Spin Defects in Spin-Peierls Systems

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We examine spin-Peierls systems in the presence of spin defects which are introduced by replacing magnetic ions Cu$^{2+}$ with non-magnetic ones Zn$^{2+}$ in CuGeO$_3$. By using the action for the bosonized Hamiltonian, it is shown directly that the antiferromagnetic state induced by the spin defects coexists with the spin-Peierls states. Further the doping dependences of both transition temperature of spin-Peierls state and the spin gap have been calculated. The transition temperature of the present estimation shows good agreement quantitatively with that observed in Cu$_{1-\delta}$Zn$_{\delta}$O$_3$ for the region of the doping rate, $\delta < 0.02$.

KEYWORDS: spin-Peierls state, impurity effect, CuGeO$_3$

§1. Introduction

The discovery of inorganic spin-Peierls (SP) system CuGeO$_3$, which has chains of Cu$^{2+}$ with spin 1/2 along $c$-axis, has attracted much attention to the role of disorder in SP systems. In the material, the antiferromagnetic (AF) exchange energy between nearest neighbor spins is estimated as $J = 183K$ from the magnetic field which corresponds to saturation of magnetization. The compound in the absence of disorder undergoes SP transition at $T_{SP} = 14K$, below which the lattices spontaneously dimerize and the magnetic susceptibility rapidly drops to zero along all the axes owing to appearance of the energy gap between the singlet ground state and the triplet excited one. The spin gap is estimated as $\Delta_S = 2.1meV$ from the inelastic neutron scattering.

The effects of the disorder on SP systems have been mainly investigated on the materials where Cu ions are replaced by Zn or Ge ions are replaced by Si. It has been observed that the doping decreases $T_{SP}$. Further, the fact that a new AF ordered phase appears below $T_{SP}$ has been now well established from measurements of the magnetic susceptibility and the neutron scattering. This fact shows that the AF states coexists with the SP state.

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In terms of the phase representation of SP Hamiltonian, Fukuyama et al. examined the states between the two impurities by assuming the boundary condition that the lattice dimerization is suppressed at the location of the impurities. Treating classical equations with renormalized quantum fluctuation, they have shown that the AF state coexists with the SP state in the presence of disorder.

In the present paper, we investigate the effect of the spin defects on SP states without the assumption for the boundary condition by deriving the action for the SP system and show the coexistence of the two kinds of states. It turns out that our results are consistent with those given by Fukuyama et al. Further, we examine the variation of both $T_{SP}$ and $\Delta_{S}$ by the increase of the doping rate. In §2, we derive the action of the SP systems with the spin defects from Peierls-Hubbard model. The transition temperature is calculated in §3. In §4, we prove the coexistence of AF state and SP one and investigate the doping dependence of $\Delta_{S}$. Section 5 is devoted to summary and discussion.

§2. Model

Since the replacement of Cu with Zn gives rise to the variation of both the charge and spin degrees of freedom, we examine the effects of the spin defects by starting the Peierls-Hubbard model in one-dimension at half filling instead of the conventional SP model. The Hamiltonian is given as

$$H = -t \sum_{l,\sigma} \left\{ 1 + \lambda (u_l - u_{l+1}) \right\} \left( c_{l,\sigma}^\dagger c_{l+1,\sigma} + h.c. \right) + \sum_{l} c_{l,\uparrow}^\dagger c_{l,\downarrow}^\dagger c_{l,\uparrow} c_{l,\downarrow} + \frac{K}{2} \sum_{l} (u_l - u_{l+1})^2,$$

where $t$ and $U$ are the hopping and the on-site Coulomb energy, respectively. The quantity $\lambda$ is the coupling constant of the electron-lattice interaction and $c_{l,\sigma}^\dagger$ is a creation operator of electrons with the site $l$ and the spin $\sigma$. The quantity $K$ is the elastic constant with $u_l$ being the lattice distortion at the site $l$.

