (visons) in the Ising gauge field condense thereby confining the spinons and chargons to form the electron. A schematic phase diagram is shown in Fig. 1. In this paper, we elucidate further some of the properties of the AF^* phase, found at half-filling.

Recent experiments by Bonn, Moler,*et al* put limits on the likelihood of this sort of spin-charge separation in $YBa_2Cu_3O_{6+x}$, although the experiments have only been performed on one sample so far [9]. The question of spin response in an antiferromagnet which is fractionalized is nevertheless well-posed and could be relevant to other materials. Also, it is quite possible that some other sort of exotic order lurks in the cuprates; this work would then serve as an illustrative calculation.

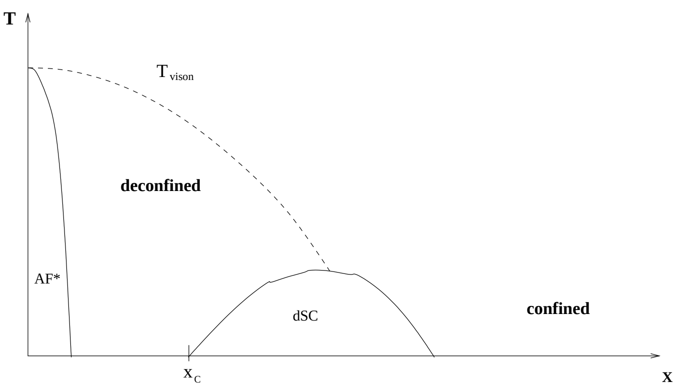


FIG. 1. Schematic phase diagram for the high T_c cuprates within a spin-charge separation scenario.

III. EFFECTIVE HAMILTONIAN FOR THE SPIN SECTOR

In this paper we work at half-filling, where the charge degrees of freedom will be gapped into a Mott insulating phase, and calculate the spin response of the system, appropriate for magnetic probes such as neutron scattering. Hence, from here on, we assume that the relevant piece of the Hamiltonian in Eq.(1) is that containing the spin degrees of freedom and we ignore the charge degrees of freedom. At temperatures much less than the vison energy, the chargons and spinons are essentially non-interacting, so this is reasonable in a fractionalized phase.

H_g (Eq.(2)) may be decoupled in a path integral, using a Hubbard-Stratonovich transformation. This gives us the following low-energy theory for the spin sector:

$$\begin{aligned} H_{spin} = &\sum_{<i,j>} [-t_s \hat{f}_i^\dagger \hat{f}_j + \Delta_{ij} \hat{f}_{i\uparrow} \hat{f}_{j\downarrow} + H.c.] \\ &-g \sum_{i \in A,\mu} \mathbf{N}_{i,\mu} \cdot \left(\hat{\mathbf{S}}_i - \hat{\mathbf{S}}_{i+\mu} \right) + \frac{g}{2} \sum_{i \in A,\mu} (\mathbf{N}_{i,\mu})^2, \end{aligned} \tag{4}$$

where $\mathbf{N}$ is a 3-component vector of classical fields living on the nearest-neighbor links of the lattice, which we have broken into its two square sublattices, labeled A and B and shown in Fig. 2. $\mu \in \{\pm\hat{x}, \pm\hat{y}\}$.

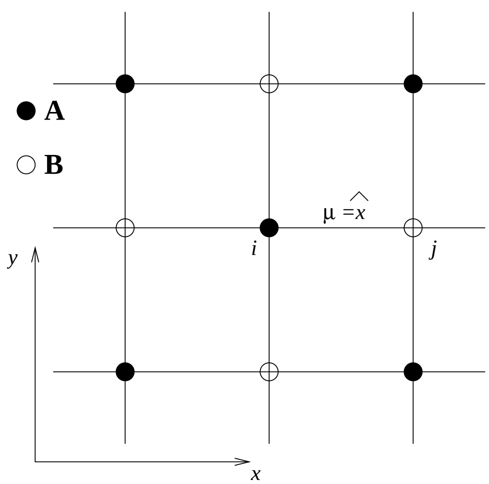


FIG. 2. The 2d square lattice with sublattices A and B marked.

We begin by analyzing Eq.(4) at the mean field level. We find antiferromagnetic Néel ordering and a quadratic theory for the spinons which can be solved exactly. We derive a self-consistency equation for the mean field approximation which connects the magnitude of the Néel order to properties of the spinons. Fluctuations about this mean field solution lead to spin-waves (as in the conventional antiferromagnet). Thus, we find that the fractionalized antiferromagnetic phase has two spin-carrying excitations: the spin-1 magnons and the spin-1/2 spinons, which interact with each other. To deal with these interactions, we treat the spinons as a perturbation: setting $t_s = \Delta = 0$, one recovers the conventional antiferromagnet and its spin-wave excitations. Integrating out the spinons to each order in t_s/g and Δ/g would give modifications of the spin-wave theory due to the spinons. If one wishes to find higher-order properties of the spinons, one may start with the mean field result and then integrate out the magnons, generating interactions between the spinons. In the limit $t_s, \Delta \ll g$, it is clear that the theory in Eq.(4) can be solved in a controlled fashion.

A. Mean Field Theory

First, we ignore the spinons, setting $t_s = \Delta = 0$ and reducing $\hat{\mathbf{S}}_i$ to the usual spin-1/2 quantum operator. Eq.(4) becomes:

$$H_g^{\mathit{eff}} = \frac{g}{2}\sum_{i\in A}\sum_{\mu}\mathbf{N}_{i,\mu}\cdot\mathbf{N}_{i,\mu} - g\sum_{i\in A}\sum_{\mu}\mathbf{N}_{i,\mu}\cdot\left(\hat{\mathbf{S}}_i - \hat{\mathbf{S}}_{i+\mu}\right). \tag{5}$$

Choosing $\hat{z}$ as the spin quantization axis, this is minimized classically by:

$$\hat{\mathrm{S}}_i^z|\uparrow\rangle_{i\in A} = \frac{1}{2}|\uparrow\rangle_{i\in A}, \tag{6}$$

$$\hat{\mathrm{S}}_j^z|\downarrow\rangle_{j\in B} = -\frac{1}{2}|\downarrow\rangle_{j\in B}, \tag{7}$$

leading to a Hamiltonian for the field $\mathbf{N}$:

$$H_g^{\mathit{eff}} = \frac{g}{2}\sum_{i\in A}\sum_{\mu}(\mathbf{N}_{i,\mu})^2 - g\sum_{i\in A}\sum_{\mu}\mathrm{N}_{i,\mu}^z. \tag{8}$$

This is minimized by: $\langle\mathrm{N}_{i,\mu}^z\rangle \equiv N_0 = 1\,\forall\, i,\mu$.

