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LETTER TO THE EDITOR

First-order transitions in the one-dimensional Kondo lattice model at quarter-filling

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Abstract

The ground state properties of the one-dimensional Kondo lattice model are studied at conduction electron quarter-filling ($n = 1/2$) in a special parameter case. The charge and spin gaps are calculated. A phase diagram is given; the local spin order in each phase is presented. Two first-order transitions are found.

Recently, the Kondo lattice model (KLM) has attracted increasing attention [1]. In this model, the conduction electron propagates by hopping to neighbouring sites and interacts with the local magnetic moment at every site. The interplay between the Kondo screening and the effective interaction among localized spins may result in a nonmagnetic Kondo singlet phase or an antiferromagnetic long range order phase.

The one-dimensional (1D) KLM has a very complicated phase diagram [1], depending on the band filling n of the conduction electron density and the strength of the Kondo interaction between the conduction electrons and the local spin. At half-filling ($n = 1$), the ground state is a spin-liquid insulator [2] for any Kondo coupling. When the conduction electron density is below half-filling ($n \leqslant 1$), things are quite different. The band filling n will play a very important role for the phase diagram. For incommensurate band filling, there is a phase transition [3] from a paramagnetic to a ferromagnetic state as the Kondo interaction increases. However, for commensurate band filling, recent works [4–7] found many new results, especially for local spin order (LSO). In a numerical calculation work [6] based on the method of the density matrix renormalization group, a spin dimerization phase for the localized spins was found in 1D KLM at quarter-filling ($n = 1/2$). This phase may provide a possible mechanism for explaining the dimerization transition observed in the quasi-one-dimensional organic compound $(Per)_2M(mnt)_2$ (M = Pt, Pd) [8]. A very recent numerical work [7] found, besides the spin dimerized phase, other magnetic phases: the island phase and the spiral-like phase. The island phase has quasi-long range order (QLRO) and zero spin gap. The spin dimerized and island phases may belong to the same universal class. These new numerical works may imply that the KLM is far from fully understood.

In view of the above considerations, we would like to study the ground state properties of the 1D KLM by a bosonization technique. This letter is organized as follows. First, we give the bosonization form of the 1D KLM. Then, under a special 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 wavefunctional [9]. We calculate the ground state energy, using which the ground state properties of the KLM are investigated at quarter-filling ($n = 1/2$). Two phase transitions are found. The spin and charge gaps are calculated for the whole parameter space. Finally, the LSO in each phase is given.

The 1D KLM can be written as

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

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-1/2 operator, $\mathbf{S}_j = \sum_{\alpha\beta}(C^{\dagger}_{j,\alpha}\boldsymbol{\sigma}_{\alpha\beta}C_{j,\beta})/2$ is the spin-density operator of the conduction electron, and $\boldsymbol{\sigma}_{\alpha\beta}$ are the Pauli matrices. After introducing the left- and right-moving electron operator $\Psi^{\dagger}_{\lambda,\sigma}(x)$ with $\lambda = \mathrm{R}, \mathrm{L}$ and linearizing the spectrum around two Fermi points, in the continuum limit, the Hamiltonian (1) is given by

$$\begin{aligned}
&H = H_0 + H_{\parallel} + H_{\perp},\\
&H_0 = -\mathrm{i}v_{\mathrm{F}}\sum_{\sigma}\int \mathrm{d}x\,\left[\Psi^{\dagger}_{\mathrm{R},\sigma}\partial_x\Psi_{\mathrm{R},\sigma} - \Psi^{\dagger}_{\mathrm{L},\sigma}\partial_x\Psi_{\mathrm{L},\sigma}\right],\\
&H_{\parallel} = J_{\parallel}\sum_{j,\lambda}S^{z}_{j}\left[\Psi^{\dagger}_{\lambda\uparrow}(R_j)\Psi_{\lambda\uparrow}(R_j) - \Psi^{\dagger}_{\lambda\downarrow}(R_j)\Psi_{\lambda\downarrow}(R_j)\right],\\
&H_{\perp} = J_{\perp}\sum_{j,\lambda,\lambda'}\left[S^{+}_{j}\Psi^{\dagger}_{\lambda\downarrow}(R_j)\Psi_{\lambda'\uparrow}(R_j) + \text{h.c.}\right],
\end{aligned} \tag{2}$$

