Stability of Insulating Phase in the Chiral Kondo Lattice Model

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In this work, the stability of the insulating phase of the 1D chiral Kondo lattice model is studied at half-filling, within the framework of self-consistent variational theory. It is found that arbitrarily small interaction would drive the system from a conducting phase to an insulating phase, in spite of the chirality of the conducting band.

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Recently, there have been considerable interests in theoretical studies of Kondo insulators and heavy fermion systems, the class of rare earth compounds [1–19]. The mechanism for these systems to become insulating is due to the interaction between the conducting electrons and the array of localized impurity spins. On a one dimensional lattice, when the electrons hop between nearest-neighboring sites, the metal-insulator phase transition in the system at half-filling described by the Kondo lattice model has been investigated with various methods [8,11,18,7,17,16]. It was found that the simple Fermi liquid fixed point of the system ($J = 0$) is unstable against infinitesimally small interaction. Arbitrarily small interaction would drive the system from conducting phase to an insulating phase.

More recently, Carruzzo and Yu develop a novel self-consistent variational approach, to investigate again whether an external magnetic field could induce a metal-insulator phase transition in the Kondo insulators [9]. It is found that the insulating gap never vanishes for any value of magnetic field, suggesting no field-induced metal-insulator transition, in contrast to the predictions by the slave boson mean field theory [12–14,9].

In the self-consistent variational theory, two scattering processes between the electrons and the impurity spins are kept in consideration: the process of no-spin-flip and zero momentum transfer ($S_1$), and that of spin-flip and $\pi$ momentum transfer ($S_2$). In absence of external magnetic field, the approach has indicated that the insulating phase is stable even for arbitrarily small interaction parameter, that is, $J_c = 0^+$, with a small but finite energy gap decaying exponentially, consistent with the previous results obtained through other methods [9]. In the following, we use their approach to study the stability of the insulating phase of the 1D chiral Kondo lattice model introduced recently by us. We find that at half-filling, the insulating phase is stable for any nonzero coupling constant. The insulating gap is computed explicitly for this system.

The 1D chiral Kondo lattice model consists of conducting electrons moving in one direction on a close chain. At each lattice site, the conducting electrons interact with a localized impurity spin through spin exchange interaction. The system is described in terms of the following Hamiltonian:
\[ H_{ck} = \sum_{k, \sigma = \uparrow, \downarrow} e(k) c_{k\sigma}^\dagger c_{k\sigma} + \sum_{i=1}^{L} c_{i\alpha}^\dagger \frac{\vec{\sigma}_{\alpha\beta}}{2} c_{i\beta} \cdot \vec{S}_f(i) - h \sum_{i} [c_{i\alpha} c_{i\alpha}^\dagger + s^z_f(i)], \]

where the conduction band spectrum is \( e(k) = -tk \), with \(-\pi(1-1/L) \leq k \leq \pi(1-1/L)\), in the momentum space. \( J \) is the coupling constant between the local impurity moments and the conducting electrons, and \( h \) is the external magnetic field. The local moments are described by the spin 1/2 operators, that is, \( [S^x_f(i), S^y_f(i)] = iS^z_f(i) \) (plus two other commutation relations obtained by the cyclic permutations of \( x, y, z \)), with the relation \( S^2_f(i) = 3/4 \), for all the sites \( i = 1, 2, \cdots, L \). In the following, for simplicity, we always restrict ourselves to the parameter range \( t > 0 \) and antiferromagnetic interaction \( J \geq 0 \). The dispersion relation of the conducting band \( e(k) = -|t|k \) yields the electron group velocity \( v = \partial e(k)/\partial k = -|t| \).

Below, we only consider the thermodynamic limit \( L \rightarrow \infty \).