The model in eq.(1) can be expressed by the phase variables as follows:

$$H = \frac{v_\rho}{4\pi} \int dx \left\{ \frac{1}{K_\rho} (\partial_x \theta_+)^2 + K_\rho (\partial_x \theta_-)^2 \right\} + \frac{v_\rho g_\rho}{\pi \alpha^2} \int dx \cos 2\theta_+ + \frac{v_\sigma}{4\pi} \int dx \left\{ \frac{1}{K_\sigma} (\partial_x \phi_+)^2 + K_\sigma (\partial_x \phi_-)^2 \right\} + \frac{v_\sigma g_\sigma}{\pi \alpha^2} \int dx \cos 2\phi_+ + B \int dx u(x) \sin \theta_+ \cos \phi_+ + \frac{2K}{a} \int dx u^2(x),$$

where $a$ is the lattice constant, $B \propto \lambda$ and $u(x) = (-1)^l u_l$ with $x = la$. The quantity $\alpha$ denotes the cut-off for the large wavenumber. The velocity of excitation of the charge (spin) is given by
\( \nu_{\rho} (\nu_{\sigma}) \). The quantities \( g_{\rho} \) and \( g_{\sigma} \) are the coupling constants of the interaction for the umklapp scattering and the backward scattering respectively. The coefficients \( K_{\rho} \) and \( K_{\sigma} \) which also include parameters of interaction characterize one-dimensional system. The phase variables, \( \theta_{\pm} \) and \( \phi_{\pm} \), express fluctuations of the charge and the spin degrees of freedom, respectively, and satisfy the commutation relations, \([\theta_{+}(x), \theta_{-}(x)] = [\phi_{+}(x), \phi_{-}(x)] = i\pi \text{sgn}(x-x')\) and the others are zero. Note that we assumed \( t > U \) in deriving eq.(2). The density of the \( z \) component of the spin is expressed by 
\[
\frac{\partial x}{\nu_{\sigma}} \frac{\phi_{+}}{\pi} + \left( -1 \right)^{l} \sin \theta_{+} \sin \phi_{+} / \pi \alpha,
\]
where the first and the second term express the slowly varying part, \( S_{0}^{z} \), and the staggered one, \( S_{z}^{\pi} \), respectively.

In the above phase Hamiltonian, the charge excitation has a gap and the phase variable \( \theta_{+} \) is fixed to the value of \( \theta_{+} = (n+1/2)\pi \) ( \( n \) : integer ). Thus, eq.(2) in the absence of disorder becomes the same as that of phase representation of the conventional SP Hamiltonian. The fact indicates that the regime of the weak interaction is analytically connected to that of the strong interaction. Therefore the parameters in eq.(2) can be read as those of phase Hamiltonian of SP model.

The defects of spins are introduced as follows. At the location where Cu\(^{2+} \) are replaced by Zn\(^{2+} \), there appears the charge defect which is expressed by as a kink of \( \theta_{+} \). Since the fluctuation of the charge density is given by \( \partial_{x} \theta_{+} / \pi \), the quantity \( \theta_{+} \) jumps by \( \pi \) at the defect where \( \sin \theta_{+} \) varies from \( \pm 1 \) to \( \mp 1 \) resulting in the change of the sign of the coupling between spin and lattice. Thus the action of SP systems in the presence of the spin defects is obtained as
\[
S = \frac{\nu_{\sigma}}{4\pi K_{\sigma}} \int d\tau dx \left\{ \left( \partial_{x} \phi_{+} \right)^{2} + \frac{1}{\nu_{\sigma}^{2}} \left( \partial_{\tau} \phi_{+} \right)^{2} \right\} + \frac{\nu_{\sigma} g_{\sigma}}{\pi \alpha^{2}} \int d\tau dx \cos 2\phi_{+} + B \int d\tau dx m(x) u(x) \cos \phi_{+} + \beta \frac{2K}{\alpha} \int dx v^{2}(x),
\]
where \( \beta \) is the inverse of temperature, \( T \). The quantity \( m(x) \), which satisfies \( |m(x)| = 1 \), changes the sign at the location of the spin defects. The staggered component of \( S_{z}^{\pi} \) is given by \(-(-1)^{l} m(x) \sin \phi_{+} / \pi \alpha \). In the following, we study the case where the spin systems are expressed by Heisenberg chains, where \( \nu_{\sigma} = \pi Ja / 2^{l} 18) \), \( K_{\sigma} \to 1 \) due to the rotational symmetry in spin space and \( g_{\sigma} \to 0 (19) \).

