Static spin configuration in the one-dimensional Kondo lattice model

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The local spin order in the one-dimensional Kondo lattice model is studied for the conduction-electron band filling $n=\frac{1}{2}$ and $\frac{1}{3}$ in a special parameter case. The local spin-dimerization ground state is confirmed for the quarter-filling case. And the spin order is studied for $n=\frac{1}{3}$. The spin and charge gaps are given for different band-filling cases.

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In recent years, the Kondo lattice model (KLM) has been extensively studied.[1] This model can be used to describe the heavy fermion materials, in which there are two kinds of electronic states corresponding to the *d* and *f* orbitals, respectively. The *d* electron can propagate by hoping to neighboring sites, while the *f* electron is localized at every site and forms a magnetic moment. In this model, the important physics arises from the interplay between the Kondo screening and the effective interaction among localized spins. These two effects may result in the nonmagnetic Kondo-singlet phase and the antiferromagnetic long-range order phase. The long-range order phase comes from the effective spin-spin Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction mediated by the conduction electrons.

The one-dimensional (1D) KLM has a complicated phase diagram,[1] depending on the band filling n of the conduction electron's density. At half filling ($n=1$), the ground state is a spin-liquid insulator[2] (or a Kondo-singlet state) for any Kondo coupling. When the conduction electron density is below half filling ($n\leqslant 1$), things are quite different. For an incommensurate band filling, there is a phase transition[3] from a paramagnetic to a ferromagnetic state as the Kondo interaction increases. However, for a commensurate band filling, the results are very interesting. In a very recent work on numerical calculation by the method of the density-matrix renormalization group,[4] a different phase is found in the 1D KLM at quarter filling $\left(n=\frac{1}{2}\right)$; there is a spin-dimerization phase for the localized spins. This phase may be a possible mechanism to explain the dimerization transition observed in the quasi-one-dimensional organic compound $(\mathrm{Per})_2M(mnt)_2$ ($\mathrm{M}=\mathrm{Pt},\mathrm{Pd}$).[5] In this phase, the local spin $\boldsymbol{\tau}_j$ dimerization order parameter $D(j)(=\langle\boldsymbol{\tau}_j\cdot\boldsymbol{\tau}_{j+1}\rangle)$ oscillates symmetrically near zero. As the conduction-electron density deviates from quarter filling $n\neq\frac{1}{2}$, $D(j)$ has no such kind of behavior, and the local spin-dimerization does not exist. Therefore, one question may be raised naturally: Is there another spin order at a commensurate band filling besides spin dimerization? This order may be improperly described by the dimerization order parameter $D(j)$.

Based on the above considerations, we intend to study the local spin configuration or spin order in the 1D KLM by the bosonization technique. This paper is organized as follows. First, we give the bosonization form of the 1D KLM. Then under a spacial parameter condition, the bosonized KLM is treated by a variational method on the basis of a trial ground state in the form of a Gaussian wave functional.[6] We calculate the ground-state energy, by which we investigate the static configuration of local spins for $n=\frac{1}{2}$ and $n=\frac{1}{3}$. For the quarter filling $\left(n=\frac{1}{2}\right)$, it is confirmed that the spin-dimerization order can exist in the 1D KLM. And for $n=\frac{1}{3}$, we show another order for the local spins. Finally, the spin and charge gaps are calculated for various band-filling cases.

