Quantum phase transition in one dimensional extended Kondo lattice model away from half filling

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Abstract

We study one dimensional extended Kondo lattice model, described by the $t - J$ Hamiltonian for conduction electrons away from half filling and the Heisenberg Hamiltonian for localized spins at half filling. Following Shankar,[1] we find an effective field theory for this model, where doped holes are represented by massless Dirac fermions (holons) and spin excitations are fractionalized into relativistic bosons (spinons). These holons and spinons interact via $U(1)$ gauge fluctuations. Effects of Berry phase to the localized spins disappear due to the presence of Kondo couplings, causing the spinon excitations gapped. Furthermore, the gauge fluctuations are suppressed by hole doping. As a result, massive spinons are deconfined to arise in the localized spins unless the Kondo hybridization is strong enough. When the Kondo hybridization strength exceeds a certain value, we find that the localized spin chain becomes critical. This indicates that the present one dimensional Kondo lattice model exhibits a phase transition from a spin-gapped phase to a critical state in the localized spin chain, driven by the Kondo interaction.

Key words: one dimensional extended Kondo lattice model, holons, spinons, gauge fluctuations, Berry phase, deconfinement, phase transition

PACS: 75.30.Hx, 71.27.+a, 71.10.Hf, 75.30.Mb

One dimensional Kondo lattice model has been studied intensively. It seems to be clearly established that in the case of the half-filled conduction band the ground state is the Kondo insulator for any non-zero Kondo coupling, which has a gap in both spin and charge excitations.[2] Away from half filling, a paramagnetic metallic phase is expected to arise.[2,3,4] However, its nature remains controversial. Some numerical and analytical studies support the Tomonaga-Luttinger liquid with dominant correlations determined by conduc-

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tion electrons.[2,3] On the other hand, the existence of spin gap was reported in the paramagnetic metallic phase[2,4].

In the present paper we investigate one dimensional extended Kondo lattice model, described by the $t - J$ Hamiltonian for conduction electrons away from half filling and the Heisenberg Hamiltonian for localized spins at half filling [Eq. (1)]. An important difference from the previous studies is that we consider strongly correlated conduction electrons described by the $t - J$ model instead of non-interacting conduction electrons. Following Shankar,[1] one can represent the one dimensional $t - J$ model in terms of bosonic spinons for spin-fractionalized excitations and fermionic holons for doped holes, interacting via $U(1)$ gauge fluctuations [Eq. (2)]. Spinons carry the spin quantum number $1/2$ without the charge quantum number while holons carry the charge quantum number $+e$ without the spin quantum number. On the other hand, the Heisenberg model for the localized spins can be represented by bosonic spinons interacting via $U(1)$ gauge fluctuations with Berry phase [Eq. (2)]. Kondo couplings between the ”conduction” spinons and ”localized” spinons are taken into account [Eq. (2)].

Based on this low energy effective Lagrangian Eq. (2), we study effects of the Kondo interactions on the fate of spinons. We find that gapped spinon excitations are deconfined to appear in the localized spin chain unless the Kondo hybridization is strong enough. This originates from the fact that the contribution of Berry phase to the localized spinons disappears due to the Kondo couplings, causing the spinon excitations gapped, and gauge fluctuations are suppressed by hole doping, allowing deconfinement of the gapped spinons. On the other hand, if the Kondo hybridization strength exceeds a certain value, we find that the spinon excitations in the localized spin chain become critical. This indicates that the present one dimensional Kondo lattice model exhibits a phase transition from a spin-gapped phase to a critical state, driven by the Kondo interaction.