In the extreme limit \( J = +\infty \), away from half-filling, we have found that the wavefunctions of the system are the RVB-type Jastrow product wavefunctions \[21\]. The interesting aspect is that in this limit various correlations of the system can be computed exactly in compact form. Moreover in this limit, the system obviously is a conductor away from half-filling, while it is an insulator at half-filling. For very large but finite \( J \) and at half-filling, each impurity spin will also attempt to form a singlet with one conduction electron at each site, to lower the energy of the system as much as possible. To transfer one electron with the long range hopping matrix element (corresponding to the chiral band) from one site to another would break two singlets, giving rise to a charge gap of the order \( O(J) \), making the system an insulator. One interesting issue is the stability of the insulating phase. In the following, we’ll investigate the stability of the insulating phase of the system when one changes \( J \), and we’ll restrict ourselves to the case of half-filling.

Following Popov and Fedotov \[20\], one first introduces fermion operators \( \{f_{j\alpha}^\dagger, f_{j\alpha}\} \), \( j \in \{1, 2, \cdots, L\}, \alpha \in \{+, -\} = \{\uparrow, \downarrow\} \) to describe the impurity spins, together with an additional term \(-\frac{i\pi}{2\beta} \sum_{j\alpha} f_{j\alpha}^\dagger f_{j\alpha} \) to take into account the constrain that every site is occupied by one impurity. The partition function of the system thus takes the following form:

\[ Z = \int Dc^\dagger Dc Df^\dagger Df \ e^{-\int_0^\beta dt \int_1^L \sum_{\alpha = \pm} c_{\alpha}(t) \partial_t c_{\alpha}(t) + \sum_{i=1}^{L} \sum_{\alpha = \pm} f_{\alpha}(t) \partial_t f_{\alpha}(t) + H(t)}, \]

(2)
where \( c \) and \( f \) are Grassman variables, and \( H(\tau) \) is given in momentum space by

\[
H(\tau) = \sum_k \sum_{\alpha=\bar{\alpha}} [c(k) - \alpha \hbar/2] c^\dagger_{\alpha}(k, \tau) c_{\alpha}(k, \tau) + \sum_k \sum_{\alpha=\bar{\alpha}} \left[ -\frac{i\pi}{2\beta} - \alpha \hbar/2 \right] f^\dagger_{\alpha}(k, \tau) f_{\alpha}(k, \tau) +
\]

\[
+ \frac{J}{4L} \sum_{k_1, \ldots, k_4: a_{\alpha}=\bar{\alpha}} \delta(k_1 - k_2 + k_3 - k_4) f^\dagger_{\alpha}(k_1, \tau) f_{\alpha}(k_2, \tau) c^\dagger_{\gamma}(k_3, \tau) c_{\delta}(k_4, \tau) \tilde{\sigma}_{\alpha\beta} \cdot \tilde{\sigma}_{\gamma\delta}.
\]

Furthermore, introducing “right” and “left” operators for electrons and impurities, i.e.

\[
\phi_{a,\alpha}(k, \tau) = \begin{cases} \phi_{R,\alpha}(k, \tau) = \phi_{\alpha}(k, \tau) & k > 0, \ a = 0 \\ \phi_{L,\alpha}(k, \tau) = \phi_{\alpha}(k - \pi, \tau) & k > 0, \ a = 1 \end{cases}
\]

with \( a \in \{ R, L \} = \{ 0, 1 \} \), and \( \phi_{a,\alpha} \) standing either for \( c_{a,\alpha} \) or for \( f_{a,\alpha} \), one can write \( H(\tau) \) as follows:

\[
H(\tau) = \sum_{k>0} \sum_{\alpha=0,1} \sum_{a=\bar{a}} [c(k - a\pi) - \alpha \hbar/2] c^\dagger_{a,\alpha}(k, \tau) c_{a,\alpha}(k, \tau) +
\]

\[
+ \sum_{k>0} \sum_{\alpha=0,1} \sum_{a=\bar{a}} \left[ -\frac{i\pi}{2\beta} - \alpha \hbar/2 \right] f^\dagger_{a,\alpha}(k, \tau) f_{a,\alpha}(k, \tau) +
\]

\[
+ \sum_{k_1, k_2>0} \sum_{a, b=0,1} \sum_{\alpha=\bar{\alpha}} f^\dagger_{a,\alpha}(k_1, \tau) \tilde{C}_{a\beta} f_{b,\beta}(k_2, \tau),
\]