The 1D KLM can be written as

$$H=-t\sum_{j,\sigma}(C^{\dagger}_{j,\sigma}C_{j+1,\sigma}+\mathrm{H.c.})+J\sum_{j}\mathbf{S}_j\cdot\boldsymbol{\tau}_j, \tag{1}$$

where t is the conduction-electron hopping strength, the operator $C^{\dagger}_{j,\sigma}$ creates an electron at site j with spin σ, $\boldsymbol{\tau}_j$ is a localized spin-$\frac{1}{2}$ operator, $\mathbf{S}_j=\Sigma_{\alpha\beta}(C^{\dagger}_{j,\alpha}\boldsymbol{\sigma}_{\alpha\beta}C_{j,\beta})/2$ is the spin-density operator of the conduction electron, and $\boldsymbol{\sigma}_{\alpha\beta}$ are the Pauli matrices. We introduce the left- and right-moving electron operator $\Psi^{\dagger}_{\lambda,\sigma}(x)$ with $\lambda=R,L$ and linearize the spectrum around two Fermi points. In the continuum limit, the Hamiltonian (1) is given by

$$\begin{aligned}
H&=H_0+H_{\parallel}+H_{\perp},\\
H_0&=-iv_F\sum_{\sigma}\int dx[\Psi^{\dagger}_{R,\sigma}\partial_x\Psi_{R,\sigma}-\Psi^{\dagger}_{L,\sigma}\partial_x\Psi_{L,\sigma}],\\
H_{\parallel}&=J_{\parallel}\sum_{j,\lambda}\tau^z_j[\Psi^{\dagger}_{\lambda\uparrow}(R_j)\Psi_{\lambda\uparrow}(R_j)-\Psi^{\dagger}_{\lambda\downarrow}(R_j)\Psi_{\lambda\downarrow}(R_j)],\\
H_{\perp}&=J_{\perp}\sum_{j,\lambda,\lambda'}[\tau^{+}_j\Psi^{\dagger}_{\lambda\downarrow}(R_j)\Psi_{\lambda'\uparrow}(R_j)+\mathrm{H.c.}],
\end{aligned} \tag{2}$$

where $v_F=2t\sin(k_Fa)$ is the Fermi velocity (a is lattice constant), and $k_F=n\pi/2a$. The local spins are located at position $R_j=ja$. H_0 is the kinetic energy of the conduction electrons. $H_{\parallel}+H_{\perp}$ is the coupling between the conduction electrons and the local spins. The anisotropic Kondo interaction is considered in this paper. $J_{\parallel}$ and $J_{\perp}$ are the longitudinal and transverse parts of the Kondo interaction, respectively. In the following bosonization process, each of them can be divided into forward- and back-scattering parts labeled by "*f*" and "*b*." So the Kondo interaction has been divided into four parts: $J^f_{\parallel}$, $J^b_{\parallel}$, $J^f_{\perp}$, and $J^b_{\perp}$.[7]

With the standard bosonization technique, we can express the conduction electrons by boson field. Here

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only the outlines of the bosonization process are given. Details can be found in Refs. 7 and 8. After introducing the boson fields $\phi_\sigma(x)$ with its conjugate momentum $\Pi_\sigma(x)$, we define $\Phi_{R(L),\sigma}(x)=[\phi_\sigma(x)\mp\int_{-\infty}^{x}\Pi_\sigma(y)dy]/2$. Then fermion operators can be expressed as $\Psi_{R(L),\sigma}=(1/\sqrt{2\pi a})\exp[\pm i\sqrt{4\pi}\Phi_{R(L),\sigma}(x)]$, whereupon the Hamiltonian (2) may be bosonized. One can rewrite the bosonized Hamiltonian by introducing the spin and charge fields, $\phi_s(x)=[\phi_\uparrow-\phi_\downarrow]/\sqrt{2}$, $\phi_c(x)=[\phi_\uparrow+\phi_\downarrow]/\sqrt{2}$. After making a unitary transformation,[9] $U=\exp[-i\sqrt{2\pi}\Sigma_j\tau_j^z\int_{-\infty}^{ja}\Pi_s(y)dy]$, we obtain a transformed Hamiltonian,

$$\tilde{H}=\frac{v_F}{2}\int dx\{[\Pi_c^2+(\partial_x\phi_c)^2]+[\Pi_s^2+(\partial_x\phi_s)^2]\}+\frac{\alpha}{a}\sum_j\tau_j^z(-1)^j\sin[\sqrt{2\pi}\phi_s(j)]\sin[\sqrt{2\pi}\phi_c(j)+2k_Fja], \tag{3}$$