We consider a hole-doped antiferromagnetic spin chain in the presence of Kondo couplings with half-filled local magnetic moments

$$H = H_c + H_m + H_K,$$

$$H_c = -t \sum_{i=1}^{N} (c_{\sigma i}^\dagger c_{\sigma i+1} + h.c.) + J \sum_{i=1}^{N} \mathbf{s}_i \cdot \mathbf{s}_{i+1},$$

$$H_m = I \sum_{i=1}^{N} \mathbf{\tau}_i \cdot \mathbf{\tau}_{i+1},$$

$$H_K = J_K \sum_{i=1}^{N} \mathbf{s}_i \cdot \mathbf{\tau}_i.$$

(1)

Here the $t - J$ Hamiltonian $H_c$ describes a hole-doped antiferromagnetic spin
chain corresponding to the conduction band in the Kondo lattice model, where \( t \) and \( J \) represent the strength of hopping and antiferromagnetic correlations for the conduction electrons, respectively. The Heisenberg Hamiltonian \( H_m \) depicts a half-filled spin chain of localized magnetic moments, where \( I \) is the strength of antiferromagnetic correlations between the localized spins. Strongly correlated conduction electrons and localized magnetic moments are antiferromagnetically correlated via the Kondo coupling \( H_K \) with the strength \( J_K \). If strong electron-electron correlations represented by the Heisenberg coupling term \( J \sum_{i=1}^{N} \mathbf{s}_i \cdot \mathbf{s}_{i+1} \) and the no-double-occupancy constraint \( \sum_{\sigma=1}^{2} c_{\sigma i}^\dagger c_{\sigma i} \leq 1 \) are neglected, this Hamiltonian is naturally reduced to the conventional Kondo lattice model. In this respect we deal with both electron-electron and electron-local moment interactions on an equal footing in the presence of hole doping.

In passing, we review physics of the one dimensional \( t - J \) Hamiltonian. In the absence of hole doping hopping of electrons is suppressed, thus the \( t - J \) Hamiltonian is reduced to the Heisenberg Hamiltonian describing the antiferromagnetic spin chain. Low energy physics of the quantum spin chain can be described by the O(3) non-linear \( \sigma \) model with Berry phase. Utilizing the \( CP^1 \) representation, one can express the non-linear \( \sigma \) model in terms of bosonic spinons interacting via compact U(1) gauge fields in the presence of the Berry phase contribution. Since the Berry phase term is ignorable in the case of integer spin, strong quantum fluctuations originating from low dimensionality lead the integer spin chain to be disordered, causing the bosonic spinons gapped.[5] These massive spinons are confined via strong gauge fluctuations, resulting in spin excitons (spinon-antispinon bound states) as elementary excitations.[5,6]

In the case of half-odd integer spin the Berry phase plays a crucial role to cause destructive interference between quantum fluctuations, thus weakening the quantum fluctuations. Owing to the Berry phase contribution the half-odd integer spin chain is expected to be ordered. But, low dimensionality leads the system to be not ordered but critical, causing the spinons gapless.[5] These massless spinons are deconfined because critical fluctuations of the spinons weaken gauge fluctuations via screening.[6,7] In this respect the half-odd integer spin chain is considered to be the Tomonaga-Luttinger liquid.[5]

When holes are doped to the antiferromagnetic spin chain, Shankar showed that doped holes can be expressed by massless Dirac fermions dubbed holons and these fermionic holons interact with the bosonic spinons via U(1) gauge fluctuations.[1] The presence of massless Dirac fermions completely alters the resulting phase in the absence of those. Massless Dirac fermions are well known to kill the Berry phase contribution.[8] Then, the bosonic spinons in the doped half-odd integer spin chain are expected to be massive like those in the undoped integer spin chain. But, these spinons are not confined in contrast to the case of the integer spin chain[8,1] because the gauge fluctuations become massive due to the massless Dirac fermions, thus ignored in the low energy
limit. A spin liquid state with gapped spinon excitations emerges in the doped antiferromagnetic spin chain. Furthermore, one can find that there are superconducting correlations of doped holes, resulting from gapless charge fluctuations (holons). It should be noted that this result is exact in the low energy limit.