where $v_{\mathrm{F}} = 2t\sin(k_{\mathrm{F}}a)$ is the Fermi velocity (a is the lattice constant) and $k_{\mathrm{F}} = n\pi/2a$. The local spins are located at position $R_j = ja$. H_0 is the kinetic energy of the conduction electrons. $J_{\parallel}$ 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, labelled with 'f' and 'b'. So the Kondo interaction has been divided into four parts: $J^{\mathrm{f}}_{\parallel}$, $J^{\mathrm{b}}_{\parallel}$, $J^{\mathrm{f}}_{\perp}$ and $J^{\mathrm{b}}_{\perp}$ [10].

The conduction electrons in the boson field can be expressed by the standard bosonization technique. Here only the outline of the bosonization process is given. Details can be found in [10, 11]. After introducing the boson fields $\phi_{\sigma}(x)$ with the conjugate momentum $\Pi_{\sigma}(x)$, we define $\Phi_{\mathrm{R(L)},\sigma}(x) = [\phi_{\sigma}(x) \mp \int_{-\infty}^{x}\Pi_{\sigma}(y)\,\mathrm{d}y]/2$. Then the fermion operators can be expressed as $\Psi_{\mathrm{R(L)},\sigma} = (1/\sqrt{2\pi a})\exp[\pm\mathrm{i}\sqrt{4\pi}\Phi_{\mathrm{R(L)},\sigma}(x)]$, whereupon the Hamiltonian (2) may be bosonized. One can rewrite the bosonized Hamiltonian by introducing the spin and charge fields, $\phi_{\mathrm{s}}(x) = [\phi_{\uparrow} - \phi_{\downarrow}]/\sqrt{2}$, $\phi_{\mathrm{c}}(x) = [\phi_{\uparrow} + \phi_{\downarrow}]/\sqrt{2}$. After making a unitary transformation [12], $U = \exp[-\mathrm{i}\sqrt{2\pi}\sum_j \tau^{z}_{j}\int_{-\infty}^{ja}\Pi_{\mathrm{s}}(y)\,\mathrm{d}y]$, we obtain a transformed Hamiltonian:

$$\begin{aligned}
\tilde{H} = \frac{v_{\mathrm{F}}}{2}\int \mathrm{d}x\,\left\{[\Pi^{2}_{\mathrm{c}} + (\partial_x\phi_{\mathrm{c}})^2] + [\Pi^{2}_{\mathrm{s}} + (\partial_x\phi_{\mathrm{s}})^2]\right\} + \sum_{j}\frac{\tau^{x}_{j}}{\pi a}\Big\{J^{\mathrm{f}}_{\perp}(-1)^{j}\cos[\sqrt{2\pi}\phi_{\mathrm{s}}(j)]\\
+ J^{\mathrm{b}}_{\perp}\cos[\sqrt{2\pi}\phi_{\mathrm{c}}(j) + 2k_{\mathrm{F}}ja]\Big\},
\end{aligned} \tag{3}$$

where we have set $\Delta J^{\mathrm{f}}_{\parallel} = J^{\mathrm{f}}_{\parallel} - \pi v_{\mathrm{F}} = 0$ and $J^{\mathrm{b}}_{\parallel} = 0$. In the following, we will always work under this parameter condition. In this way, the operator $\{\tau^{x}_{j}\}$ can commute with $\tilde{H}$. So $\{\tau^{x}_{j}\}$ are good quantum numbers. Thus we can treat them as constant numbers $\tau^{x}_{j} = \pm 1/2$. The

configuration of $\{\tau_j^x\}$ should be properly selected in order to minimize the ground state energy. As $n < 1$, $J_\perp^{\rm b}$ and $J_\perp^{\rm f}$ may lead to different phases and orders for the conduction electron band and local spin. The phase diagram of the above Hamiltonian can be roughly understood on the basis of the competition between $J_\perp^{\rm b}$ and $J_\perp^{\rm f}$ in two limits: in the limit $J_\perp^{\rm b} = 0$, the charge part is free and the spin part is gapped. The local spin is antiferromagnetically ordered, because of the factor $(-1)^j$. In the limit $J_\perp^{\rm f} = 0$, the spin part will be gapless and have LRO. The order of the local spins may be modulated by $\cos(2k_{\rm F} ja)$.

