Magnetic ordering in doped coupled frustrated quantum spin-$1/2$ chains with 4-spin exchange.

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Abstract

The role of various magnetic inter-chain couplings has been investigated recently by numerical methods in doped frustrated quantum spin chains. A non-magnetic dopant introduced in a gapped spin chain releases a free spin-1/2 soliton. The formation of a local magnetic moment has been analyzed in term of soliton confinement. A four-spin coupling which might originate from cyclic exchange is shown to produce such a confinement. Dopants on different chains experience an effective space-extended non-frustrating pairwise spin interaction. This effective interaction between impurity-spins is long-ranged and therefore is expected to play a crucial role in the mechanism of antiferromagnetic (AF) long-range ordering (LRO) observed in spin-Peierls (SP) compounds such as CuGeO$_3$ doped with non-magnetic impurities.

Key words: Quantum magnetism, Impurities effect, spin-Peierls systems.

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1. Introduction

Doping a spin liquid system with non-magnetic impurities leads to very surprising new features. For example in the doped quasi one-dimensional compound Cu$_{1-x}$M$_x$GeO$_3$ (M=Zn or Mg), the discovery of coexistence between dimerization and AF LRO at small impurity concentration $x$ has motivated extended experimental [1] and theoretical [2,3,4,5,6,7] investigations. The impurity-induced AF LRO has been observed in other doped spin liquid materials such as the 2-legs ladder Sr(Cu$_{1-x}$Zn$_x$)$_2$O$_3$ [8], the Haldane compound Pb(Ni$_{1-x}$Mg$_x$)$_2$V$_2$O$_8$ [9] or the coupled spin dimer system TiCu$_{1-x}$Mg$_x$Cl$_3$ [10].

Replacing a spin-$1/2$ in a spontaneously dimerised (isolated) spin chain by a non magnetic dopant (described as an inert site) liberates a free spin $1/2$, named a soliton, which does not bind to the dopant [2]. On the other hand, a static bond dimerisation produces an attractive potential between the soliton and the dopant [2,3] and consequently leads, under doping, to the formation of local magnetic moments [2,5] as well as a rapid suppression of the spin gap [4]. However, a coupling to a purely one-dimensional (1D) adiabatic lattice [6] does not produce confinement in contrast to more realistic models including an elastic inter-chain coupling (to mimic 2D or 3D lattices) [6,7].

Frustration and inter-chains effects are necessary to understand the impurity-induced AF ordering in the doped spin-Peierls (SP) material Cu$_{1-x}$M$_x$GeO$_3$. In section 2 we report numeri-
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2. Impurity induced local moment

formation in doped coupled frustrated spin

Let us first consider a model of coupled frus-

trated spin-\frac{1}{2} antiferromagnetic chains (see Fig.1). Following Schulz [12], a mean-field (MF) treat-

ment of the inter-chain couplings has been per-

formed [11] and the resulting Hamiltonian is given by

\[ H_{\text{eff}}(\alpha, J_\perp, J_4) = J \sum_{i,a} \left[ (1 + \delta J_{i,a}) \mathbf{S}_{i,a} \cdot \mathbf{S}_{i+1,a} \right. 
\left. + \alpha \mathbf{S}_{i,a} \cdot \mathbf{S}_{i+2,a} + h_{i,a} \mathbf{S}_{i,a}^z + \text{constant} \right] \tag{1} \]

where

\[ h_{i,a} = J_\perp \left( \langle S_{i,a+1}^z \rangle + \langle S_{i,a-1}^z \rangle \right) \tag{2} \]

accounts for first-order effects in the inter-chain magnetic coupling \( J_\perp \), and

\[ \delta J_{i,a} = J_4 \{ \langle \mathbf{S}_{i,a+1} \cdot \mathbf{S}_{i+1,a+1} \rangle + \langle \mathbf{S}_{i,a-1} \cdot \mathbf{S}_{i+1,a-1} \rangle \} \tag{3} \]

takes a generic form because it might have multiple origins; although a four-spin cyclic ex-

change [13,14] provides the most straightforward derivation of it [11], \( J_4 \) can also mimic higher or-

der effects in \( J_\perp \) [15] or the coupling to a 2D (or 3D) lattice [6]. \( i \) is a lattice index along the chain

of size \( L \) and \( a \) labels the \( M \) chains (\( L \) and \( M \) chosen to be even). Periodic boundary conditions will

be assumed in both directions. The energy scale is

set by the coupling along the chains \( J = 1 \) and \( \alpha \) is the relative magnitude of the NNN frustrating

coupling.