Plugging this mean field solution for $\mathbf{N}$ back into Eq.(4) gives a Hamiltonian for the spin sector at the mean field level which is quadratic in the spinons:

$$H_{spin}^{\mathrm{MFT}} = \sum_{<i,j>}[-t_s\hat{f}_{i\alpha}^\dagger\hat{f}_{j\alpha} + \Delta_{ij}\hat{f}_{i\uparrow}\hat{f}_{j\downarrow} + H.c.] - 4g\sum_i N_0\hat{z}\cdot\hat{\mathbf{S}}_i^{\boldsymbol{\pi}} + \frac{g}{2}\sum_{i\in A,\mu}N_0^2, \tag{9}$$

where we have retained $\hat{z}$ as the spin quantization axis and have written $\sum_i(-1)^{x+y}\hat{\mathbf{S}}_i \equiv \sum_i\hat{\mathbf{S}}_i^{\boldsymbol{\pi}} = \frac{1}{2}\sum_{\mathbf{k}}\hat{f}_{\mathbf{k}+\boldsymbol{\pi}}^\dagger\boldsymbol{\sigma}\hat{f}_{\mathbf{k}}$. The lattice spacing has been set to unity.

The full solution to this quadratic spinon Hamiltonian has been given elsewhere [5,10] and here we reproduce only the dispersion:

$$\mathcal{E}_{\mathbf{k}}^2 = N_g^2 + \epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2, \tag{10}$$

with

$$N_g = 2gN_0, \tag{11}$$

$$\epsilon_{\mathbf{k}} = -2t_s(\cos k_x + \cos k_y), \tag{12}$$

$$\Delta_{\mathbf{k}} = -\Delta(\cos k_x - \cos k_y). \tag{13}$$

B. Self-Consistency of the Mean Field Solution

The mean field solution with $N_0 = 1$ is found formally in the limit $t_s = \Delta = 0$, and one expects the spinons to reduce the Néel order from this maximum value. We therefore take a mean field solution of the form $\langle\mathrm{N}_{i,\mu}^z\rangle = N_0$ and demand that it be a saddle point of the full theory, Eq.(9):

$$Z[N_0] = \mathrm{Tr}_{\{\hat{f},\hat{f}^\dagger\}}e^{-\beta H^{\mathrm{MFT}}[N_0,\hat{f},\hat{f}^\dagger]}, \tag{14}$$

$$Z[N_0] \equiv e^{-S^{\mathrm{MF}}[N_0]}. \tag{15}$$

Tracing out the quadratic spinons gives an expression for $S^{\mathrm{MF}}[N_0]$ and the saddle point condition, $\delta S^{\mathrm{MF}}/\delta N_0 = 0$, gives a self-consistent equation for N_0. At zero temperature, this is:

$$1 = 2g\int\frac{d^2k}{(2\pi)^2}\,\frac{1}{\mathcal{E}_k[N_0]}, \tag{16}$$

with $\mathcal{E}_k[N_0]$ given in Eq.(10).

It is easy to check that for $t_s = \Delta = 0$, Eq.(16) gives $N_0 = 1$. For $t_s, \Delta \ll g$, one finds the perturbative result:

$$N_0 \simeq 1 - \frac{(2t_s)^2 + \Delta^2}{8g^2} + \cdots. \tag{17}$$

At large values of t_s/g and Δ/g, one expects the spinons to drive the Néel order to zero, even at zero temperature. In order to keep our calculations controlled, we work in the limit $t_s, \Delta \ll g$ and treat the spinons as a perturbation. The reasonableness of this limit for the physical systems in question will be discussed later.

C. Fluctuations About the Mean Field

We see from the self-consistent mean field calculation of the previous section that the Néel order is reduced at zero temperature by the spinons. Even in the absence of the spinons (i.e. in the pure-spin model with $t_s = \Delta = 0$) we know that fluctuations in the order parameter are important and lead to magnons. This suggests the following program for calculating the spin excitations in AF^* beyond the mean field level. First, set $t_s = \Delta = 0$ and work with the spin-1/2 quantum operator, $\hat{\mathbf{S}}_i$. "Integrating out" these operators on each site leads to an effective theory of fluctuations in the field $\mathbf{N}$ and gives the spin-wave dispersion. Then, one may integrate out the spinons perturbatively in t_s/g and Δ/g. This will lead to interactions between the magnons and give corrections to the magnon dispersion.

With t_s and Δ set to zero, the effective spin Hamiltonian, Eq.(4), reduces to $H_g^{\mathit{eff}}[\mathbf{N},\hat{\mathbf{S}}]$, Eq.(5). In this section we look at fluctuations of the field $\mathbf{N}$ around the mean field solution. We therefore set $\mathrm{N}^z = 1$ on all links and look at the fluctuations, $\mathbf{N} - \hat{z}\mathrm{N}^z \simeq \mathbf{N}^\perp$. H_g^{eff} can then be written in the following form:

$$H_g^{eff} = \frac{g}{2}\sum_{i\in A}\sum_{\mu}\left(\mathbf{N}^{\perp}_{i,\mu}\right)^2 + H^{\rm int}, \tag{18}$$

$$H^{\rm int} = H_0 + H_1, \tag{19}$$

$$H_0 = -4g\sum_{i\in A}\hat{\rm S}^z_i + 4g\sum_{j\in B}\hat{\rm S}^z_j, \tag{20}$$

$$H_1 = -g\sum_{i\in A,\mu}\hat{\mathbf{S}}^{\perp}_i\cdot\mathbf{N}^{\perp}_{i,\mu} + g\sum_{j\in B,\mu}\hat{\mathbf{S}}^{\perp}_j\cdot\mathbf{N}^{\perp}_{j-\mu,\mu}. \tag{21}$$