where $\alpha=2J_\parallel^b/\pi$. In (3), we have set $\Delta J_\parallel^f=J_\parallel^f-\pi v_F=0$ and $J_\perp^f=J_\perp^b=0$. In the following, we will always work under this parameter condition. In this way, the operator $\{\tau_j^z\}$ can commutate with $\tilde{H}$. So $\{\tau_j^z\}$ are good quantum numbers. Thus we can treat them as constant numbers $\tau_j^z=\pm1/2$. It should be noted that the configuration of $\{\tau_j^z\}$ should be properly selected in order to minimize the ground-state energy.

Since the Hamiltonian (3) cannot be solved exactly, one can simulate it by the following exactly solvable reference model.[10]

$$H_{ref}=H_s+H_c,$$

$$H_s=\frac{v_F}{2}\int dx\{\Pi_s^2+(\partial_x\phi_s)^2+m_s^2\phi_s^2\}, \tag{4}$$

$$H_c=\frac{v_F}{2}\int dx\{\Pi_c^2+(\partial_x\phi_c)^2+m_c^2\phi_c^2\},$$

where m_c and m_s are the charge and spin gaps, respectively. They will be determined variationally. The field $\phi_{c(s)}$ and its canonical $\Pi_{c(s)}$ can be expanded as

$$\phi_{c(s)}(x)=\sum_\mu\frac{1}{\sqrt{2\varepsilon_{\mu,c(s)}}}u_{\mu,c(s)}(x)[a_{\mu,c(s)}+a_{\mu,c(s)}^\dagger],$$

$$\Pi_{c(s)}(x)=-i\sum_\mu\sqrt{\frac{\varepsilon_{\mu,c(s)}}{2}}u_{\mu,c(s)}(x)[a_{\mu,c(s)}-a_{\mu,c(s)}^\dagger]. \tag{5}$$

With a bilinear form, the Hamiltonian H_{ref} can be exactly diagonalized as

$$H_{ref}=\sum_{\mu,l=c,s}\varepsilon_{\mu,l}\left(a_{\mu,l}^\dagger a_{\mu,l}+\frac{1}{2}\right). \tag{6}$$

The eigenfunction $\{u_{\mu,c(s)}(x)\}$ and eigenvalue $\{\varepsilon_{\mu,c(s)}\}$ are obtained by the following differential equation:

$$\left[-\frac{d^2}{dx^2}+m_{c(s)}^2\right]u_{\mu,c(s)}(x)=\varepsilon_{\mu,c(s)}^2u_{\mu,c(s)}(x). \tag{7}$$

The ground state of H_{ref} in Eq. (6) satisfies the condition,

$$a_{\mu,l}|\psi\rangle=\frac{1}{\sqrt{2}}\int dxu_{\mu,l}(x)\left[\sqrt{\varepsilon_{\mu,l}}\phi_l(x)+i\frac{1}{\sqrt{\varepsilon_{\mu,l}}}\Pi_l(x)\right]|\psi\rangle=0,\quad\text{for all }\mu\text{ and }l. \tag{8}$$

In the representation of $\phi_l(x)$, $\Pi_l(x)=(1/i)[\delta/\delta\phi_l(x)]$, the solution is a Gaussian wave functional,

$$|\psi\rangle=\mathcal{N}\prod_{l=c,s}\exp\left(-\frac{1}{2}\int\int dxdy\{[\phi_l(x)-\phi_{l,0}]K_l^{-1}(x,y)[\phi_l(y)-\phi_{l,0}]\}\right), \tag{9}$$

where $\phi_{c(s),0}$ is a variational parameter that represents the local classical value of the field $\phi_{c(s)}$. Without losing generalization, we restrain $\phi_{c(s),0}$ in the region of $[0,\pi]$. $\mathcal{N}$ is the normalization coefficient. The kernel in wave-function (9) is defined as