Since the Hamiltonian (3) cannot be solved exactly, it can be simulated using the following exactly solvable reference model [13, 14]:

$$\begin{aligned} H_{\rm ref} &= H_{\rm s} + H_{\rm c}, \\ H_{\rm s} &= \frac{v_{\rm F}}{2}\int {\rm d}x\, \left\{\Pi_{\rm s}^2 + (\partial_x\phi_{\rm s})^2 + m_{\rm s}^2\phi_{\rm s}^2\right\}, \\ H_{\rm c} &= \frac{v_{\rm F}}{2}\int {\rm d}x\, \left\{\Pi_{\rm c}^2 + (\partial_x\phi_{\rm c})^2 + m_{\rm c}^2\phi_{\rm c}^2\right\}, \end{aligned} \tag{4}$$

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

$$\begin{aligned} \phi_{\rm c(s)}(x) &= \sum_\mu \frac{1}{\sqrt{2\varepsilon_{\mu,{\rm c(s)}}}} u_{\mu,{\rm c(s)}}(x)\left[a_{\mu,{\rm c(s)}} + a_{\mu,{\rm c(s)}}^\dagger\right], \\ \Pi_{\rm c(s)}(x) &= -{\rm i}\sum_\mu \sqrt{\frac{\varepsilon_{\mu,{\rm c(s)}}}{2}}\, u_{\mu,{\rm c(s)}}(x)\left[a_{\mu,{\rm c(s)}} - a_{\mu,{\rm c(s)}}^\dagger\right]. \end{aligned} \tag{5}$$

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

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

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

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

The ground state of $H_{\rm ref}$ in equation (6) satisfies the condition

$$\begin{aligned} a_{\mu,l}\,|\psi\rangle &= \frac{1}{\sqrt{2}}\int {\rm d}x\, u_{\mu,l}(x)\left[\sqrt{\varepsilon_{\mu,l}}\phi_l(x) + {\rm i}\frac{1}{\sqrt{\varepsilon_{\mu,l}}}\Pi_l(x)\right]|\psi\rangle \\ &= 0, \qquad \text{for all } \mu \text{ and } l. \end{aligned} \tag{8}$$

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

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

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

$$\int K_l(x,y)K_l^{-1}(x',y)\,{\rm d}y = \delta(x - x'),$$

and takes the form

$$K_l^{-1}(x,y) = \sum_\mu \varepsilon_{\mu,l}u_{\mu,l}(x)u_{\mu,l}(y), \tag{10}$$

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

$$K_l(x, y) = \sum_{\mu} \frac{u_{\mu,l}(x)u_{\mu,l}(y)}{\varepsilon_{\mu,l}}. \tag{11}$$

From the wavefunction of equation (9), one can obtain the density of the ground state energy for Hamiltonian (3):

$$E_g(\phi_{c,0}, m_c, \phi_{s,0}, m_s) = \left\langle \psi(\phi_{c,0}, m_c, \phi_{s,0}, m_s) \left| H \right| \psi(\phi_{c,0}, m_c, \phi_{s,0}, m_s) \right\rangle = E_1 + E_2, \tag{12}$$

where

$$E_1 = \frac{v_F}{8\pi a}\left[\sqrt{\left(1 + m_c^2 a^2\right)} + \sqrt{\left(1 + m_s^2 a^2\right)}\right], \tag{13}$$