§3. Temperature of Spin-Peierls Transition

We calculate \( T_{SP} \) from the softening of phonon with \( q = \pi \). The complete softening takes place at \( T = T_{SP} \) resulting in the vanishing of the effective elastic constant, \( K_{eff} \), which comes from the renormalization of \( K \) in eq.(3) through the electron-phonon coupling. By integrated out the spin degree of freedom up to the second order, \( K_{eff} \) is given as follows,
\[
K_{eff} = K - \frac{a}{\omega_{c}} B^{2} \int_{0}^{\infty} dx h(x) e^{-x/\xi} K(e^{-2x/\xi}),
\]

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where $\omega_c = v_\sigma \alpha^{-1}$, $\xi = v_\sigma / (\pi T)$ and $K(k)$ is the complete elliptic integral of the first kind. The function $h(x)$ is defined by $(1/L) \int dX \langle m(X + x/2)m(X - x/2) \rangle_{\text{imp}}$ with $\langle \cdots \rangle_{\text{imp}}$ expressing the impurity average. By noting that $h(x)$ is given by $1 - 2\delta|x|/a$ for $2\delta|x|/a \ll 1$ and $h(x \to \pm \infty) = 0$, we make use of the approximation given by $e^{-2\delta|x|/a}$ where $\delta$ denotes the doping rate. Then $T_{SP}/T_{SP}^0$ with $T_{SP}^0$, being the transition temperature in the absence of the impurities is determined self-consistently by the following equation,

$$
\frac{T_{SP}}{T_{SP}^0} = \frac{1}{C_1} \int_0^1 duu(J\delta/T_{SP}^0)/(T_{SP}/T_{SP}^0)K(u^2),
$$

where $C_1 \equiv \int_0^1 dtK(t^2) \simeq 1.72$. The asymptotic behavior is given as follows,

$$
\frac{T_{SP}}{T_{SP}^0} \lesssim \begin{cases} 
1 - \frac{C_2}{C_1} \frac{J\delta}{T_{SP}^0} & \text{for } \frac{J\delta}{T_{SP}^0} \ll 1 \\
4 \frac{J\delta}{T_{SP}^0} \exp \left\{ - \left( 2C_1 \frac{J\delta}{T_{SP}^0} - \gamma \right) \right\} & \text{for } \frac{J\delta}{T_{SP}^0} \gg 1 
\end{cases}
$$

where $C_2 \equiv -\int_0^1 dt \ln tK(t^2) \simeq 1.59$ and $\gamma \simeq 0.577$ is Euler’s constant. We show $T_{SP}/T_{SP}^0$ as a function of $J\delta/T_{SP}^0$ in Fig.1(a). According to the measurements of magnetic susceptibility and neutron scattering, $T_{SP}$ of Cu$_{1-\delta}$Zn$_\delta$GeO$_3$ decreases linearly for $\delta < 0.02$ and saturates from $\delta \simeq 0.02$ to at least $\delta \simeq 0.05$ [14]. In Fig.1(b), by substituting the values of $J = 183K$ and $T_{SP}^0 = 14K$ into eqs.(5) and (6), the present result (solid curve and dashed line) is compared with the experimental one given by the measurements of the neutron scattering (open circles) and the magnetic susceptibility (filled circles) which is shown in Fig.1 of ref.10. Figure 1(b) shows good agreement between the present result and the experimental one for $\delta \lesssim 0.02$. However, our result cannot explain the saturation of the transition temperature in the region of the doping rate of $0.02 < \delta < 0.05$.

