Spin-Peierls mechanism for the non-trivial magnetization plateaux in two-leg spin ladders

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Abstract

We propose the spin-Peierls mechanism for the the non-trivial magnetization plateaux at $M_s/4$ and $(3/4)M_s$ (M_s is the saturation magnetization) of the two-leg $S = 1$ spin ladder, bearing in mind the recent experiment on the BIP-TENO.

Key words: spin ladder; spin gap; magnetization plateau; spin-Peierls transition

A new organic tetraradical, 3,3',5,5'-tetrakis(*N-tert*-butylaminoxyl)biphenyl, abbreviated as BIP-TENO, has been synthesized recently [1]. This material can be regarded as an $S = 1$ antiferromagnetic two-leg spin ladder. The magnetization curve of BIP-TENO measured at low temperatures in high magnetic fields up to 50T [2], and up to 70T very recently [3] In these experiments the magnetization plateau at $M_s/4$ (M_s is the saturation magnetization) is observed between 45 T and 65 T.

This plateau should be non-trivial. because this must occur with a two-fold degeneracy in the ground state, associated with the spontaneous breakdown of the translational symmetry, based on the necessary condition of the magnetization quantization [4]. We have already proposed the "dimer mechanism"for this plateau due to the third-neighbor interactions [5,6] and succeeded to explain the magnetization curve semiquantitatively. However, the required strength of the third neighbor interactions is fairly larger. In consideration of these situations, we propose another mechanism for the $M_s/4$ plateau, the spin-Peierls mechanism

A simplified model [1] of BIP-TENO is shown in Fig. 1, although the real material is more complicated.

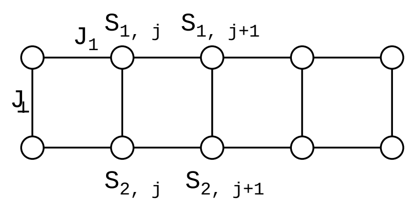

Fig. 1. Simplified model of BIP-TENO. Open circles represent $S = 1$ spins.

Both coupling constants are thought to be antiferromagnetic. In experimental estimation, it seems $J_\perp \gg J_1$.

The Hamiltonian of Fig. 1 is expressed as

$$H = J_1 \sum_{l=1,2} \sum_{j=1}^{L} \boldsymbol{S}_{l,j} \cdot \boldsymbol{S}_{l,j+1} + J_\perp \sum_{j=1}^{L} \boldsymbol{S}_{1,j} \cdot \boldsymbol{S}_{2,j} - h \sum_{l=1,2} \sum_{j=1}^{L} S^z_{l,j} \qquad (1)$$

where $\boldsymbol{S}$ denotes the spin-1 operator, j the rung number and $l = 1, 2$ the leg number. The last term is the Zeeman energy in the magnetic field h.

In the opposite limit $J_\perp \gg J_1$ we can use the degenerate perturbation theory [7]. When $J_1 = 0$, all the rung spin pairs are mutually independent. Thus, at

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$M = M_s/4$, half of the rung spin pairs are in the state

$$\psi(0,0) = \frac{1}{\sqrt{3}} \left(\left| \begin{matrix} \uparrow \\ \downarrow \end{matrix} \right\rangle + \left| \begin{matrix} \downarrow \\ \uparrow \end{matrix} \right\rangle - \left| \begin{matrix} 0 \\ 0 \end{matrix} \right\rangle \right), \tag{2}$$

and the remaining half pairs are in the state

$$\psi(1,1) = \frac{1}{\sqrt{2}} \left(\left| \begin{matrix} \uparrow \\ 0 \end{matrix} \right\rangle + \left| \begin{matrix} 0 \\ \uparrow \end{matrix} \right\rangle \right), \tag{3}$$