In the pure case (i.e. without impurity), all the

chains are equivalent and the problem is therefore

reduced to a single chain problem in a staggered

magnetic field \( h_i = -2J_\perp < S_i^z > \) and with its

NN exchange modulated by \( \delta J_i = J_4 \langle \mathbf{S}_{i} \cdot \mathbf{S}_{i+1} \rangle \)

if \( J_4 < 0 \) or \( \delta J_i = J_4 \langle \mathbf{S}_{i+1} \cdot \mathbf{S}_{i+2} \rangle \) if \( J_4 > 0 \).

Using Lanczos ED up to the convergence of the MF

procedure [17], we can identify two different phases

in the \((\alpha, J_\perp)\) plane. A dimerised SP phase and an

AF ordered phase separated by a transition line

\( J_\perp = J_4^2(\alpha) \) (see Fig.2). ED have been performed

on small systems (\( L \leq 16 \)) for different values of \( J_4 \).

Fortunately, the finite size effects (FSE) are small

in the gapped regime. The modulation created by \( J_4 \) stabilizes the SP phase, as we can observe on

Fig.2

Let us now turn to the doped case. A non-
magnetic dopant is described here as an inert

site decoupled from its neighbors. Under doping

the system becomes non-homogeneous so that we

define a local mean staggered magnetization,

\[ M_{i,a}^{\text{stag}} = \frac{1}{4}(-1)^i \alpha \left( 2\langle S_{i,a}^z \rangle - \langle S_{i+1,a}^z \rangle - \langle S_{i-1,a}^z \rangle \right) \tag{4} \]

Following the method used in Ref. [7], the MF

equations are solved self-consistently on finite \( L \times M \) clusters and lead to a non-uniform solution. At

each step of the MF iteration procedure, we use

Lanczos ED techniques to treat exactly (although independently) the \( M \) non-equivalent finite chains

and compute \( \langle S_{i,a}^z \rangle \) for the next iteration step un-
til the convergence is eventually achieved. We first

consider the case of a single dopant. Whereas in the

case \( J_4 = 0 \) the soliton remains de-confined as can be seen from Fig.3, a very small \( J_4 \neq 0 \)
is sufficient to produce a confining string which

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{SP-AF phase diagram in the \((\alpha, J_\perp)\) plane from ED of chains of length up to 16 sites. Symbols correspond to different values of \( J_4 \geq 0 \) as indicated on plot. Typically, FSE are smaller than the size of the symbols. The computed transition lines are extended by tentative transition lines (dashed lines) in the region where FSE become large. At \( J_4 = 0 \) we have plotted a few points in the vicinity of the MG point [16] for \( L = 12 \) and \( L = 16 \) (reprinted from Ref.[11]).}
\end{figure}
binds the soliton to the dopant. Note that the interchain coupling induces a "polarization cloud" with strong antiferromagnetic correlations in the neighboring chains of the doped one; we can therefore define a typical length scale in the transverse direction $\xi_\perp$ which is $\sim 1$ in the case $J_\perp = 0.1$, as we will study in the last part of next section. A confinement length in the chain direction $\xi_\parallel$ can also be extracted. Defined by

$$\xi_\parallel = \frac{\sum_i |S_i^z|}{\sum_i |S_i^z|},$$

we have calculated it for a $16 \times 8$ system with $\alpha = 0.5$ and $J_\perp = 0.1$, and we show its variation as a function of $J_4$ in Fig.4. FSE decrease for increasing $J_4$. Note that $\xi_\parallel(J_4) \neq \xi_\parallel(-J_4)$ and a power law [3] with different exponents $\eta$ is expected when $J_4 \rightarrow 0$. A fit gives $\eta \sim 0.33$ if $J_4 < 0$ and $\eta \sim 0.50$ for $J_4 > 0$ (Fig.4). This asymmetry can be understood from opposite renormalisations of $J_4$ for different signs of $J_4$. Indeed, if $J_4 < 0$ then $\delta J_{i,a} > 0$ and the nearest neighbor MF exchange becomes larger than the bare one. Opposite effects are induced by $J_4 > 0$.