Integrating out the operators $\hat{\mathbf{S}}_i$ on each site amounts to performing perturbation theory in $H^{\rm int}$. To second order, the resulting effective action for $\mathbf{N}^{\perp}$ is:

$$exp\{-S^{eff}[\mathbf{N}^{\perp}]\} = {\rm Tr}_{\{\hat{\mathbf{S}}\}}e^{-\beta H_g^{eff}[\mathbf{N},\hat{\mathbf{S}}]}, \tag{22}$$

$$\begin{aligned} S^{eff}[\mathbf{N}^{\perp}] \simeq \int_0^{\infty} d\tau \Bigg[\frac{g}{2}\sum_{i\in A,\mu}|\mathbf{N}^{\perp}_{i,\mu}|^2 \\ -\frac{g}{16}\left(\sum_{i\in A}|\textstyle\sum_{\mu}\mathbf{N}^{\perp}_{i,\mu}|^2 + \displaystyle\sum_{j\in B}|\textstyle\sum_{\mu}\mathbf{N}^{\perp}_{j-\mu,\mu}|^2\right) \\ +\frac{1}{64g}\left(\sum_{i\in A}|\textstyle\sum_{\mu}\partial_\tau\mathbf{N}^{\perp}_{i,\mu}|^2 + \displaystyle\sum_{j\in B}|\textstyle\sum_{\mu}\partial_\tau\mathbf{N}^{\perp}_{j-\mu,\mu}|^2\right)\Bigg], \end{aligned} \tag{23}$$

where τ is imaginary time and we have set the temperature to zero.

Since we are interested in obtaining a long-wavelength theory for the spin-waves, we make the coarse-graining: $\mathbf{N}^{\perp}_{i,\mu} \to \mathbf{N}^{\perp}_i$, $i \in A$. This amounts to working in the basis of the Goldstone modes of the theory. With this approximation, we arrive at the effective action:

$$\begin{aligned} S^{eff}[\mathbf{N}^{\perp}] \simeq \int_0^{\infty} d\tau \Bigg[\sum_i\left(\frac{3g}{4}|\mathbf{N}^{\perp}_i|^2 + \frac{5}{16g}|\partial_\tau\mathbf{N}^{\perp}_i|^2\right) \\ +\sum_{\langle i,i'\rangle}\left(-\frac{g}{4}\mathbf{N}^{\perp}_i\cdot\mathbf{N}^{\perp}_{i'} + \frac{1}{16g}\partial_\tau\mathbf{N}^{\perp}_i\cdot\partial_\tau\mathbf{N}^{\perp}_{i'}\right) \\ +\sum_{\langle\langle i,i''\rangle\rangle}\left(-\frac{g}{8}\mathbf{N}^{\perp}_i\cdot\mathbf{N}^{\perp}_{i''} + \frac{1}{64g}\partial_\tau\mathbf{N}^{\perp}_i\cdot\partial_\tau\mathbf{N}^{\perp}_{i''}\right)\Bigg], \end{aligned} \tag{24}$$

where all sites are on the A sublattice, $\langle\cdots\rangle$ refers to nearest-neighbor pairs, and $\langle\langle\cdots\rangle\rangle$ refers to next-nearest-neighbor pairs. Fourier transforming to $\mathbf{k}$ and (imaginary) ω gives:

$$S^{eff} = \int_{\mathbf{k},\omega} g|\mathbf{N}^{\perp}(\mathbf{k},\omega)|^2\left[\left(1-\gamma^2_{\mathbf{k}}\right) + \frac{\omega^2}{4g^2}\left(1+\gamma^2_{\mathbf{k}}\right)\right], \tag{25}$$

with

$$\gamma_{\mathbf{k}} \equiv \frac{1}{2}(\cos k_x + \cos k_y). \tag{26}$$

This immediately gives the lowest-order magnon dispersion, $\omega_k = 2g\sqrt{(1-\gamma^2_k)/(1+\gamma^2_k)}$. This dispersion is similar to the usual one found using, for instance, Holstein-Primakov bosons (see, for instance, Ref. [11]), but the ratio of the spin-wave velocity to the maximum of the dispersion is different. Even neglecting spinons entirely, this is only a lowest-order result for fluctuations of the field $\mathbf{N}$. Working to higher orders in the perturbation theory of Eqns.(19-21) will generate a more realistic spin-wave theory of the conventional antiferromagnet. For the purposes of calculating the INS response, we satisfy ourselves with the lowest-order result for the magnons.

The lowest-order effect of the spinons, as we have seen in Section III B, will be to reduce $\langle {\rm N}^z\rangle$ from unity. At higher order, we expect interactions with the spinons to further affect the magnon dispersion. However, it would be wise for the purposes of comparing the magnon and spinon INS responses to take into account this over-all reduction of the Néel order by the spinons. Therefore, we make the substitution: $g \to gN_0$, where N_0 is set by the self-consistency condition, Eq.(16), giving a "self-consistent" magnon dispersion:

$$\omega_{\mathbf{k}} = 2gN_0\sqrt{\frac{1-\gamma^2_{\mathbf{k}}}{1+\gamma^2_{\mathbf{k}}}}\,. \tag{27}$$

One important consequence of this calculation is that it allows one to set the parameter g in terms of experimentally-measured properties of the magnon spectrum. Because it is probably less sensitive to details of magnon interactions, we choose to set g by the maximum of the magnon dispersion rather than by the spin-wave velocity near $\mathbf{k} = (0,0)$. In the Heisenberg model, the maximum of the magnon dispersion is $2J$; we therefore make contact with this model by identifying $J = gN_0$. Many experimental probes of the undoped cuprates find J to be around 150 meV [12–15].