$$\int dyK_l(x,y)K_l^{-1}(x',y)=\delta(x-x'), \tag{10}$$

and takes the form as

$$K_l^{-1}(x,y)=\sum_\mu\varepsilon_{\mu,l}u_{\mu,l}(x)u_{\mu,l}(y), \tag{11}$$

whose inverse $K_l(x,y)$ can be expressed as

$$K_l(x,y)=\sum_\mu\frac{u_{\mu,l}(x)u_{\mu,l}(y)}{\varepsilon_{\mu,l}}. \tag{12}$$

By the trial wave function of Eq. (9), we obtain the ground-state energy of Hamiltonian (3)

$$E_g(\phi_{c,0},m_c,\phi_{s,0},m_s)=\langle\psi(\phi_{c,0},m_c,\phi_{s,0},m_s)|H|\psi(\phi_{c,0},m_c,\phi_{s,0},m_s)\rangle=E_1+E_2, \tag{13}$$

where

$$E_1=\frac{v_FL}{8\pi a^2}[\sqrt{(1+m_c^2a^2)}+\sqrt{(1+m_s^2a^2)}], \tag{14}$$

$$E_2=\frac{\alpha}{a}\exp\left[-\frac{1}{4}(\beta_s^2K_s+\beta_c^2K_c)\right]\mathcal{J}, \tag{15}$$

and

$$\mathcal{J}=\sum_j\mathcal{J}_j, \tag{16}$$

$$\mathcal{J}_j=\tau_j^z(-1)^j\sin(\beta_c\phi_{c,0}+2k_Fja)\sin(\beta_s\phi_{s,0}), \tag{17}$$

$$K_{c(s)} = \frac{1}{2\pi} \ln\left(\frac{1 + \sqrt{1 + m_{c(s)}^2 a^2}}{m_{c(s)} a} \right). \tag{18}$$

In the above equations, $\beta_c = \beta_s = \sqrt{2\pi}$. $L = Na$ is the length of the system and N is the total number of lattice sites. By the ground-state energy equation (13), one can investigate the ground-state properties of the KLM. The four parameters $\phi_{c,0}, m_c, \phi_{s,0}, m_s$ and the configuration of local spins may be obtained by minimizing the ground-state energy.

By carefully analyzing the second part of the ground-state energy equation (13), one may find that this part is the total energy contributed by the interaction of conduction electrons and local spins. The classical path of the spin sector $\phi_{s,0}$ is obtained by $\partial E / \partial \phi_{s,0} = 0$, which will result in $\cos(\beta_s \phi_{s,0}) = 0$ or $\sin(\beta_s \phi_{s,0}) = 1$. Let us pay more attention to the term $\mathcal{J}_j$. As $n = \frac{1}{2}$ ($2k_F ja = j\pi/2$), it is easy to find that

$$\mathcal{J}_j = \begin{cases} \tau_j^z (-1)^{(j/2)} \sin(\beta_c \phi_{c,0}), & (j \in \text{Even}) \\ \tau_j^z (-1)^{[(j+1)/2]} \cos(\beta_c \phi_{c,0}), & (j \in \text{Odd}). \end{cases} \tag{19}$$

For a given set of parameters $\{\phi_{c,0}, m_c, \phi_{s,0}, m_s\}$, $\min(\mathcal{J}_j) = -|\mathcal{J}_j|/2$. If $\mathcal{J}_j$ is written in the form $\mathcal{J}_j = \tau_j^z \mathcal{G}_j$, we obtain the minimal $\mathcal{J}_j$ by selecting $\tau_j^z = -|\mathcal{G}_j|/(2\mathcal{G}_j)$. This kind of selection will ensure that $\mathcal{J}$ is minimal, that is to say, the total ground-state energy is minimal. Thus we have

$$\mathcal{J} = -N[|\sin(\beta_c \phi_{c,0})| + |\cos(\beta_c \phi_{c,0})|]/4. \tag{20}$$