where

\[
\tilde{C}_{a\beta} = \frac{J}{4L} \sum_{k_3, k_4>0} \sum_{c,d=0,1} \sum_{\alpha=\bar{\alpha}} \sum_{\gamma, \delta=\bar{\delta}} c^\dagger_{c,\gamma}(k_3, \tau) c_{d,\delta}(k_4, \tau) [\tilde{\sigma}_{a\beta} \cdot \tilde{\sigma}_{\gamma\delta}] \times
\]

\[
\times \delta(k_1 - k_2 + k_3 - k_4 - (a - b + c - d)\pi),
\]

with \( \tilde{\sigma}_{a\beta} \cdot \tilde{\sigma}_{\gamma\delta} = \alpha\gamma\delta_{a,\beta}\delta_{\gamma,\delta} + 2\delta_{a,-\beta}\delta_{\gamma,-\delta} \), and we have neglected the \( k = 0 \) terms.

Following Ref. [9], we shall keep only the scattering processes:

\[
S_1 : \ k_1 = k_2, \ k_3 = k_4, \ a = b, \ c = d, \alpha = \beta, \gamma = \delta, \]

\[
S_2 : \ k_1 = k_2, \ k_3 = k_4, \ a = b + 1, \ c = d + 1 \ (\text{mod} 2), \alpha = -\beta, \gamma = -\delta.
\]

The two scattering processes correspond to the following effective interaction: \( S_1 : \)

\[
\frac{J}{4L} \sum_{j, \gamma} (-1)^j c^\dagger_{j,\gamma} c_{j,\gamma}, \quad S_2 : \]

\[
\frac{J}{4L} \sum_{j, \gamma} (-1)^j f^\dagger_{j,\alpha} f_{j,\alpha} \sum_{j, \gamma} (-1)^j c^\dagger_{j,\gamma} c_{j,\gamma}. \]

Therefore, \( \tilde{C} \) is the \( 4 \times 4 \) matrix given in this approximation by
\[ \tilde{C} = \begin{pmatrix} \tilde{C}_{++}^{ab} & \tilde{C}_{+-}^{ab} \\ \tilde{C}_{-+}^{ab} & \tilde{C}_{--}^{ab} \end{pmatrix} = \begin{pmatrix} \tilde{C}_{++} & \tilde{C}_{+-} \sigma_x \\ \tilde{C}_{-+} \sigma_x & \tilde{C}_{--} + \tilde{1} \end{pmatrix}, \] (8)

with matrix elements given by

\[ \tilde{C}_{++} = \frac{J}{4L} \sum_{k>0} \sum_{b=0,1} \sum_{\gamma=\pm} c_{b,\gamma}^\dagger(k,\tau) c_{b,\gamma}(k,\tau) \gamma, \]
\[ \tilde{C}_{+-} = \frac{J}{2L} \sum_{k>0} \sum_{b=\pm} c_{-b,-}^\dagger(k,\tau) c_{b,+}(k,\tau), \]
\[ \tilde{C}_{-+} = \frac{J}{2L} \sum_{k>0} \sum_{b=\pm} c_{-b,+}^\dagger(k,\tau) c_{b,-}(k,\tau). \] (9)

Introducing 4-vector \( f^\dagger = (f_0^\dagger, f_1^\dagger, f_0^\dagger, f_1^\dagger) \), the interaction term is thus given by

\[ H_I(\tau) = \sum_{k>0} f(k,\tau) \tilde{C} f(k,\tau). \] (10)

We can then rewrite the partition function in terms of following functional integral

\[ Z \approx \int Dc^\dagger Dc Df^\dagger Df \exp\{-[S_{oc}[c^\dagger, c] + S_{of}[f^\dagger, f] + S_{fc}[c^\dagger, c, f^\dagger, f]]\}, \] (11)