The present problem is more complex than the above owing to the presence of Kondo couplings with local magnetic moments. Following Shankar, we obtain an effective Lagrangian for Eq. (1)

\[
S_{\text{eff}} = S_c + S_m + S_K,
\]

\[
S_c = \int d^2x \left[ (|\partial_\mu - ia_\mu| z_\sigma|^2 + m_z^2 z_\sigma|^2 + \frac{u_z}{2} (|z_\sigma|^2)^2 + \frac{1}{2g_z^2} |\epsilon_{\mu\nu}\partial_\mu a_\nu|^2 - iS\epsilon_{\mu\nu}\partial_\mu a_\nu \right]
\]

\[
+ \int d^2x \left[ \bar{\psi}_A \gamma_\mu (\partial_\mu + ia_\mu) \psi_A + \bar{\psi}_B \gamma_\mu (\partial_\mu - ia_\mu) \psi_B \right],
\]

\[
S_m = \int d^2x \left[ (|\partial_\mu - ic_\mu| b_\sigma|^2 + m_b^2 b_\sigma|^2 + \frac{u_b}{2} (|b_\sigma|^2)^2 + \frac{1}{2g_b^2} |\epsilon_{\mu\nu}\partial_\mu c_\nu|^2 - iS\epsilon_{\mu\nu}\partial_\mu c_\nu \right]
\]

\[
S_K = \sum \int d^2x \frac{J_K}{4} \gamma_\alpha \gamma_\beta z_\sigma \cdot \gamma_\gamma \gamma_\delta b_\sigma.
\]

Here \(z_\sigma\) and \(\psi_A(B)\) represent a bosonic spinon with spin \(\uparrow, \downarrow\) and a fermionic holon in a sublattice \(A(B)\) in the conduction chain, respectively. The spinons and holons interact via the U(1) gauge field \(a_\mu\) with the coupling strength \(g_z\). \(m_z\) and \(u_z\) are the mass and local interaction strength of the conduction spinons, respectively. \(S\) in the Berry phase term \(iS\epsilon_{\mu\nu}\partial_\mu a_\nu\) represents the value of spin 1/2. \(b_\sigma\) is a bosonic spinon in the chain of local magnetic moments. These spinons interact with each other via the other U(1) gauge field \(c_\mu\) with the coupling strength \(g_b\). \(m_b\) and \(u_b\) are the mass and local interaction strength of the local spinons, respectively.

New physics would arise from the Kondo coupling term \(S_K\) between the two spinons, \(z_\sigma\) and \(b_\sigma\). In order to treat the Kondo coupling term, we perform the usual Hubbard-Stratonovich transformation, and obtain the following one body effective action\[10,11\] \(S_K = \sum \int d^2x \left[ \frac{J_K}{4} \Delta_0^2 - \Delta_0 e^{i\phi} z_\sigma \right] - h.c. \). Here \(\Delta_0\) is an amplitude of the hybridization order parameter \(\Delta = \Delta_0 e^{i\phi}\) between the \(z_\sigma\) and \(b_\sigma\) spinons, and \(\phi\) is its phase-fluctuation field. The amplitude is given by \(\Delta_0 = \frac{\lambda_{M}}{4} |z_\sigma| |b_\sigma|^2 \). In the present paper we concentrate on phase fluctuations of the hybridization order parameter. They are controlled by the low energy effective action \(S_\phi = \sum \int d^2x \frac{\rho}{2} |\partial_\mu \phi - a_\mu + c_\mu|^2\), where \(\rho\) is the stiffness parameter proportional to \(\Delta_0^2\).[11]