IV. INELASTIC NEUTRON SCATTERING RESPONSE

What is the difference in spin response between the model given in Eq.(1) and a spin-charge confined antiferromagnet? The lowest energy spin excitations in both systems are the spin-1 magnons dictated by Goldstone's theorem in this symmetry-broken phase. For the confined insulator, the lowest-energy spin-1/2 excitations would presumably be something like single electrons, which have a huge Mott gap (on the order of a few eV in the cuprates). In contrast, we see immediately that provided one is in the regime where Eq.(1) holds (*i.e.* at temperatures and energies small compared to the vison gap), the lowest energy spin-1/2 excitations are spinons which propagate as independent excitations above the Néel (and d-wave) gap which is on the order of $J \sim 0.1$ eV. In the previous sections, we have laid out a theory of the spin degrees of freedom in a fractionalized insulator with long-range Néel order. Now, we calculate the INS signal in AF^* using the lowest-order theories of the magnons, Eq.(25), and spinons, Eq.(9).

A. Magnetic Neutron Scattering Cross-Section

The differential cross-section for neutrons scattering by wave-vector $\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i$ and energy ω off electronic spins is [16]:

$$\frac{d^2\sigma}{d\Omega d\omega} \sim \frac{|k_f|}{|k_i|} F^2(\mathbf{q}) \sum_{\alpha,\beta} \left(\delta_{\alpha\beta} - \frac{q_\alpha q_\beta}{q^2} \right) \mathcal{S}^{\alpha\beta}(\mathbf{q}, \omega) \quad (28)$$

(α,$\beta = x, y, z$), where $F^2(\mathbf{q})$ is a form factor and the spin structure factor is:

$$\mathcal{S}^{\alpha\beta}(\mathbf{q}, \omega) = \frac{1}{\pi} \frac{1}{1 - e^{-\omega/k_B T}} \mathrm{Im}\chi^{\alpha\beta}(\mathbf{q}, \omega), \quad (29)$$

where

$$\chi^{\alpha\beta}(\mathbf{q}, i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau \hat{\mathrm{S}}^\alpha_{\mathbf{q}}(\tau) \hat{\mathrm{S}}^\beta_{-\mathbf{q}}(0) \rangle \quad (30)$$

is the imaginary-time spin-spin correlation function. At temperatures such that $k_B T \ll \omega$, we can take the zero-temperature limit:

$$\frac{1}{1 - e^{-\omega/k_b T}} \to \Theta(-\omega) \quad (31)$$

with $\Theta(x)$ the Heavyside-step function. The spin-1/2 operators are given by the usual expression with electron operators replaced by spinon operators: $\hat{\mathbf{S}}(\mathbf{q}, \tau) = \sum_{\mathbf{k}} \hat{f}^\dagger_{\mathbf{q}+\mathbf{k}}(\tau) \boldsymbol{\sigma} \hat{f}_{\mathbf{k}}(\tau)$.

The model outlined in the sections above provides a theory of the spin response in AF^*. In the next section, we use the lowest-order results to calculate the magnon and spinon signals (respectively) in inelastic neutron scattering. We include a brief discussion of higher-order effects.

B. Magnon Response

Starting from the $t_s = \Delta = 0$ spin Hamiltonian, Eq.(5), it is straightforward to calculate the spin-spin response function by including a source term in the effective action of the form: $\sum_i \hat{\mathbf{S}}_i \cdot \mathbf{K}_i$. The result, to lowest order in fluctuations of $\mathbf{N}$ is:

$$\mathcal{S}^{+-}_{\mathrm{magnons}}(\mathbf{q}, \omega) = \frac{4}{(1 + \gamma^2_{\mathbf{q}})^2} \frac{(1 - \gamma_{\mathbf{q}})^2}{\sqrt{1 - \gamma^4_{\mathbf{q}}}} \delta(\omega - \omega_{\mathbf{q}}), \quad (32)$$

with $\gamma_{\mathbf{q}}$ and $\omega_{\mathbf{q}}$ given in Eqns.(26-27). While the exact form of this response function differs from that found in, say, the Holstein-Primakov formalism, it has the same universal features. By universal properties we mean that the limits of both the response function and the spin-wave dispersion as $\mathbf{q} \to (0, 0)$ and $\mathbf{q} \to (\pi, \pi)$ are the same for all calculational methods because they are dictated by symmetries. Including intra-spin-wave interactions modifies the non-universal aspects of the dispersion (*e.g.* the spin-wave velocity near $\mathbf{q} = \mathbf{0}$) and yields direct multi-magnon contributions to the spin structure factor. These direct multi-magnon processes are of a much lower weight than the single magnon processes and so we ignore them.

To first order then, the magnon response to neutron scattering in AF^* has the same universal features as in a conventional antiferromagnet. This calculation allows us to fix the parameters in our theory: we have seen in Section III C that the energy scale $gN_0 = J$ to this order. Additionally, the magnitude of the direct spinon signal can be compared with the magnitude of this well-established magnon signal.

C. Spinon Response

As detailed in Section III A, at the mean field level, the spinon part of the Hamiltonian in Eq.(1) is quadratic and has been solved elsewhere [5,10]. The spin-flip and longitudinal structure factors for the spinons are as follows:

$$\begin{aligned} \mathcal{S}^{+-}_f(\mathbf{q}, \omega) &= \int_{\mathbf{k}} \Bigg[\left(1 - \frac{\epsilon_{\mathbf{q}-\mathbf{k}}}{\mathcal{E}_{\mathbf{q}-\mathbf{k}}}\right) \left(1 + \frac{\epsilon_{\mathbf{k}}}{\mathcal{E}_{\mathbf{k}}}\right) - \frac{\Delta_{\mathbf{q}-\mathbf{k}} \Delta_{\mathbf{k}}}{\mathcal{E}_{\mathbf{q}-\mathbf{k}} \mathcal{E}_{\mathbf{k}}} \\ &\quad + \frac{N_g^2}{\mathcal{E}_{\mathbf{q}-\mathbf{k}} \mathcal{E}_{\mathbf{k}}} \Bigg] \times \delta(\omega - \mathcal{E}_{\mathbf{q}-\mathbf{k}} - \mathcal{E}_{\mathbf{k}}), & (33) \\ &= \mathcal{S}^{-+}_f(\mathbf{q}, \omega), & (34) \\ \mathcal{S}^{zz}_f(\mathbf{q}, \omega) &= \frac{1}{2} \int_{\mathbf{k}} \Bigg[\left(1 - \frac{\epsilon_{\mathbf{q}-\mathbf{k}}}{\mathcal{E}_{\mathbf{q}-\mathbf{k}}}\right) \left(1 + \frac{\epsilon_{\mathbf{k}}}{\mathcal{E}_{\mathbf{k}}}\right) - \frac{\Delta_{\mathbf{q}-\mathbf{k}} \Delta_{\mathbf{k}}}{\mathcal{E}_{\mathbf{q}-\mathbf{k}} \mathcal{E}_{\mathbf{k}}} \\ &\quad - \frac{N_g^2}{\mathcal{E}_{\mathbf{q}-\mathbf{k}} \mathcal{E}_{\mathbf{k}}} \Bigg] \times \delta(\omega - \mathcal{E}_{\mathbf{q}-\mathbf{k}} - \mathcal{E}_{\mathbf{k}}) \\ &\quad + \text{elastic (Bragg) response}, & (35) \end{aligned}$$