where the various actions are given by

\[ \begin{cases} S_{oc} = \frac{1}{\beta} \sum_{k>0} \sum_\omega c^\dagger(k,\omega) D_0 c(k,\omega) \\ (D_0)^{ab}_{\alpha\beta} = \delta_{a,b} \delta_{\alpha,\beta} [i\omega - \alpha \hbar/2 + e(k - a\pi)] \end{cases} \]
\[ \begin{cases} S_{of} = \frac{1}{\beta} \sum_{k>0} \sum_\omega f^\dagger(k,\omega) F_0 f(k,\omega) \\ (F_0)^{ab}_{\alpha\beta} = \delta_{a,b} \delta_{\alpha,\beta} [i\omega - \frac{\pi}{2\beta} - \alpha \hbar/2] \end{cases} \] (12)

and \( \phi(k,\tau) = \frac{1}{\beta} \sum_{\omega=(2n+1)\pi} \phi(k,\omega) e^{i\omega \tau} \). Keeping only the terms with \( \omega_1 = \omega_2 \) (thus \( \omega_3 = \omega_4 \)) as considered in Ref. \[9\], we have

\[ \begin{cases} S_{fc} = \frac{1}{\beta^2} \sum_{k>0} \sum_\omega f^\dagger(k,\omega) C f(k,\omega) \\ C = \begin{pmatrix} \tilde{C}_{++} & \tilde{C}_{+-} \sigma_x \\ \tilde{C}_{-+} \sigma_x & \tilde{C}_{--} + \tilde{1} \end{pmatrix} \end{cases} \] (13)

with matrix elements:

\[ \tilde{C}_{++} = \frac{J}{4L\beta} \sum_{k>0} \sum_{\omega} \sum_{b,\gamma} c_{b,\gamma}^\dagger(k,\omega) c_{b,\gamma}(k,\omega) \gamma, \]
\[ \tilde{C}_{+-} = \frac{J}{2L\beta} \sum_{k>0} \sum_{\omega} \sum_{b} c_{-b,-}^\dagger(k,\omega) c_{b,+}(k,\omega), \]
\[ \tilde{C}_{-+} = \frac{J}{2L\beta} \sum_{k>0} \sum_{\omega} \sum_{b} c_{-b,+}^\dagger(k,\omega) c_{b,-}(k,\omega). \] (14)
For this chiral Kondo lattice model, we follow the self-consistent variational approach of Carruzzo and Yu. To find the quasi-particle spectrum of the electron degrees of freedom, one first integrates out the impurity degrees of freedom, to obtain the effective action of the electrons. When integrating out the Popov-Fedotov fermions for the impurity spins, one replaces the bare propagator with its dressed version, taking into account the effects of the conduction electrons on the impurity spins themselves. After some algebraic manipulation, we obtain the effective functional integral for the electron degrees of freedom:

$$Z = \int Dc^\dagger Dc \exp \left( -S_{eff}[c^\dagger, c] \right),$$

with the effective action

$$S_{eff} = \frac{1}{\beta} \sum_\omega \sum_{k>0} c^\dagger(k, \omega) D(k, \omega) c(k, \omega),$$

where using the same approximation of Ref. [9], the corresponding matrix $D$ is found to be

$$D = \begin{pmatrix}
i\omega - \bar{h} + e(k) & 0 & 0 & -\frac{JC_\pi}{4\lambda} \\
0 & i\omega - \bar{h} + e(k - \pi) & -\frac{JC_\pi}{4\lambda} & 0 \\
0 & -\frac{JC_\pi}{4\lambda} & i\omega + \bar{h} + e(k) & 0 \\
-\frac{JC_\pi}{4\lambda} & 0 & 0 & i\omega + \bar{h} + e(k - \pi)
\end{pmatrix},$$

where $e(k) = -kt$, $C_0$ and $C_\pi$ are the mean field parameters

$$C_0 = \lim_{\beta \to \infty} \frac{<C_{++}>}{\beta}, C_\pi = \lim_{\beta \to \infty} \frac{<C_{+-}>}{\beta},$$

and

$$\lambda = [(h/2 - C_0)^2 + C_\pi^2]^{1/2}, \bar{h} = h/2 - \frac{J}{4\lambda} \left( \frac{h}{2} - C_0 \right).$$