In order to take phase fluctuations in the Kondo coupling term, we perform the gauge transformation of \(\tilde{b}_\sigma = e^{i\phi} b_\sigma\) and \(\tilde{c}_\mu = c_\mu + \partial_\mu \phi\).[11] Then, Eq. (2) reads
\[
S_{\text{eff}} = \int d^2x \left[ \left( \partial_\mu - ia_\mu \right) z_\sigma \right]^2 + m^2 z_\sigma^2 + \frac{u_z}{2} \left( |z_\sigma| \right)^2 + \frac{1}{2g_z^2} \epsilon_{\mu\nu} \partial_\mu a_\nu \right]^2 - iS\epsilon_{\mu\nu} \partial_\mu a_\nu \right] 
+ \int d^2x \left[ \bar{\psi}_A \gamma_\mu (\partial_\mu + ia_\mu) \psi_A + \bar{\psi}_B \gamma_\mu (\partial_\mu - ia_\mu) \psi_B \right] 
+ \int d^2x \left[ \left( \partial_\mu - ic_\mu \right) b_\sigma \right]^2 + m_b^2 |b_\sigma| \right]^2 + \frac{ub}{2} \left( |b_\sigma| \right)^2 \right] 
+ \frac{1}{2g_b^2} \epsilon_{\mu\nu} \partial_\mu \bar{c}_\nu - \epsilon_{\mu\nu} \partial_\mu \partial_\nu \phi \right|^2 
+ \frac{1}{2g_b^2} \epsilon_{\mu\nu} \partial_\mu \bar{c}_\nu - \epsilon_{\mu\nu} \partial_\mu \partial_\nu \phi \right] - iS\epsilon_{\mu\nu} \partial_\mu \bar{c}_\nu + iS\epsilon_{\mu\nu} \partial_\mu \partial_\nu \phi \right] 
+ \int d^2x \left[ \frac{\rho}{2} |a_\mu - \bar{c}_\mu|^2 - \Delta_0 z_\sigma^{\dagger} b_\sigma - h.c. + \frac{4}{J_K} \Delta_0^2 \right]. \tag{3}
\]

In the action of the renormalized local spinons \( \bar{b}_\sigma \), the Berry phase-induced term \( iS \int d^2x \epsilon_{\mu\nu} \partial_\mu \partial_\nu \phi \) can be expressed by \( iS \int d^2x \epsilon_{\mu\nu} \partial_\mu \partial_\nu \phi = iS \int dx \partial_\mu \phi = i2\pi S n = i\pi n. \) This is nothing but a vortex contribution in the phase field \( \phi \). \( n \) is an integer representing a vortex charge. Vortex excitations would break phase coherence, making the hybridization disappear. But, the Berry phase-induced term plays a role to suppress single vortex excitations. When a single vortex configuration appears, this complex phase term gives a factor \(-1\) to the partition function of the action Eq. (3). This destructive interference originating from the Berry phase contribution for single vortex excitations leads to suppression of single vortex excitations, indicating no vortex condensation. As a result, phase coherence is sustained, i.e., \( \langle e^{i\phi} \rangle \neq 0 \), resulting in the hybridization of the two spinons.

This mechanism is similar to that for the suppression of strong gauge fluctuations (instantons) between topologically inequivalent gauge vacua owing to the Berry phase contribution in the half-odd integer spin chain,\([6]\) as discussed before. The suppression of instanton excitations in gauge fluctuations increases the tendency of antiferromagnetic ordering. In a different angle the condensation of the order parameter \( \Delta \) means that the Kondo couplings are relevant in the context of renormalization group. The relevance of the Kondo couplings causes the mass term \( \frac{\rho}{2} |a_\mu - \bar{c}_\mu|^2 \). This is nothing but the Anderson-Higgs mechanism, allowing us to set \( \bar{c}_\mu = a_\mu \) in the low energy limit. Then, we obtain the following effective action

\[
S_{\text{eff}} = \int d^2x \left[ \left( \partial_\mu - ia_\mu \right) z_\sigma \right]^2 + m^2 z_\sigma^2 + \frac{u_z}{2} \left( |z_\sigma| \right)^2 + \frac{1}{2g_z^2} \epsilon_{\mu\nu} \partial_\mu a_\nu \right]^2 
+ \int d^2x \left[ \bar{\psi}_A \gamma_\mu (\partial_\mu + ia_\mu) \psi_A + \bar{\psi}_B \gamma_\mu (\partial_\mu - ia_\mu) \psi_B \right] 
+ \int d^2x \left[ \left( \partial_\mu - ia_\mu \right) \bar{b}_\sigma \right]^2 + m_b^2 |b_\sigma| \right]^2 + \frac{ub}{2} \left( |b_\sigma| \right)^2 \right] 
+ \frac{1}{2g_b^2} \epsilon_{\mu\nu} \partial_\mu \bar{b}_\sigma - \epsilon_{\mu\nu} \partial_\mu \partial_\nu \phi \right] 
+ \frac{4}{J_K} \Delta_0^2 - \Delta_0 z_\sigma^{\dagger} b_\sigma - h.c. \right]. \tag{4}
\]