**3. Effective interaction between impurity-spins**

We now turn to the investigation of the effective interaction between dopants. Each impurity releases an effective spin $\frac{1}{2}$, localized at a distance $\sim \xi_\parallel$ from it due to the confining potential set by $J_4$. We define an effective pairwise interaction $J_{\text{eff}}$ as the energy difference of the $S = 1$ and the $S = 0$ GS. When $J_{\text{eff}} = E(S = 1) - E(S = 0)$ is positive (negative) the spin interaction is AF (ferromagnetic). Let us first consider the case of two dopants in the same chain. (i) When the two vacancies are on the same sub-lattice the moments experience a very small ferromagnetic $J_{\text{eff}} < 0$ as seen in Fig. 5 with $\Delta a = 0$ so that the two effective spins $\frac{1}{2}$ are almost free. (ii) When the two vacancies sit on different sub-lattices, $\Delta i$ is odd and the effective coupling is AF with a magnitude close to the singlet-triplet gap. Fig. 5 with $\Delta a = 0$ shows that the decay of $J_{\text{eff}}$ with distance is in fact very slow for such a configuration. The behavior of the pairwise interaction of two dopants located on different chains ($\Delta a = 1, 2, 3$) is shown in Fig. 5 for $\Delta a = 1, 2, 3$ for $J_4 > 0$. When dopants are on opposite sub-lattices the effective interaction is antiferromagnetic. At small dopant separation $J_{\text{eff}}(\Delta i)$ increases with the dopant separation as the overlap between the two AF clouds increases until $\Delta i \sim 2\xi_\parallel$. For larger separation, $J_{\text{eff}}(\Delta i)$ decays rapidly. If dopants are on the same sub-lattice, solitons are located on the same side of the dopants [18] and the effective exchange $J_{\text{eff}}(\Delta i)$ is ferromagnetic and decays rapidly to become negligible when $\Delta i > 2\xi_\parallel$. The key feature here is the fact that the effective pairwise interaction is not frustrating (because of its sign alternation with distance) although the frustration is present in the microscopic underlying model. AF ordering is then expected (at $T = 0$) as seen for a related system of coupled Spin-Peierls chains [7].

Our next step is to fit the numerical data in order to derive an analytic expression for $J_{\text{eff}}$ and a long ranged non frustration effective model for diluted
spins $\frac{1}{2}$ on a $L_x \times L_y$ square lattice,
\[ \mathcal{H}_{\text{eff}} = \sum_{\mathbf{r}_1, \mathbf{r}_2} \epsilon_{\mathbf{r}_1} \epsilon_{\mathbf{r}_2} J_{\text{eff}}(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{S}_{\mathbf{r}_1} \cdot \mathbf{S}_{\mathbf{r}_2}, \tag{6} \]
with $\epsilon_{\mathbf{r}} = 1$ ($0$) with probability $x$ ($1-x$), $x$ being the dopant concentration. Using only five parameters, two energy scales and three length scales, we can fit ED data with very simple mathematical expressions. When $\Delta \alpha = 0$ (same chain), $J^\text{eff}$ approximately fulfills $J_{\text{eff}}(\Delta \alpha, 0) = J_0 (1 - \Delta \alpha / \xi_\parallel^0)$ for $\Delta \alpha$ even and $\Delta \alpha < \xi_\parallel^0$, and $J_{\text{eff}}(\Delta \alpha, 0) = 0$ otherwise. For dopants located on different chains and on the same sub-lattice ($\Delta \alpha = 0$ even) one has,
\[ J_{\text{eff}}(\Delta \alpha, 0) = -J'_0 \exp(-\Delta \alpha / \xi_\parallel) \exp(-\Delta \alpha / \xi_\perp), \tag{7} \]
while if the dopants are on opposite sub-lattices, one gets
\[ J_{\text{eff}}(\Delta \alpha, 0) = J'_0 \frac{\Delta \alpha}{2\xi_\parallel} \exp(-\Delta \alpha / \xi_\perp), \tag{8} \]
for $\Delta \alpha \leq 2\xi_\parallel$ and
\[ J_{\text{eff}}(\Delta \alpha, 0) = -J'_0 \exp(-\Delta \alpha / 2\xi_\parallel) \exp(-\Delta \alpha / \xi_\perp), \tag{9} \]
for $\Delta \alpha > 2\xi_\parallel$. The fitting parameters are $J_0 = 0.52$, $J'_0 = 0.3$, $\xi_\parallel^0 = 17.33$, $\xi_\parallel = 2.5$ and $\xi_\perp = 1$ in the case considered here : $\alpha = 0.5$, $J_\perp = 0.1$ and $J_\parallel = 0.08$ (see Fig.5).

4. Conclusion

We can conclude this study by mentioning some preliminary results obtained by the way of QMC simulations [19] performed on the effective diluted model Eq.(6) with a great number of spins $N \leq 256$. Even at very small concentrations $x$, a Néel type AF LRO at $T = 0$ is observed as a result of the simulations; details about this study will be reported elsewhere [20].

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