$$E_2 = \frac{1}{N}\sum_j \tau_j^x \mathcal{J}_i, \tag{14}$$

and

$$\mathcal{J}_i = \alpha_s(-1)^j \cos\left(\beta_s \phi_{s,0}\right) + \alpha_c \cos\left(\beta_c \phi_{c,0} + 2k_F j a\right), \tag{15}$$

$$\alpha_s = \frac{J_\perp^f}{\pi a} \exp\left(-\frac{\beta_s^2 K_s}{4}\right), \tag{16}$$

$$\alpha_c = \frac{J_\perp^b}{\pi a} \exp\left(-\frac{\beta_c^2 K_c}{4}\right), \tag{17}$$

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

In the above equations, $\beta_c = \beta_s = \sqrt{2\pi}$. N is the total number of lattice sites. From the ground state energy (12), 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. The classical path $\phi_{c(s),0}$ can obtained from $\partial E_g/\partial \phi_{c(s),0} = 0$, which may result in $\beta_s \phi_{s,0} = 0$. And $\beta_c \phi_{c,0}$ can be obtained from the following calculation. As $n = 1/2$ ($2k_F j a = j\pi/2$), one can find that

$$\mathcal{J}_j = (-1)^{\mathrm{mod}(j/4)} \alpha_s + \alpha_c \cos(\beta_c \phi_{c,0} + j\pi/2). \tag{19}$$

For a given set of parameters $\{m_c, m_s\}$, $\min(\tau_j^x \mathcal{J}_j) = -|\mathcal{J}_j|/2$, from selecting

$$\tau_j^x = -\left|\mathcal{J}_j\right| / \left(2\mathcal{J}_j\right). \tag{20}$$

This kind of selection will ensure that $\tau_j^x \mathcal{J}_j$ is minimal, that is to say, the total ground state energy is minimal. By carefully analysing equation (19), one can find that $\beta_c \phi_{c,0}$ has three possible values 0, $\pi/4$ and $\pi/2$. The ground state energy can be written as

$$E_g = \begin{cases} E_1 - \alpha_s/2, & \alpha_c < \alpha_s \\ E_1 - (\alpha_s + \alpha_c)/4, & (\sqrt{2} - 1)\alpha_c < \alpha_s < \alpha_c \\ E_1 - \sqrt{2}\alpha_c/4, & \alpha_s < (\sqrt{2} - 1)\alpha_c. \end{cases} \tag{21}$$

The pattern of local spin should be obtained from the sign of $\mathcal{J}_j$. Up to now, one can get the values of m_c and m_s by minimizing the ground state energy (21).

In figure 1, we plot the ground state energy dependence on the variational parameters m_c and m_c for $J_\perp^f = 1.0$, $J_\perp^b = 0.75$. From this figure, one can find that there are three minimal points in the parameter space. m_c and m_c should be selected for the minimal point with lowest energy. As $\alpha_c < \alpha_s$, the second part of (21) is equal to $-\alpha_s/2$. This means that the interaction

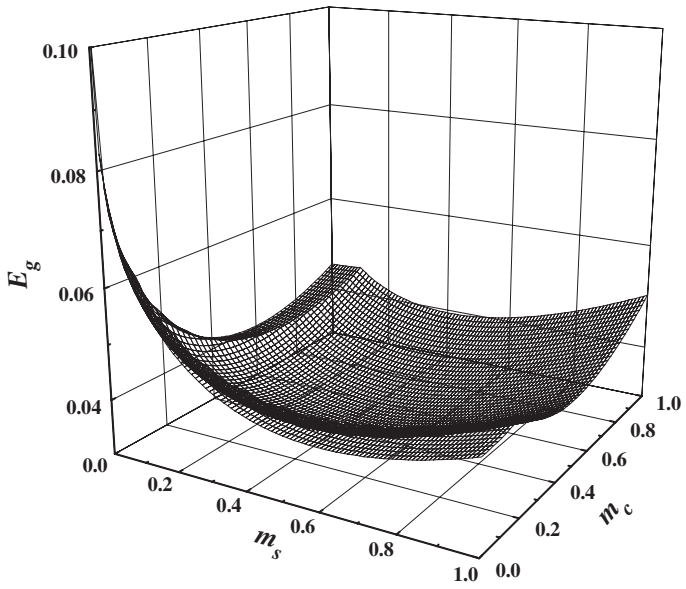

Figure 1. The ground state energy dependence of m_c and m_s for $J_\perp^f = 1.0$, $J_\perp^b = 0.75$.