Surprisingly, only one gauge fluctuations remain as a result of the relevant
Kondo coupling. A similar result is also obtained in Ref. [11]. Furthermore, considering $2S = 1$, one can easily find that the following result
\[ i S \epsilon_{\mu\nu} \partial_\mu a_\nu + i S \epsilon_{\mu\nu} \partial_\mu \tilde{c}_\nu = i 2 S \epsilon_{\mu\nu} \partial_\mu a_\nu \]
yields the Berry phase contribution to vanish. This is well known in the non-linear $\sigma$ model approach to the spin-ladder system.[12]

We check whether our present analysis reproduces the known results in the absence of hole doping. Considering a half-filled conduction chain, the present problem is the same as the two-leg-ladder problem. It is well known that the ground state is the phase of Kondo singlets.[13] Elementary excitations are singlet to triplet excitations with spin 1.[13] Eq. (4) without massless Dirac fermions recovers these well known properties. As discussed earlier, Eq. (4) shows condensation of the hybridization order parameter $< \Delta >$ ≠ 0, indicating the presence of Kondo singlets. The formation of Kondo singlets gives a mass gap to both the $z_\sigma$ and $\tilde{b}_\sigma$ spinons. These massive spinons are confined via strong gauge fluctuations $a_\mu$.[5] As a result, elementary excitations are Kondo triplet excitations $z_\sigma^\dagger \tilde{b}_\sigma$ with spin 1.

Now we investigate the role of hole doping in this system. In order to treat massless Dirac fermions, we utilize the well known bosonization technique[1,8]

\[
\bar{\psi}_A \gamma_\mu \partial_\mu \psi_A = \frac{1}{2} (\partial_\mu \theta_A)^2, \quad \bar{\psi}_B \gamma_\mu \partial_\mu \psi_B = \frac{1}{2} (\partial_\mu \theta_B)^2, \\
\bar{\psi}_A \gamma_\mu \psi_A = \frac{1}{\sqrt{\pi}} \epsilon_{\mu\nu} \partial_\nu \theta_A, \quad \bar{\psi}_B \gamma_\mu \psi_B = \frac{1}{\sqrt{\pi}} \epsilon_{\mu\nu} \partial_\nu \theta_B, \\
\tag{5}
\]

where $\theta_A$ and $\theta_B$ are bosonic fields in each sublattice. These bosonic field variables are associated with collective density fluctuations of the Dirac fermions.

Inserting these into the above action Eq. (4), we obtain an effective action

\[
S_{\text{eff}} = \int d^2x \left[ \left( \partial_\mu - i a_\mu \right) z_\sigma \right]^2 + m_z^2 |z_\sigma|^2 + \frac{u_z}{2} (|z_\sigma|^2)^2 + \frac{1}{2 g_z^2} |\epsilon_{\mu\nu} \partial_\mu a_\nu|^2 \\
+ \int d^2x \left[ \frac{1}{2} (\partial_\mu \theta_+)^2 + \frac{1}{2} (\partial_\mu \theta_-)^2 + i \sqrt{\frac{2}{\pi}} \epsilon_{\mu\nu} \partial_\mu a_\nu \right] \\
+ \int d^2x \left[ \left( \partial_\mu - i a_\mu \right) \tilde{b}_\sigma \right]^2 + m_z^2 |\tilde{b}_\sigma|^2 + \frac{u_b}{2} (|\tilde{b}_\sigma|^2)^2 + \frac{1}{2 g_b^2} |\epsilon_{\mu\nu} \partial_\mu a_\nu|^2 \\
+ \int d^2x \left[ \frac{4}{J_K} \Delta_0^2 - \Delta_0 z_\sigma^\dagger \tilde{b}_\sigma - \text{h.c.} \right] \\
\tag{6}
\]