where $N_g, \epsilon_k, \Delta_k$, and $\mathcal{E}_k$ are defined in Eqns. (10-13).

These formulas have a few salient features. Spin-flip neutron scattering leaves a spin-1 excitation in the sample with momentum $\mathbf{q}$ and energy ω. The expression for $\mathcal{S}^{+-}_f$ simply sums the ways of destroying a spin-down (-up) spinon at momentum $-\mathbf{k}$ and creating a spin-up (-down) spinon at momentum $\mathbf{q} - \mathbf{k}$, with the constraint that the energy cost for this process must be ω. The rest of the expression is the zero-temperature probability that the state at $-\mathbf{k}$ is occupied and the one at $\mathbf{q}-\mathbf{k}$ is unoccupied, appropriate for fermions. If one takes $N_g = 0$ (corresponding to no Néel order), the full spin-rotation invariance of the spinon system is restored and $\mathcal{S}^{+-} = \mathcal{S}^{zz}$, as expected.

For INS using unpolarized neutrons, the differential cross section is a combination of these two signals, but it is possible using polarized neutrons to obtain signals from these two channels separately (albeit at a large cost to the intensity). It is worth noting that, provided one aligns the polarized neutron spins along the direction of the staggered magnetization, the signal due to single magnons is only in the "spin-flip" sector, i.e. $\mathcal{S}^{zz}_{1\ \mathrm{magnon}} = 0$. The first contribution to $\mathcal{S}^{zz}$ from spin-waves alone occurs in the two-magnon channel which is of a greatly reduced weight compared to the single magnon signal. The spinons then constitute the only magnetic signal of reasonable weight in this channel at energy scales of order J.

A discussion of parameters is wise at this point. Working in units of $gN_0 = J$, we will use $t_s = \Delta = J$ to calculate $\mathcal{S}^{\alpha\beta}$ for the spinons. This gives numerical values of these constants which are reasonable for the undoped cuprates. However, one may wonder whether they violate our above working assumptions $t_s/g, \Delta/g \ll 1$. Indeed, it is not immediately obvious how to set the parameter g. Here, we take the following tack: the quantity gN_0 is set by comparison between the magnon dispersion in Eq. (27) and the maximum of the magnon dispersion in INS experiments. This gives $gN_0 = J \simeq 150meV$. The parameters t_s and Δ may similarly be set by experiments and we use the values given above. With these two constraints, the self-consistency equation, Eq. (16), becomes an equation for the parameter g. It is clear that if the values of t_s and Δ are too large, the equation for g will have no solutions. For the parameters above, using the expansion (valid for small t_s/g and Δ/g) in Eq.(17) as a first iteration yields $g \simeq 1.4J$. Plugging the resultant values of t_s/g and Δ/g into the full self-consistent equation for N_0, the right hand side of Eq.(16) can be numerically integrated for various values of N_0. The result is shown in Fig. 3. It is clear from the graph that the value of N_0 which satisfies the self-consistent equation is $N_0 \simeq 0.7$. This gives $gN_0 = .98J \simeq J$, and we have our self-consistent parameters. We note that the value $N_0 \simeq 0.7$ is still rather close to the "no spinon" mean field value of unity, so that treating the spinons as a perturbation is somewhat justified [17].

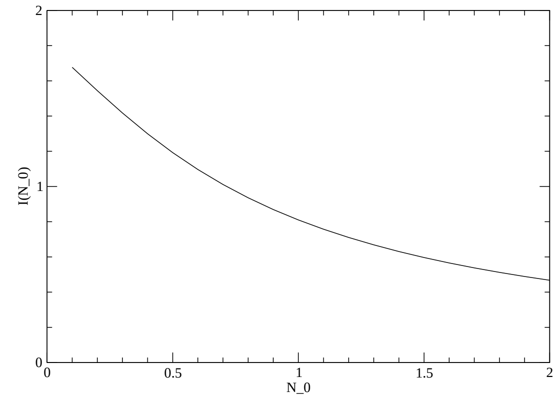


FIG. 3. Results of numerically integrating the RHS of Eq.(16), called $I(N_0)$, for $t_s/g = \Delta/g = 0.7$. The self-consistent value of N_0 is the one for which $I = 1$.

The above expression for $\mathcal{S}^{+-}_f$ can be numerically integrated to obtain the spinon response. This has been performed, approximating the δ-function in energy with a Lorentzian of width $\epsilon = 0.01J$. None of the salient features of the results were influenced by the specific values of parameters (such as t_s, Δ, ϵ).

D. INS Signal

In Figs. 5 and 6 we present the lowest-order results for $\mathcal{S}^{+-} = \mathcal{S}^{+-}_f + \mathcal{S}^{+-}_{\mathrm{magnons}}$, corresponding to spin-flip neutron scattering. All energies are in units of $J = gN_0$. Note that we have taken the staggered magnetization to point in the $\hat{z}$-direction, but since our theory does not contain terms which couple the spin and spatial variables (as, say, a spin-orbit coupling would), the spin axes can be rotated independently of the spatial axes.