of the charge part disappears. So the charge part is free. As $(\sqrt{2}-1)\alpha_c < \alpha_s < \alpha_c$, the second part of (21) is $-(\alpha_s + \alpha_c)/4$, which will result in spin and charge gaps. As $\alpha_s < (\sqrt{2}-1)\alpha_c$, the interaction of the spin part disappears and the spin excitations are gapless. For a pair $(J_\perp^f, J_\perp^b)$, the energy of E_g can be divided into three regions in the space of (m_c, m_s) by the lines $\alpha_s = \alpha_c$ and $(\sqrt{2}-1)\alpha_c = \alpha_s$. In each region, there is a minimal point for the ground state energy. One can easily find that these three points are $(m_{1,c}, m_{1,s})$, $(m_{2,c}, m_{2,s})$ and $(m_{3,c}, m_{3,s})$, for which

$$m_{1,c} = 0, \tag{22}$$

$$m_{1,s}^2 = \frac{J_\perp^f \beta_s^2}{2\pi v_F}\left(\frac{m_{1,s}}{1+\sqrt{1+m_{1,s}^2}}\right)^{\beta_s^2/8\pi}, \tag{23}$$

$$m_{2,c}^2 = \frac{J_\perp^b \beta_c^2}{4\pi v_F}\left(\frac{m_{2,c}}{1+\sqrt{1+m_{2,c}^2}}\right)^{\beta_c^2/8\pi}, \tag{24}$$

$$m_{2,s}^2 = \frac{J_\perp^f \beta_s^2}{4\pi v_F}\left(\frac{m_{2,s}}{1+\sqrt{1+m_{2,s}^2}}\right)^{\beta_s^2/8\pi}, \tag{25}$$

and

$$m_{3,c}^2 = \frac{\sqrt{2}J_\perp^b \beta_c^2}{4\pi v_F}\left(\frac{m_{3,c}}{1+\sqrt{1+m_{3,c}^2}}\right)^{\beta_c^2/8\pi}, \tag{26}$$

$$m_{3,s} = 0. \tag{27}$$

In our calculation, one should carefully compare the energy of these three points and select the points with lowest energy as the true charge and spin gaps.

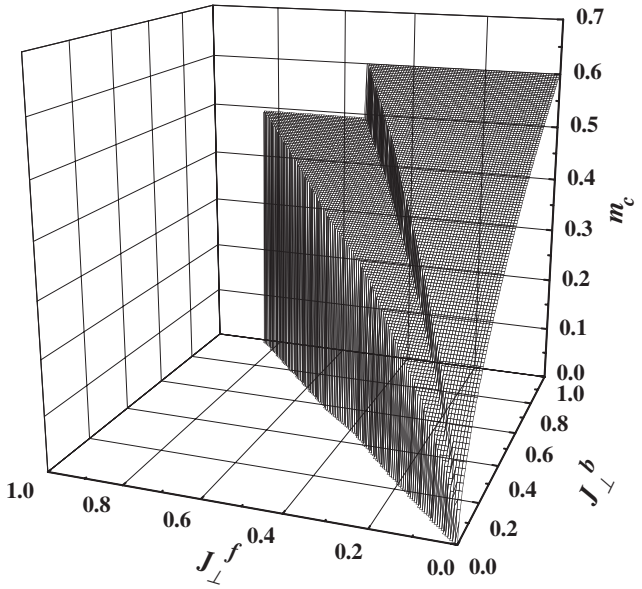

Figure 2. The charge gap dependence of $J_\perp^{\mathrm{f}}$ and $J_\perp^{\mathrm{b}}$.