§4. The Case of $T \ll T_{SP}$

In this section, we examine the coexistence of the AF state and the SP state in the presence of the spin defects and calculate the doping dependence of $\Delta_S$ based on the action given by eq.(3).

We note that the change of the sign of the spin-lattice interaction at the location of the spin defects can be reexpressed as $m(x) \cos \phi_+(x) \rightarrow \cos \{ \phi_+(x) + n(x)\pi \}$ and $m(x) \sin \phi_+(x) \rightarrow \sin \{ \phi_+(x) + n(x)\pi \}$ where the integer $n(x)$ jumps alternatively by $\pm 1$ at the spin defects. By rewriting $\phi_+ + n(x)\pi$ as $\phi$, the action, $S$, can be given as follows,

$$
S = \frac{v_\sigma}{4\pi} \int d\tau dx \left\{ \left( \partial_\tau \phi \right)^2 + \frac{1}{v_\sigma^2} \left( \partial_x \phi \right)^2 \right\}
$$

$$
- \frac{v_\sigma}{2} \int d\tau \sum_i p_i \partial_\tau \phi(x_i) + \beta \frac{\pi v_\sigma}{4} \sum_{i,j} p_ip_j \delta(x_i - x_j)
$$
Fig. 1. (a) The critical temperature of spin-Peierls transition normalized by that without doping as a function of $(J/T_{SP}^0)\delta$. The dotted (dashed) curve shows an asymptotic form for $J\delta/T_{SP}^0 \ll 1$ ($\gg 1$) given by eq.(6). (b) Comparison of the present result with the experimental result (open and filled circles) in ref.[10] where $J = 183K$ and $T_{SP}^0 = 14K$. Here the open and the filled circles express $T_{SP}$ determined by the measurements of the neutron scattering and the magnetic susceptibility, respectively.

\[ + B \int d\tau dxu(x) \cos \phi + \beta \frac{2K}{a} \int dxu^2(x), \]

where $x_i$ is the position of the spin defects. With the use of the number $p_i = \pm 1$, $\partial_x n(x) = \sum_i p_i \delta(x - x_i)$ and $p_ip_{i+1} = -1$. In eq.(7), we divide the lattice distortion as $u(x) = -u + \bar{u}(x)$
where \( \bar{u}(x) \) denotes the spatial variation around the uniform value, \( u \). Correspondingly, the action \( S \) is divided as \( S = S_1[u] + S_2[u, \bar{u}(x)] \). We apply the variational method to \( S_1[u] \), whose trial action \( S_0[u] \) is given by

\[
S_0[u] = \frac{v \sigma}{4\pi} \int d\tau dx \left\{ (\partial_x \phi)^2 + q_0^2 \phi^2 + \frac{1}{v \sigma^2} (\partial_\tau \phi)^2 \right\} - \frac{v \sigma}{2} \int d\tau \sum_i p_i \partial_x \phi(x_i) + \beta \pi v \sigma \sum_{i,j} p_i p_j \delta(x_i - x_j) + \beta L \frac{2K}{a} u^2. 
\] (8)

Here \( L \) is the system size, and \( q_0 \) is related to the spin gap in the presence of the disorder \( \Delta_S \) as

\[
\Delta_S = v \sigma q_0. 
\]

The quantities \( q_0 \) and \( u \) are determined by minimizing the following Free energy

\[
F_{tr} = F_0 - Bu \int dx \langle \cos \phi \rangle_{S_0} - \frac{v \sigma q_0^2}{4\pi} \int dx \langle \phi^2 \rangle_{S_0}, 
\] (9)

where \( \langle \cdots \rangle_{S_0} \) expresses the average with respect to \( S_0[u] \). On the other hand, \( \bar{u}(x) \) is determined by minimizing the quantity,

\[
- \ln \langle \exp \{-S_2[u, \bar{u}(x)]\} \rangle_{S_0} 
\]

with respect to \( \bar{u}(x) \).

