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# DMRG study of the impurity–induced transition from the spin-Peierls state to the antiferromagnetic state

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**Abstract**

We investigate impurity effects in the spin-Peierls systems coupled with an interchain exchange interaction. The density matrix renormalization group method is used. The interchain interaction is treated within the mean field approximation. In the impurity-free case, the ground state makes a first-order transition from the spin-Peierls (SP) state to the antiferromagnetic (AF) state at a critical strength of the interchain interaction. Impurities are doped to the spin-Peierls system which is located close to the SP-AF phase boundary in the phase diagram. A single impurity suppresses the bond alternation and induces a staggered magnetic moment locally around the doped site. If the impurity density is larger than a critical value, the spin-Peierls system makes a transition to the antiferromagnetic state. It is shown that a two-impurity problem is essential to understand the physical mechanism of the phase transition.

*Keywords:* Semi-empirical models and model calculations, Computer simulations, Structural phase transition, Magnetic phase transition

## 1. Introduction

Impurity effects in conducting polymers have been studied extensively. It is widely known [1] that the conducting polymers make a phase transition from the Peierls insulator to the highly conductive metallic state. Recently, impurity effects in spin-gapped materials have attracted much attention. The spin-Peierls system belongs to this class of materials.

The spin-Peierls compound $CuGeO_3$ can be doped with non-magnetic impurities such as zinc or magnesium atoms.[2] Copper atoms in $CuGeO_3$ are partially substituted by the impurities. It is remarkable that substitution of a small fraction of copper atoms induces a phase transition from the spin-Peierls state to the antiferromagnetic state.[3, 4, 5] $CuGeO_3$ can also be doped with silicon atoms, by which germanium atoms are replaced. In this case also, the doped impurities induce the phase transition to the antiferromagnetic state.[6]

Impurity effects in spin-Peierls systems have been theoretically studied.[7, 8, 9, 10] It is found that a single impurity suppresses the bond alternation of the spin-Peierls state and induces a staggered magnetic moment locally. However there are few theoretical works on the mechanism of the phase transition to the antiferromagnetic state.[11] In the present paper, we study the spin-Peierls system doped with randomly distributed impurities, using the density matrix renormalization group method.[12, 13] We will show that an intuitive scenario of the phase transition can be obtained by considering two-impurity problems.

## 2. Model

We study the one-dimensional Heisenberg model that is generalized to include the spin-lattice coupling and the interchain exchange interaction[14]

$$H = J\sum_{i=1}^{N}[1-\lambda(u_{i+1}-u_i)]\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1} + \frac{K}{2}\sum_{i=1}^{N}(u_{i+1}-u_i)^2 - zJ_\perp\sum_{i=1}^{N}m_i(S_i^z-\frac{m_i}{2}), \quad (1)$$

where $\lambda$ is the spin-lattice coupling, $u_i$ being lattice displacement of the $i$-th ion. The second term is elastic energy of the classical lattice. The last term is the interchain exchange coupling which is treated within the mean-field approximation, $z$ being the coordination

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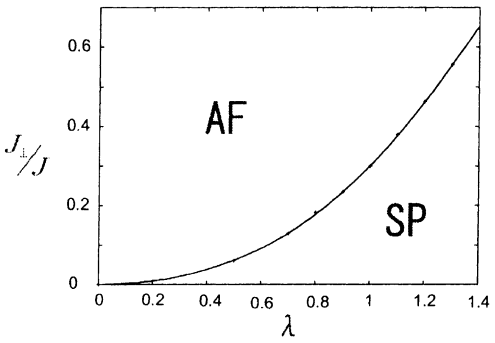


Fig. 1. The phase diagram in the impurity-free case. The ground state makes a first-order transition from the spin-Peierls (SP) phase to the antiferromagnetic (AF) phase at a critical value of the interchain interaction $J_{\perp c}(\lambda)$.