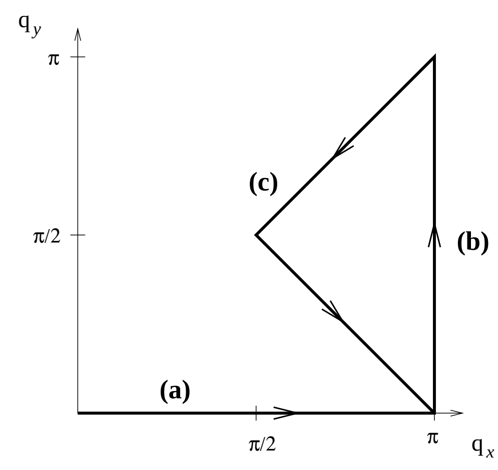


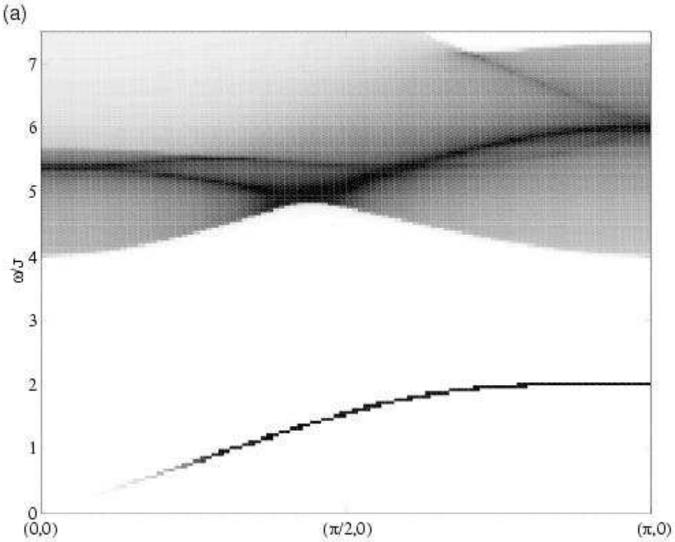
FIG. 4. Contours in the q_x, q_y plane.

As $\mathcal{S}^{\alpha\beta}(\mathbf{q},\omega)$ is a function of three variables (for the effectively two-dimensional cuprates of interest), we show here a few views of this function. Fig.5, shows contour plots of the intensity as a function of distance along cuts in the (q_x, q_y) plane (shown in Fig.4) and energy. For the magnon signal, the δ-function in Eq.(32) has been replaced with a "box" function:

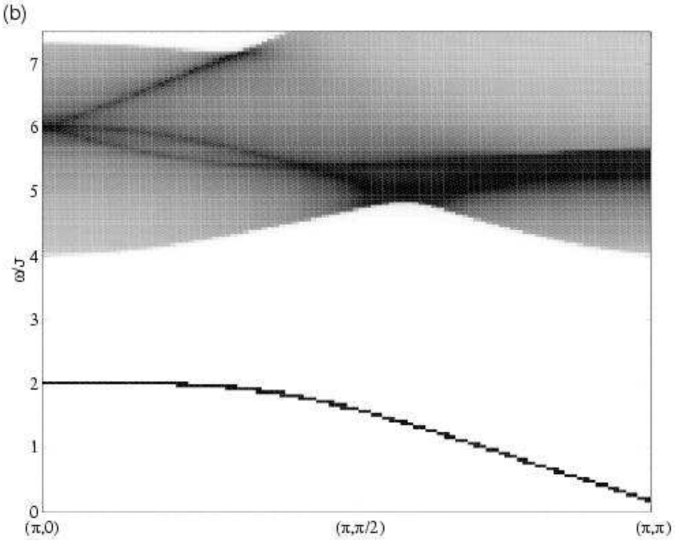
$$\delta(x) = \begin{cases} 1/\epsilon & \text{for} - \epsilon/2 < x < \epsilon/2, \\ 0 & \text{else,} \end{cases} \tag{36}$$

with $\epsilon = 0.06J \simeq 10meV$. In these plots, we see the magnon dispersion with zeros at $\mathbf{q} = (0,0)$ and (π,π) and a vanishing weight near $(0,0)$. Above this, we see the spinon continuum turn on with a lower-bound which is modulated with twice the period of the magnon dispersion. We see in this plot that the spinon signal is appreciable.

(a)



(b)



(c)

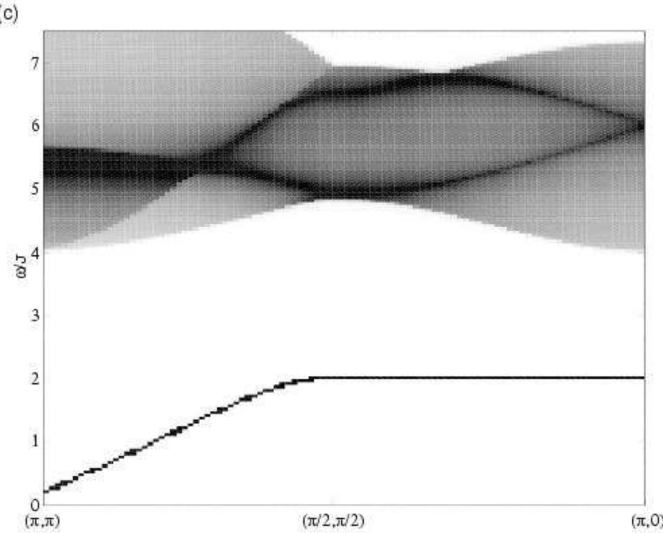
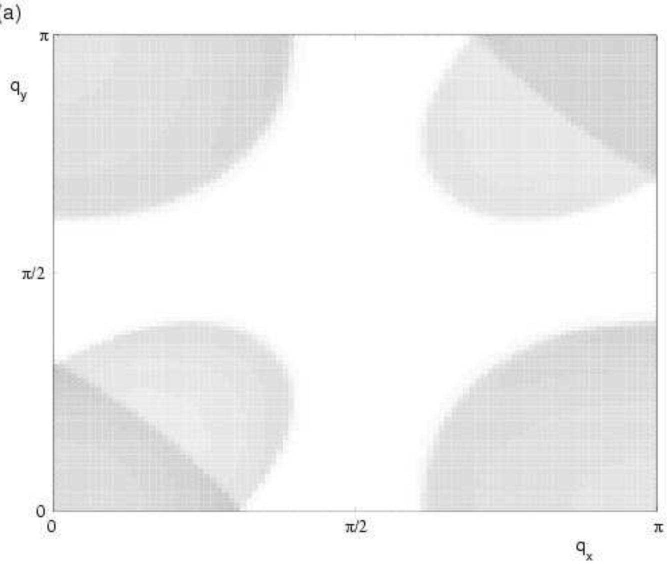


FIG. 5. $\mathcal{S}^{+-}(\mathbf{q},\omega)$ along cuts (a),(b),and (c) in Fig. 4. Energies are in units of J. White regions are zero intensity and black regions are high intensity.