where $\psi(S_{\rm tot}, S^z_{\rm tot})$ is the wave function of with the quantum numbers $S_{\rm tot}$ and $S^z_{\rm tot}$. These two wave functions have the lowest energies in the subspace of $S^z_{\rm tot} = 0$ and $S^z_{\rm tot} = 1$, respectively. The $M_s/4$ state is highly degenerate as far as $J_1 = 0$, because there is no restriction for the configurations of these two states. This degeneracy is lifted up by the introduction of J_1. To investigate the effect of J_1, we introduce the pseudospin $\boldsymbol{T}$ with $T = 1/2$. The $|\Uparrow\rangle$ and $|\Downarrow\rangle$ states of the $\boldsymbol{T}$ spin correspond to $\psi(1,1)$ and $\psi(0,0)$, respectively. Neglecting the other seven states for the rung spin pairs, the effective Hamiltonian can be written as, through straightforward calculations

$$H_{\rm eff} = \sum_j \left\{ J^{xy}_{\rm eff}(T^x_j T^x_{j+1} + T^y_j T^y_{j+1}) + J^z_{\rm eff} T^z_j T^z_{j+1} \right\}, \tag{4}$$

in the lowest order of J_1, where

$$J^{xy}_{\rm eff} = (8/3)J_1, \qquad J^z_{\rm eff} = (1/2)J_1, \tag{5}$$

Thus, the $M_s/4$ plateau problem of the original model in a magnetic field is mapped onto the $M = 0$ problem of the $T = 1/2$ antiferromagnetic XXZ spin chain with the nearest-neighbor interaction in the absence of magnetic field.

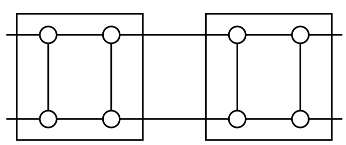

Fig. 2. Physical picture of the spin-Peierls mechanism. The distance between neighboring two spins on a leg changes alternatingly. This is the origin of the bond-alternation. The rectangle denote the effective singlet pair of two $\boldsymbol{T}$ spins.

Let us introduce the bond-alternation to $H_{\rm eff}$, coming from the lattice distortion to $H_{\rm eff}$, as

$$J^{xy,z}_{\rm eff} \Rightarrow J^{xy,z}_{\rm eff}\{1 + (-1)^j \delta\} \tag{6}$$

where δ is the magnitude of the bond-alternation. The energy gain of the $\boldsymbol{T}$-system due to the bond-alternation is proportional to δ^a where [8,9]

$$a = 4/(4-\eta), \qquad \eta = 2/[(1 + (2/\pi)\sin^{-1}\Delta_{\rm eff}] \tag{7}$$

with $\Delta_{\rm eff} \equiv J^z_{\rm eff}/J^{xy}_{\rm eff}$. Since the energy loss of the lattice distortion is proportional to δ^2, the condition for the occurrence of the spontaneous lattice distortion is $a < 2$. This mechanism is essentially the same as that of the spin-Peierls transition. Thus we call our mechanism "spin-Peierls mechanism". In our case, we can see

$$a = 1.81 < 2 \tag{8}$$

which means that the spin-Peierls mechanism is possible from the consideration of the energy. Our preliminary numerical calculation based on the $S = 1$ model shows that the a is very close to 1.8 as conjectured in (8).

We can develop a similar consideration for the $(3/4)M_s$ plateau case, where $|\Downarrow\rangle$ and $|\Uparrow\rangle$ should be modified to

$$|\Downarrow\rangle = \frac{1}{\sqrt{2}} \left(\left| \begin{matrix} \uparrow \\ 0 \end{matrix} \right\rangle + \left| \begin{matrix} 0 \\ \uparrow \end{matrix} \right\rangle \right), \qquad |\Uparrow\rangle = \left| \begin{matrix} \uparrow \\ \uparrow \end{matrix} \right\rangle \tag{9}$$

respectively. In this case, we see

$$\Delta_{\rm eff} = 1/4, \qquad a = 1.76 < 2 \tag{10}$$

which also results in the possibility of the spin-Peierls mechanism. A similar analysis can be applied also to the $M_s/2$ plateau of the two-leg $S = 1/2$ spin ladder.

We have proposed the spin-Peierls mechanism for the $M_s/4$ and $(3/4)M_s$ plateaux of the $S = 1$ two-leg ladder. The spin-Peierls mechanism and the third neighbor interaction may work in a cooperative way to form singlet dimer pairs of the $\boldsymbol{T}$ picture . However, more detailed investigations may be required for the full understanding of the magnetization curve of the BIP-TENO.

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