Finding the inverse of the matrix $D$, with the analytical continuation $i\omega \to w$, the poles of the propagators yield the quasiparticle dispersion relations. We have found that there also exist four bands $E_1(k), E_2(k), E_3(k)$ and $E_4(k)$, given below:

$$E_1(k) = kt - \pi t/2 - [(\pi t/2 + |\bar{h}|)^2 + (JC_\pi/4\lambda)^2]^{1/2},$$

$$E_2(k) = kt - \pi t/2 - [(\pi t/2 - |\bar{h}|)^2 + (JC_\pi/4\lambda)^2]^{1/2},$$

$$E_3(k) = kt - \pi t/2 + [(\pi t/2 - |\bar{h}|)^2 + (JC_\pi/4\lambda)^2]^{1/2},$$

$$E_4(k) = kt - \pi t/2 + [(\pi t/2 + |\bar{h}|)^2 + (JC_\pi/4\lambda)^2]^{1/2}.$$
Let us only consider the case of no external magnetic field \( h = 0 \). For sufficiently large coupling constant \( J \), when the system is in the insulating phase, the upper two bands \( E_3(k) \) and \( E_4(k) \) are positive, the lower two bands \( E_1(k) \) and \( E_2(k) \) are negative. The energy gap of the system is given by

\[
\Delta = E_3(0) - E_2(\pi).
\]

The self-consistent equations for the mean field parameters \( C_0 \) and \( C_\pi \) are given by:

\[
\begin{align*}
\lambda &= \frac{J^2}{16} \int_0^\pi \frac{dk}{2\pi} \left[ \frac{1}{E_3} + \frac{1}{E_4} \right], \\
C_0 &= \frac{J}{4} \int_0^\pi \frac{dk}{2\pi} \left[ \frac{\hbar + \pi t/2}{E_4} + \frac{\hbar - \pi t/2}{E_3} \right],
\end{align*}
\]

where \( \lambda = (C_0^2 + C_\pi^2)^{1/2} \), \( \hbar = JC_0/(4\lambda) \). If the quasi-particle energy gap \( \Delta \) is greater than zero, the insulating phase is stable. However, as the coupling constant \( J \) is small enough, the energy gap approaches to zero, and the system becomes conducting at this critical point.

In order for the theory to be self-consistent, the definitions of the mean field parameters \( C_\pi \) and \( C_0 \) must satisfy the condition \( |C_\pi| \leq J/4, |C_0| \leq J/4 \). The self-consistent Eq. (22) can be solved for \( C_0 \) and \( C_\pi \). One can find that \( C_0 = 0 \). The value of \( C_\pi \) is determined by the following equation:

\[
|C_\pi| = \left( \frac{J^2}{16} \right) \int_0^\pi \frac{dk}{\pi} \left[ \frac{1}{kt - \pi t/2 + [(\pi t/2)^2 + (J/2)^2]^{1/2}} \right]
= \frac{J}{8} f(|\frac{J}{\pi t}|),
\]

where the function \( f(x) = x \ln \frac{1+1+x^2}{x} \). Since \( 0 \leq f(x) < 1 \) for any \( x > 0 \), one sees that \( |C_\pi| < \frac{J}{8} \), a physically acceptable solution. For any coupling \( J \), the quasi-particle energy gap at half-filling is found to be

\[
\Delta = -\pi t + [(\pi t)^2 + J^2/4]^{1/2}.
\]

The above result indicates that the system is always in an insulating state for any nonzero coupling \( J \) and \( h = 0 \). Hence, we conclude that \( |J_c| = 0^+ \), in spite of the chirality of conducting band ( corresponding to long range hopping matrix ). In the strong interaction
limit, the energy gap is $\Delta \approx |J|/2$. In the weak interaction limit, the energy gap becomes $\Delta \approx J^2/(8\pi t)$.

In summary, the stability of the insulating phase of the 1D chiral Kondo lattice model at half-filling is studied, within the framework of self-consistent variational theory. It is found that the insulating phase is stable for any nonzero impurity-electron interaction, and the critical point of metal-insulator phase transition is at $J = 0$ in zero external magnetic field. It would be very interesting to validate the conclusion of the critical point through other approaches. Further work is necessary for study of the behavior of the chiral Kondo lattice model in nonzero magnetic field.

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