If $0 \leqslant \beta_c \phi_{c,0} \leqslant \pi/2$, the pattern of the local spin may be given as

$$\tau_j^z = \begin{cases} \dfrac{(-1)^{(j/2+1)}}{2}, & (j \in \text{Even}) \\ \dfrac{(-1)^{[(j-1)/2]}}{2}, & (j \in \text{Odd}). \end{cases} \tag{21}$$

As $\pi/2 \leqslant \beta_c \phi_{c,0} \leqslant \pi$, the configuration of the local spin takes the form,

$$\tau_j^z = \begin{cases} \dfrac{(-1)^{(j/2+1)}}{2}, & (j \in \text{Even}) \\ \dfrac{(-1)^{[(j-1)/2+1]}}{2}, & (j \in \text{Odd}). \end{cases} \tag{22}$$

The above two local spin configurations are degenerated because their ground-state energies are equal. After the configuration of the local spins is fixed, the value of the local spin-dimer-order parameter $D(j) = \langle \boldsymbol{\tau}_j \cdot \boldsymbol{\tau}_{j+1} \rangle$ can be calculated. It is convenient to find that $D(j) = -(-1)^j/4$ or $D(j) = (-1)^j/4$ by the expression of the local spin configuration [(21) and (22)]. It means that there is an exact spin-dimerization ground state. The value of our result for $D(j)$ is very close to the numerical result ($|D(j)| \approx 0.21$) in Ref. 4. At the same time, m_c and m_s can be determined by $\partial E / \partial m_s = \partial E / \partial m_c = 0$, which will yield the following equations:

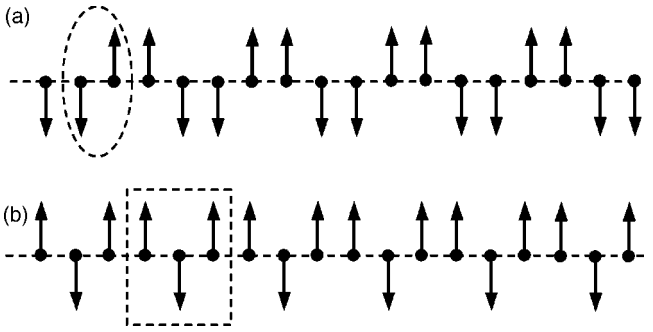

FIG. 1. The static, local spin configuration. (a) The conduction band filling $n = \frac{1}{2}$. The spins in the dashed circle area form a spin dimer. (b) The conduction band filling $n = \frac{1}{3}$. The spins in the dashed square area form a period of the spin configuration.

$$m_c^2 = m_s^2 = \frac{\alpha' \beta_c^2}{v_F} \left(\frac{m_c}{1 + \sqrt{1 + m_c^2}} \right)^{\beta_c^2/8\pi} \left(\frac{m_s}{1 + \sqrt{1 + m_s^2}} \right)^{\beta_s^2/8\pi}, \tag{23}$$

in which $\alpha' = \alpha \min(\mathcal{J})/N = \alpha\sqrt{2}/4$. Since the spin and charge in the reference Hamiltonian are symmetrical, the value of the renormalization mass m_c and m_s are the same. And $\beta_c \phi_{c,0} = \pi/4$ or $3\pi/4$, which is given by $\partial E / \partial \phi_{c,0} = 0$ or $\partial(\mathcal{J}) / \partial \phi_{c,0} = 0$. Up to now, our calculations show that the ground state is a static, local spin dimerization at $\Delta J_{\parallel}^f = 0$, $J_{\perp}^f = J_{\perp}^b = 0$.