In Fig.6, we show contour plots of the spinon intensity as a function of q_x and q_y at constant values of the energy. We see that the spinon intensity at turn-on ($\omega = 4J$) is largest near the corners at $(0,0)$, (π,π), etc. For comparison, Fig. 6(d) shows plots of the single magnon weight (Eq.(32)) as a function of q_x and q_y.

(a)



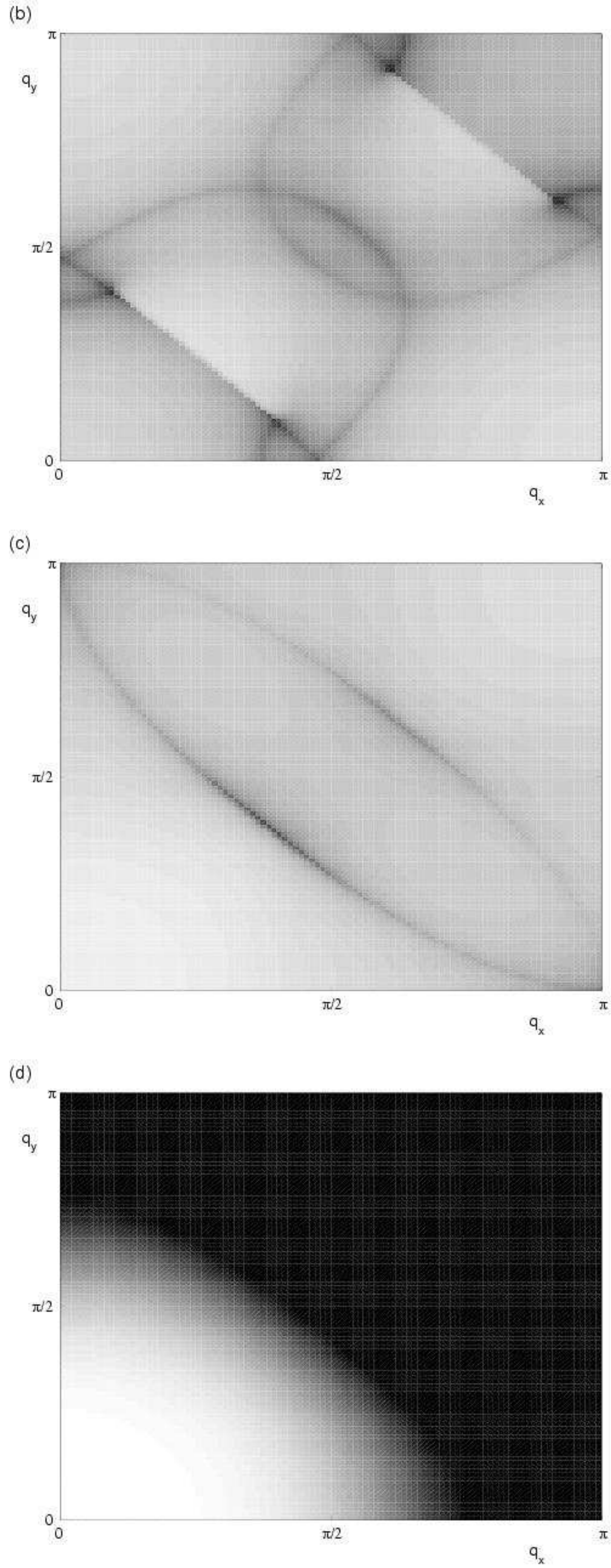


FIG. 6. Spinon $\mathcal{S}^{+-}(\mathbf{q},\omega)$ at energies ω/J = (a) 4.5 (b)5.0 (c)6.0 . The single magnon weight, Eq.(32), is shown in (d). White regions are low intensity and black regions are high intensity.

In Fig. 7 we present contour plots of $S_f^{zz}(\mathbf{q},\omega)$ sequentially along the cuts in Fig. 4. We note again that, to first order, there is no magnon contribution to this correlation function and so the two-spinon continuum visible in these plots should in principle be the primary magnetic source of INS in this channel.

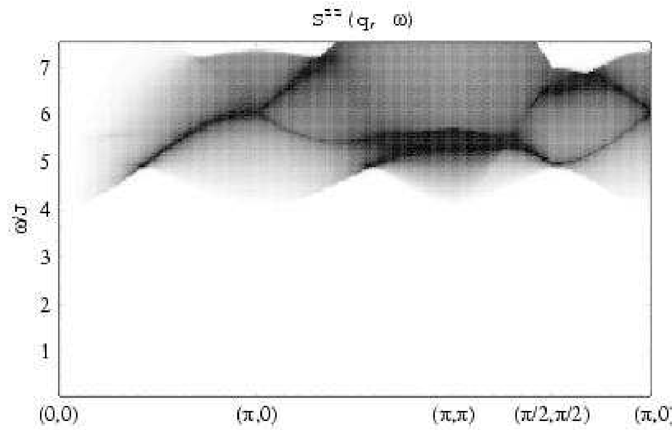


FIG. 7. $\mathcal{S}^{zz}(\mathbf{q},\omega)$ along a cut (a)+(b)+(c) in Fig. 4. Energies are in units of J and the color scheme is the same as in Figs. 5 and 6.