In order to calculate the various quantities averaged by \( S_0 \), we first calculate the generating function,

\[
W[J(x,\tau)] = \exp \left\{ -\frac{1}{2} \int d\tau \int dx \int d\tau' \int dx' H(x-x',\tau-\tau';T)J(x,\tau)J(x',\tau') \right\} \times \exp \left\{ -i \int d\tau dx F(x)J(x,\tau) \right\}, 
\] (10)

where

\[
H(x-x',\tau-\tau';T) = \frac{1}{\beta L} \sum_{q,\omega_n} \exp \left\{ -iq(x-x') + i\omega_n(\tau-\tau') \right\} \frac{v \sigma}{2\pi} \left( q^2 + q_0^2 + \omega_n^2 \right) 
\] (11)

and

\[
F(x) = \frac{\pi}{2} \sum_i p_i \frac{\pi}{L} \sum_q \frac{iq \exp \left\{ iq(x_i - x) \right\}}{q^2 + q_0^2} = \frac{\pi}{2} \sum_i p_i e^{-q_0|x-x_i|} \text{sgn}(x-x_i), 
\] (12)

with \( \omega_n = 2n\pi T \ (n: \text{integer}) \). Equations (10)-(12) lead the following results,

\[
S_\pi^x(x) = -\frac{(-1)^l}{\pi \alpha} \langle \sin \phi \rangle_{S_0}
\]
\begin{equation}
= - \frac{(-1)^l}{\pi \alpha} \exp \left\{ - \frac{1}{2} H(0,0;T) \right\} \sin F(x),
\end{equation}

\begin{equation}
u(x) = - \frac{aB}{4K} \cos \phi \left. S_0 \right. 
= - \frac{aB}{4K} \exp \left\{ - \frac{1}{2} H(0,0;T) \right\} \cos F(x).
\end{equation}

with \( x = la \). Here the first line in eq.(14) is derived by minimizing \(- \ln \{ \exp \{ - S_2[u, \bar{u}(x)] \} \} \) with respect to \( \bar{u}(x) \). The function \(|F(x)|\) takes almost a value of \( \pi/2 \) near the location of the spin defects and decreases rapidly to zero far from the location. Thus, without the assumption of the boundary condition, we obtain that the lattice dimerization is suppressed and AF moments appear near the location of the spin defects. The characteristic length of the spatial dependence is given by \( 1/q_0 \). Equations (13) and (14) show the facts that the phase \( \phi(x) \) can be divided as \( \phi(x) = \phi_{cl}(x) + \phi_q(x) \) where \( \phi_{cl}(x) \) is the classical part and \( \phi_q(x) \) expresses the quantum fluctuation around \( \phi_{cl}(x) \) where \( \phi_{cl}(x) = F(x) \) and \( \left< \phi_q^2(x) \right> = H(0,0;T) \). In Fig.2, we compare the classical part of the phase obtained in the present study and that derived by solving the classical equation in the case of two defects. Here the distance between the impurities, \( l_{imp} \) is 159a (a) and 79a (b) and \( 1/(q_0a) \) is chosen as 11.8 which corresponds to undoped CuGeO. The solid curve expresses \( \theta_{cl}(x) = F(x) + \pi/2 \) and the dotted curve is obtained from the classical equations with the boundary conditions of \( \theta_{cl}(0) = \theta_{cl}(l_{imp}) = F(0) + \pi/2 \). Note that we have chosen the region of \( F(0) = F(l_{imp}) \simeq - \pi/2 \). Figure 2 shows the following facts. Our treatment that the cosine term is replaced by the term proportional to \( \phi^2 \) underestimates the correlation between the impurities. Our result is valid for the case of the small doping, \( q_0a/\delta \gg 1 \).