One may ask if there exists a similar static spin configuration at other band fillings. As an example, the case of $n = \frac{1}{3}$ is considered. When $n = \frac{1}{3}$, a similar calculation is still held. We obtain

$$\mathcal{J} = -\frac{N}{6} \left[\left| \sin\left(\beta_c \phi_{c,0} - \frac{2\pi}{3} \right) \right| + |\sin(\beta_c \phi_{c,0})| + \left| \sin\left(\beta_c \phi_{c,0} + \frac{2\pi}{3} \right) \right| \right]. \tag{24}$$

The local spin configuration is

$$\tau_j^z = \frac{1}{2} (-1)^{\text{mod}(j/3)}. \tag{25}$$

In this case, the form of the solution (23) for the spin and charge gap is unchanged but $\alpha' = \alpha/3$ with $\beta_c \phi_{c,0} = \pi/6$. The static, local spin configuration is shown in Fig. 1(b). Although this result is obtained at our special parameter condition, we hope that such kinds of spin configurations may still be retained for isotropic KLM. We expect that this point can be confirmed in future studies.

Before closing this paper, we would like to give a plot for the spin and charge gaps dependent on the band filling. In Fig. 2, we give the energy gap as $J_{\parallel}^b = 0.5$ and $n = 1/m$ ($m = 2, 3, \ldots$). Each dot represents one kind of band filling. The line is just a guide line. By this figure, one may find that the spin or charge gap $m_c = m_s \approx 0.26$ is $n = \frac{1}{2}$. This value is a little larger than the results in Ref. 4. The reason is that we just consider the case of $\Delta J_{\parallel}^f = 0$ and $J_{\perp}^f = J_{\perp}^b = 0$. However, $\Delta J_{\parallel}^f$, $J_{\perp}^f$, and $J_{\perp}^b$ all have finite values in Ref. 4. These kinds of

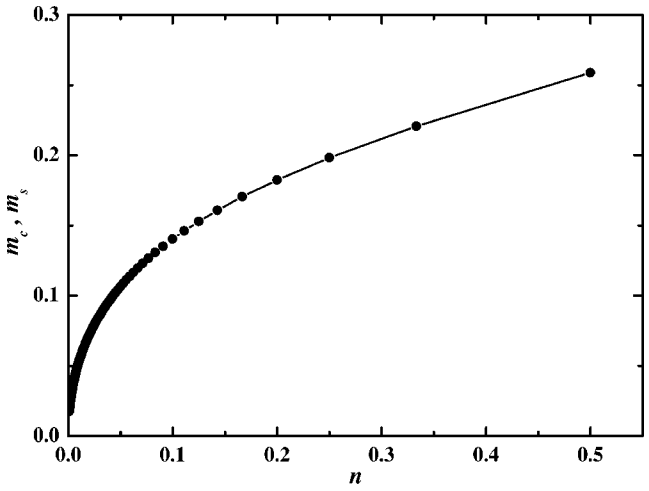

FIG. 2. The spin- and charge-gap dependence of the band filling ($n=1/m$, $m=2,3,\ldots$) at $J_{\parallel}^{b}=0.5$.

interactions may reduce the energy gaps. From this figure, one can also find that the energy gap will be decreased as the band filling is lowered.

In conclusion, we study the local spin order in a special parameter case by the bosonization technique. It is confirmed that there exists a spin-dimerization order in quarter filling in 1D KLM. Although our work is restrained in a special parameter case, we argue that the local spin-ordered ground state may still exist in 1D KLM for the general case. Furthermore, other kinds of band fillings are also considered in this paper. We find that, for a commensurate band filling, there still may exist other kinds of local spin order that cannot be described simply by order parameter. As an example, the case for $n=\frac{1}{3}$ is studied, and the local spin configuration is given. In the end, we calculate the spin and charge gap in different band fillings. It is found that the energy gaps are lowered by reducing the band fillings. This point may imply that a state with a static spin configuration will be unstable as the band filling is low. It may be very easily destroyed by the interactions, which are not considered in our treatment.

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