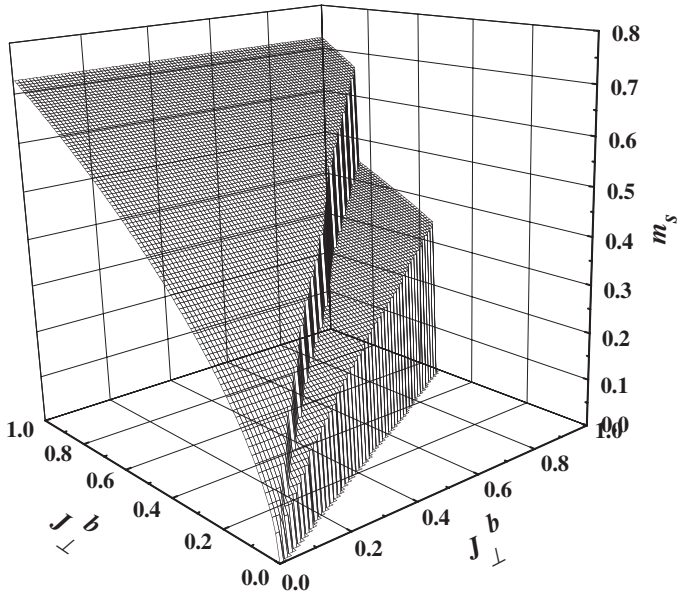

Figure 3. The spin gap dependence of $J_\perp^{\mathrm{f}}$ and $J_\perp^{\mathrm{b}}$.

In figures 2 and 3, we give the charge and spin gap dependence on $J_\perp^{\mathrm{f}}$ and $J_\perp^{\mathrm{b}}$. From these two figures, one can find that, as $J_\perp^{\mathrm{b}}$ is small enough, the charge gap (shown in figure 2) has zero value and the spin gap (shown in figure 3) has a finite value for a given $J_\perp^{\mathrm{f}}$. As $J_\perp^{\mathrm{b}}$ is increased to a critical value, the charge gap m_{c} will jump to a finite value. At the same time, the spin gap will jump down. With further increase of $J_\perp^{\mathrm{b}}$, the charge gap will jump to another greater value and the spin gap will be closed. These phenomena indicate that there occur two

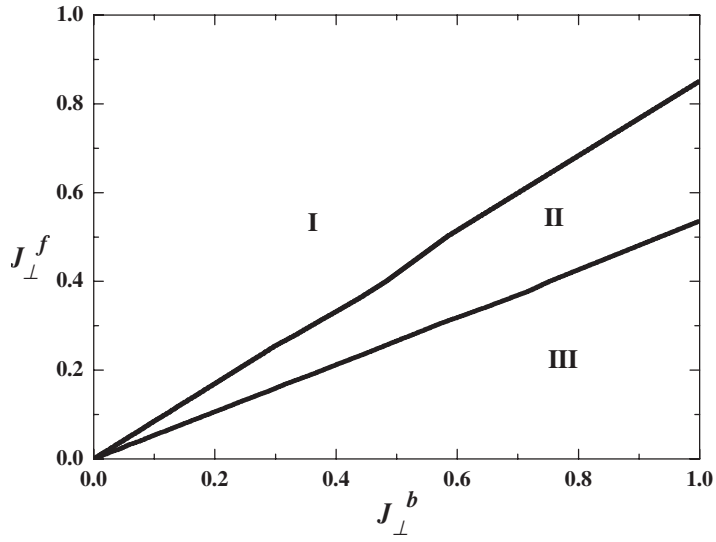

Figure 4. The phase diagram of our model. In region I, $m_c = 0$, $m_s \neq 0$. In region II, $m_c, m_s \neq 0$. In region III, $m_s = 0$, $m_c \neq 0$.