The free energy of eq.(13) per unit length, \( f_{tr} \equiv F_{tr}/L \) is easily calculated as

\begin{equation}
f_{tr} = \frac{1}{L} \sum_q \frac{E_q}{2} + \frac{1}{\beta L} \sum_q \ln (1 - e^{-\beta E_q})
+ \frac{\pi \nu \sigma q_0^2}{16} \sum_{ij} p_i p_j (1 + q_0 |x_i - x_j|) e^{-q_0 |x_i - x_j|}
+ \frac{2K}{a} u^2 - B u e^{-\frac{1}{2} H(0,0;T)} \frac{1}{L} \int dx \cos F(x)
- \frac{\nu \sigma q_0^2}{4\pi} H(0,0;T),
\end{equation}

where \( E_q = \nu \sigma \sqrt{q^2 + q_0^2} \) is the excitation spectrum of spin fluctuation. In the following, we consider the case of \( T = 0 \) and \( q_0a/\delta \gg 1 \). Then the energy per unit length, \( \epsilon_{tr} \equiv f_{tr}(T = 0) \), can be calculated as follows,

\begin{equation}
\epsilon_{tr} = \frac{v_\sigma}{2\pi \alpha^2} \left( \frac{\alpha q_0}{2} \right)^2 + \frac{v_\sigma}{\pi \alpha^2} \frac{\alpha \pi^2}{8a} \delta \left( \frac{\alpha q_0}{2} \right) + \frac{2K}{a} u^2
- B u \left( \frac{\alpha q_0}{2} \right)^{1/2} \left\{ 1 - \frac{\alpha}{a(\alpha q_0/2)} \tan(\frac{\pi}{2} \delta) \right\},
\end{equation}

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Fig. 2. Spatial dependence of the classical part of the phase, $\theta_{cl}$, in the case of two impurities, where the distance between the two impurities are chosen as $159a(a)$ and $79a(b)$ with $a$ being the lattice distance. The solid (dotted) curves express the classical part of the phase obtained from the present study (the classical equation in ref.14).

where $Cin(\pi/2) = \int_{0}^{\pi/2} dt (1 - \cos t)/t \simeq 0.5568$. In deriving eq.(16), we used $q_0 \alpha \ll 1$. By minimizing eq.(16) with respect to $u$ and $\alpha q_0/2$, and defining $\Delta^0_S$ and $u_0$ as the spin gap and the lattice dimerization in the absence of the disorder, quantities $\Delta_S/\Delta^0_S$ and $u/u_0$ in the case of
$J\delta/\Delta S \ll 1$ are given as follows,

\[
\frac{\Delta S}{\Delta S_0} = 1 - \frac{\pi^2}{8} \left( \frac{J\pi}{\Delta S_0} \right) \delta, \tag{17}
\]

\[
u = 1 - \left\{ \frac{\pi^2}{16} + C\sin(\frac{\pi}{2}) \right\} \left( \frac{J\pi}{\Delta S_0} \right) \delta. \tag{18}
\]

Note that eq. (18) is consistent with eq. (14) in the sense that the spatial average of eq. (14) leads to eq. (18). Thus the spin gap and the lattice dimerization are suppressed linearly as a function of doping as is seen in the transition temperature. The ratio, $\Delta S/T_{SP}^0$, is given as

\[
\frac{\Delta S}{T_{SP}} = \frac{\Delta S_0}{T_{SP}^0} \left\{ 1 - \left( \frac{\pi^2}{8} \frac{\pi J}{\Delta S_0} - \frac{C_2}{C_1} \frac{J}{T_{SP}^0} \right) \delta \right\}. \tag{19}
\]

For the case of Cu$_{1-\delta}$Zn$_\delta$GeO$_3$, the quantity $\Delta S/T_{SP}$ decreases with increase of the doping rate, i.e., $\Delta S/T_{SP} \simeq \Delta S_0/T_{SP}^0(1 - 17\delta)$. The decrease of the spin gap originates from the fact that the coupling between the spins decreases due to the suppression of the lattice dimerization around the spin defects. Such a result indicates that the model having the constant lattice dimerization with the value in the absence of the impurities is hard to explain the suppression of the spin gap.

§5. Summary and Discussion

We have derived the action for the SP system in the presence of the spin defects, and have shown that the lattice dimerization is suppressed and the AF moments appear around the location of the defects. The doping dependences of both the transition temperature and the spin gap were calculated based on the action.