with $\theta_+ = \frac{1}{\sqrt{2}} (\theta_A + \theta_B)$ and $\theta_- = \frac{1}{\sqrt{2}} (\theta_A - \theta_B)$. The presence of massless Dirac fermions results in a mass gap to the U(1) gauge field $a_\mu$.[8,1,9] Integrating over the $\theta_-$ fields, one can see that a mass term of the gauge field appears, allowing to ignore the U(1) gauge fluctuations in the low energy limit. This causes deconfinement of the massive spinons in contrast to the half-filled case.
The resulting low energy effective action is given by

\[
S_{\text{eff}} = \int d^2x \left[ |\partial_\mu z_\sigma|^2 + m_z^2 |z_\sigma|^2 + |\partial_\mu \tilde{b}_\sigma|^2 + m_\tilde{b}^2 |\tilde{b}_\sigma|^2 + \frac{4}{J_K} \Delta_0^2 - \Delta_0 z_\sigma \tilde{b}_\sigma - \text{h.c.} \right] + \int d^2x \frac{1}{2} (\partial_\mu \theta_\sigma)^2. \tag{7}
\]

Performing the canonical transformation for the \(z_\sigma\) and \(\tilde{b}_\sigma\) bosons, one can solve the Kondo hybridization to find Bogliubov quasispinons. The mass gap of the quasispinon excitation is given by \(M_\pm^2 = \frac{1}{2} \left( m_z^2 + m_\tilde{b}^2 \pm \sqrt{(m_z^2 - m_\tilde{b}^2)^2 + (2\Delta_0)^2} \right)\), originating from electron-electron and electron-local moment interactions. Unless the Kondo hybridization \(\Delta_0\) is strong enough to satisfy \(\Delta_0 \geq m_z m_\tilde{b}\), both quasispinon excitations are gapped although this spin gap is exponentially small. This indicates that despite half filling the massive spinons are deconfined to emerge in the local spin chain, allowed by the relevant Kondo coupling and hole doping to the conduction chain. On the other hand, if \(\Delta_0 \geq m_z m_\tilde{b}\) is satisfied, low energy quasispinons become condensed owing to electron-electron and electron-local moment interactions. Unless the Kondo hybridization \(\Delta_0\) is strong enough to satisfy \(\Delta_0 \geq m_z m_\tilde{b}\), both quasispinon excitations are gapped although this spin gap is exponentially small. This indicates that despite half filling the massive spinons are deconfined to emerge in the local spin chain, allowed by the relevant Kondo coupling and hole doping to the conduction chain. On the other hand, if \(\Delta_0 \geq m_z m_\tilde{b}\) is satisfied, low energy quasispinons become condensed owing to electron-electron and electron-local moment interactions. Because low dimensionality prohibits the localized spin chain from ordering, it would be critical. In this case the Tomonaga-Luttinger liquid is expected. Introducing an electromagnetic field \(A_\mu\), we obtain the coupling term of \(i\sqrt{2} \theta_\pm \epsilon_{\mu \nu} \partial_\mu A_\nu\). A mass of the electromagnetic field arises when the \(\theta_\pm\) fields are integrated out. This implies superconductivity in the doped spin chain, consistent with the result of Shankar.[1]

In this paper we found that the present one dimensional Kondo lattice model [Eq. (1)] shows a phase transition from a spin-gapped phase to a spin-critical state as increasing the Kondo coupling strength. Resorting to the effective field theory [Eq. (2)] for this model, we showed that Berry phase vanishes due to Kondo couplings [Eq. (4)] and U(1) gauge fluctuations are suppressed by hole doping [Eq. (6)]. From the resulting effective action [Eq. (7)] we found that gapped spinon excitations can emerge in the half-filled antiferromagnetic spin chain when the Kondo hybridization is not strong enough, while the spinon excitations can be critical if the Kondo hybridization strength is beyond a certain value. We expect that the present formulation can be easily extended in two spacial dimensions.[14] It will be interesting to examine the issue of the spinon deconfinement in the two dimensional Kondo lattice model.

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