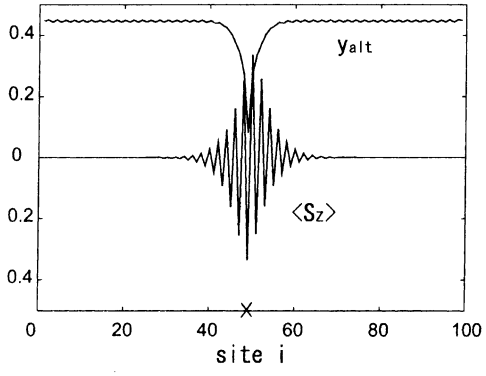


Fig. 2. The bond configuration $y_{alt} = (-1)^i y_i$ and the spin density $\langle S_z \rangle$ in the presence of a bond impurity. The parameters are $\lambda = 1.3$, $\lambda_{imp}/\lambda = 1/3$ and $J_\perp/J = 0.54$.

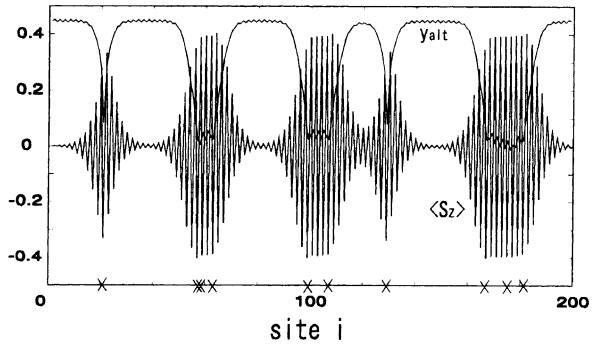


Fig. 3. The bond configuration $y_{alt} = (-1)^i y_i$ and the spin density $\langle S_z \rangle$ for the impurity density of 5%. The parameters are the same as in Fig.2.

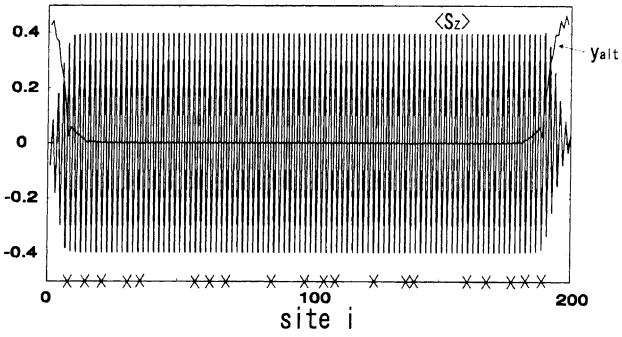


Fig. 4. The bond configuration $y_{alt} = (-1)^i y_i$ and the spin density $\langle S_z \rangle$ for the impurity density of 10%. The parameters are the same as in Fig.2.

number in the direction perpendicular to the spin chain. We take an open boundary condition for each spin chain that consists of $N$ lattice points. We set $J = 1$, $K = 1$ and $z = 2$.

We determine the bond configuration $u_i$ by minimizing the total energy of the Hamiltonian. The self-consistent equations for $u_i$ and $m_i$ are given by

$$y_i = \frac{\lambda J}{K}\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}\rangle - \frac{\lambda J}{KN}\sum_{i=1}^{N}\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}\rangle \qquad (2)$$

and

$$m_i = \langle S_z \rangle, \qquad (3)$$

where $y_i \equiv u_{i+1} - u_i$. The bracket $\langle\ \rangle$ means the expectation value with respect to the ground state of the Hamiltonian (1). The expectation value is numerically estimated by the density matrix renormalization group (DMRG) method. We have chosen $m = 32$, $m$ being the number of states kept during the DMRG calculation. The coupled equations (1), (2) and (3) are solved iteratively.

A similar model has been very recently studied using the numerical transfer-matrix method, which loses accuracy at low temperatures.[14] The present study at absolute zero temperature will give an alternative insight to the impurity-induced phase transition.

## 3. Impurity-free Case

First, we consider the impurity-free case. If the interchain interaction is absent, the ground state is in the spin-Peierls phase. The ground state makes a first-order transition to the antiferromagnetic phase at a critical value of the interchain exchange coupling $J_{\perp c}(\lambda)$.[15] The phase diagram is shown in Fig. 1.

## 4. Single Impurity

Next, we consider a bond-type impurity, which is doped to the spin-Peierls system located near the SP-