The action was obtained from the Peierls-Hubbard model which includes not only spin but also charge degrees of freedom, because the substitution of non-magnetic ion for magnetic ion influences both degrees of freedom. The resulting action given in eq. (3) is equal to that of SP model with spin-lattice coupling which changes the sign at the location of the defects due to the kink of the charge.

The transition temperature of the present calculation shows good agreement with the experimental result of Cu$_{1-\delta}$Zn$_\delta$GeO$_3$ for $\delta < 0.02$. However there is a discrepancy in the sense that the saturation of $T_{SP}$ appears in the experiments for $\delta > 0.02$ while $T_{SP}$ of the present calculation decreases exponentially by the increase of $\delta$. Further theoretical studies are needed in order to understand the saturation of the transition temperature of the SP state under doping.

By applying the variational method to the action, the coexistence of the AF state and the SP one at $T = 0$ was demonstrated without the assumption of the boundary condition at the spin defect. The present results are consistent with the assumption and the result by Fukuyama et al. In addition, it was shown that the spin gap and the spatially averaged lattice dimerization decrease by the doping. The decrease of the spin gap is due to the suppression of the lattice dimerization near the spin defects.
Finally we comment on the low energy excitation in the spin gap. It is very complicated to discuss the excitation by the variational method. However the existence of the excitation in the present action of eq.(3) could be understood qualitatively by the following discussion. According to the renormalization group analysis, the coefficient $B$ in eq.(3) tends to strong coupling for $K_\sigma < 4$, which shows that the system described by eq.(3) with $K_\sigma < 4$ belongs to the same universality class. In the special case of $K_\sigma = 2$, the Hamiltonian of the spin sector corresponding to eq.(3) can be mapped into that of non-interacting Dirac Fermions systems with the mass, $m_0(x)$,

$$
H = v_\sigma \int dx \left\{ \psi_1^\dagger (-i\partial_x) \psi_1 - \psi_2^\dagger (-i\partial_x) \psi_2 \right\} + \int dx \left\{ m_0(x) \left( \psi_1^\dagger \psi_2 + \psi_2^\dagger \psi_1 \right) \right\}, \tag{20}
$$

where $m_0(x) = \pi a B m(x) u(x)$. The term proportional to $\cos 2\phi_+$ is neglected because the term is less divergent compared to that proportional to $\cos \phi_+$. In the case where $m_0(x)$ takes periodically two values $\phi_0$ and $-\phi_0$ with the same interval $l_{int}$, the gap near the zero energy vanishes, because $m_0(q=0) = \int_0^{2l_{int}} dx m(x) = 0$. We also note another case that $m_0(x)$ takes two values $\phi_0$ and $\phi_1$ alternatively with the random distribution of the interval length $l$. When the distribution is given by $f_0(l) = \theta(l)n_0 e^{-n_0 l}$ and $f_1(l) = \theta(l)n_1 e^{-n_1 l}$, i.e., $1/n_0$ and $1/n_1$ being the mean length for $\phi_0$ and $\phi_1$ respectively, the integrated density of states and the localization length can be calculated exactly. Fabrizio and Melin have noticed that the Hamiltonian of SP system of XY chain with doping of Zn is given by eq.(20) and showed the midgap states by applying the above method. For the quantitative discussion, one must take into account the fact that the spatial variation of the mass, $m_0(x)$, is not exactly the telegraph type but changes the sign with the characteristic length of the order of $1/q_0$ due to $u(x) \propto \cos F(x)$, and that the magnitude of the mass depends on the doping rate. The further exploration is needed in order to understand the low energy excitation in the presence of spin defects.

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The diagrams illustrate the comparison between classical equations and the authors' approach for two different values of $l_{\text{imp}}/a$.

(a) $l_{\text{imp}}/a = 159$

- Classical eq.
- Ours

(b) $l_{\text{imp}}/a = 79$

- Classical eq.
- Ours

The graphs show the variation of $\theta_{\text{cl}}$ with $x/a$ for each case.