E. Higher Order Effects

At higher orders in the perturbation theory of Eqns. (19 -21), we would expect spin wave interactions (present and important for detailed features even when t_s and Δ are zero) to modify the magnon dispersion and lead to multi-magnon signals in both the $\mathcal{S}^{+-}$ and $\mathcal{S}^{zz}$ channels. This calculation would be the same as for a conventional antiferromagnet (since $t_s = \Delta = 0$) and would presumably lead to the actual spin-wave response in a conventional antiferromagnetic system. At higher orders in t_s/g and Δ/g, we would obtain magnon interactions mediated by spinons, which are not present in conventional antiferromagnets. Being gapped excitations, the spinons are inherently a "high energy" phenomena as far as the spin-waves are concerned. We might therefore expect them to influence most heavily the high-energy portions of the magnon dispersion. One can see from the graphs given in Section IV D that the lower edge of the spinon continuum has a minimum near $(\pi,0)$, where the magnon dispersion has one of its maxima. One would expect interactions between these two excitations to effect the dispersions most heavily near these points of closest approach. While the effect of unconventional excitations such as spinons can in principle be seen in the spin-wave response, we have chosen in this paper to focus on the direct spinon contribution to inelastic neutron scattering, shown in the previous section. The spin-waves will also affect the spinon signal at higher orders, however, probably not in any dramatic fashion.

V. CONCLUSIONS

In this paper we have presented a theory of the spin excitations of the fractionalized antiferromagnet, AF^*, in the limit where the visons can be ignored. This theory is Eq.(4). This phase has both long-ranged antiferromagnetic order and the topological order associated with fractionalization [18]. It contains two spin-carrying excitations: the spin-1 magnons and the spin-1/2 spinons, which interact with each other. The theory is well-defined and can be solved in a controlled manner in the limit $t_s/g, \Delta/g \ll 1$. In this paper, we have found the lowest-order theories of these two excitations and have calculated the dynamic spin-spin response functions of each, appropriate for inelastic neutron scattering experiments.

To lowest order, the magnon signal is the same as in a conventional antiferromagnet, but higher-order effects of the spinons should lead to modifications of the dispersion, particularly near $(\pi, 0)$. The main anomalous feature of the INS signal from AF^* is the presence of a spinon continuum at energies $\sim 4J$, which exists even in the longitudinal response, where the magnons are expected to be absent at lowest-order.

We are grateful to Gabe Aeppli, Radu Coldea, Steve Girvin, Steve Nagler, Doug Scalapino, Alan Tennant, and Senthil Todadri for helpful discussions. This research was supported by the NSF under Grants DMR-9704005 and PHY-9907949.

---

[1] P.W. Anderson, Science, **235**, 1196 (1987); S. Kivelson, D.S. Rokhsar, and J. Sethna, Phys. Rev. **B35**, 8865 (1987) .

[2] N. Read and S. Sachdev, Phys. Rev. Lett. **66**, 1773 (1991); S. Sachdev and N. Read, Int. J. Mod. Phys. B **5**, 219 (1991); R. Jalabert and S. Sachdev, Phys. Rev. **B44**, 686 (1991); S. Sachdev and Matthias Vojta, J. Phys. Soc. Japan, **69** Suppl B, 1 (2000); X.G. Wen, Phys. Rev. **B44**, 2664 (1991); C. Mudry and E. Fradkin, **B49**, 5200 (1994).

[3] T. Senthil and M.P.A. Fisher, J. Phys. A, **34**, L119 (2001); cond-mat/0008082.

[4] L. Balents, M.P.A. Fisher, and S.M. Girvin, cond-mat/0110005; T. Senthil and O. Motrunich, cond-mat/0201320.

[5] C. Lannert, M.P.A. Fisher, and T. Senthil, Phys. Rev. **B64**, 014518 (2001).

[6] T. Senthil and Matthew P.A. Fisher, Phys. Rev. **B62**, 7850 (2000).

[7] L. Balents, M.P.A. Fisher, and C. Nayak, Phys. Rev. **B60**, 1654 (1999); L. Balents, M.P.A. Fisher, and C. Nayak, Phys. Rev. **B61**, 6307 (2000).

[8] T. Senthil and M.P.A. Fisher, cond-mat/9912380; cond-mat/0008082.

[9] Wynn J.C., Bonn D.A., Gardner B.W., Lin Y.J., Liang R.X., Hardy W.N., Kirtley J.R., Moler K.A., Phys. Rev. Lett. **87**, 197002 (2001); Bonn D.A., Wynn J.C., Gardner B.W., Lin Y.J., Liang R., Hardy W.N., Kirtley J.R., Moler K.A., Nature **414**, 887-889 (2001)

[10] G.J. Chen, Robert Joynt, F.C. Zhang, and C. Gros, Phys. Rev. **B42**, 2662 (1990).

[11] A. Auerbach, *Interacting Electrons and Quantum Magnetism*, Springer-Verlag New York, New York (1994).

[12] R. Coldea, S.M. Hayden, G. Aeppli, T.G. Perring, C.D. Frost, T.E. Mason, S.-W. Cheong, and Z. Fisk, Phys. Rev. Lett. **86** 5377 (2001).

[13] K.B. Lyons, P.E. Sulewski, P.A. Fleury, H.L. Carter, A.S. Cooper, G.P. Espinosa, Z. Fisk, and S.-W. Cheong, Phys. Rev. **B39**, 9693 (1989); R.R.P. Singh, P.A. Fleury, K.B. Lyons, and P.E. Sulewski, Phys. Rev. Lett. **62**, 2736 (1989); Y. Tokura, S. Koshihara, T. Arima, H. Takagi, S. Ishibashi, T. Ido, and S. Uchida, Phys. Rev. **B41**, 11657 (1990).

[14] T. Thio, T.R. Thurston, N.W. Preyer, P.J. Picone, M.A. Kastner, H.P. Jenssen, D.R. Gabbe, C.Y. Chen, R.J. Birgeneau, and A. Aharony, Phys. Rev. **B38**, 905 (1988).

[15] J. Lorenzana, J. Eroles, and S. Sorella, Phys. Rev. Lett. **83** 5122 (1999).

[16] G.L. Squires, *Introduction to the Theory of Thermal Neutron Scattering*, Cambridge University Press, Cambridge, 1978.

[17] Indeed the values $t_s/g = \Delta/g = 0.7$, while not $\ll 1$, are at least < 1.

[18] T. Senthil and M.P.A. Fisher, cond-mat/0008082.