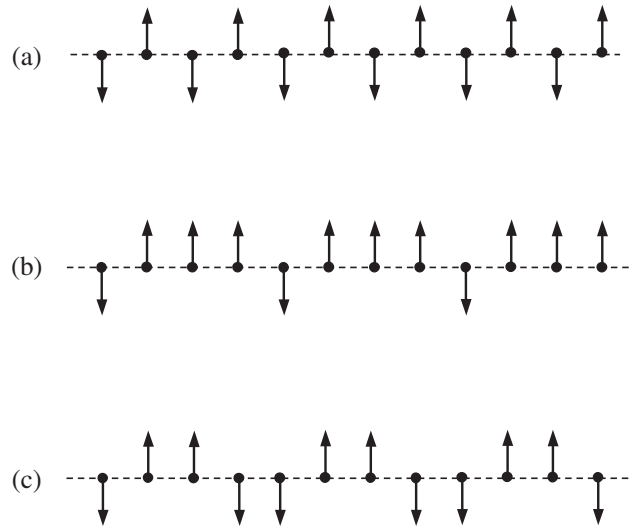

Figure 5. The static local spin configuration: (a) the local spin order in phase I, (b) the local spin order in phase II and (c) the local spin order in phase III.

phase transitions. Combining the results presented in figure 1, one can conclude that these transitions are first order.

A phase diagram is presented in figure 4. In this figure, the parameter space of $(J_\perp^f, J_\perp^b)$ can be divided into three regions. In region I, $m_c = 0$, $m_s \neq 0$; this means that it is a metal phase without QLRO in the spin part. In region II, the values of m_c and m_s are all nonzero; this is an insulating phase without QLRO. In region III, $m_c \neq 0$, $m_s = 0$; in this phase the spin excitation is free and has a QLRO.

Since the values of m_c and m_s can be calculated, via (20) we can give LSO of each phase, which is shown in figure 5. For the metal phase I, the LSO is shown in figure 5(a).

The local spins are arranged antiferromagnetically: $\tau_j^x = -(-1)^j$. This is just like the classical Néel order. For the insulating phase II, the LSO is given in figure 5(b). This kind of LSO can be viewed as a special kind of island phase with a spin gap. The LSO in phase III is given in figure 5(c). This phase without a spin gap is the true spin island phase [7] or spin dimerization [6] phase. These three phases can be understood on the basis of the competition of interactions in (3) as follows: in the metal phase I, $J_\perp^{\mathrm{f}}$ favours a staggered local magnetic moment, which can be treated as a staggered external magnetic field. The effective field may result in a spin gap and has no effect on the charge part. So there is only a spin gap, whereas the charge part is gapless. In this phase, only $J_\perp^{\mathrm{f}}$ contributes to the ground state. For the insulating phase II, the effects of $J_\perp^{\mathrm{b}}$ will appear. The order of the local spin will change to make the interaction of the charge part become nonzero. Thus, the charge gap will be opened. Comparing with the staggered local spin order in metal phase, one may find that the LSO in this insulating phase can be treated as a small departure from the staggered order. So the spin gap will be reduced. In the island phase III, the effects of $J_\perp^{\mathrm{f}}$ will totally disappear. The remainder of the interaction is $J_\perp^{\mathrm{b}}$, which will result in a charge gap and close the spin gap. The LSO is modulated by $\cos(\beta_{\mathrm{c}}\phi_{c,0} + 2k_{\mathrm{F}}ja)$, which reflects the conduction electron band filling. So the QLRO in this island phase is the contribution of $J_\perp^{\mathrm{b}}$. The phase evolution from I to III arises from the competition of $J_\perp^{\mathrm{f}}$ and $J_\perp^{\mathrm{b}}$. Phase II can be treated as a mixture of or phase intermediate between I and III.

In conclusion, we study the 1D Kondo lattice model in a special parameter case by the bosonization technique. It is confirmed that there does indeed exist an island phase with QLRO. In addition, we find that there may exist two other types of LSO. With changing model parameter, there are two first-order transitions. Although our work is restricted to a special parameter case, we argue that the local spin ordered ground state may still exist in the 1D KLM for the general case. For band quarter-filling ($n = 1/2$), there may exist yet other types of LSO.

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