Instability to partial Kondo-singlet state in the Kondo necklace model on frustrated lattices

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Abstract. We present our theoretical results on the Kondo necklace model, which is known to give a good description of the half-filled state of the Kondo lattice model, on geometrically frustrated lattices. We employ the Lanczos exact diagonalization method as well as the bond-operator mean-field approximation to clarify the magnetic state at zero temperature. We examine a possibility of relieving severe frustration by making a spatially-periodic arrangement of magnetic ordered sites and nonmagnetic ones, i.e., the magnetic moments vanish periodically due to the Kondo singlet formation. We call the composite of magnetic and Kondo-singlet subsystems ‘partial Kondo-singlet state’, by analogy with the partial order in frustrated spin systems. We demonstrate that small clusters of 1D and 2D frustrated models show a tendency to exhibit the partial Kondo-singlet formation, and compare the results with those by the bond-operator mean-field approximation.

1. Introduction
In localized spin systems, geometrical frustration of underlying lattice structure often prevents the system from stabilizing a simple magnetic order, and results in residual entropy at low temperatures due to macroscopic number of degenerate ground states. The fate of the high entropy state is diversified; nontrivial magnetic orders stabilized by quantum and thermal fluctuations, some glassy states with freezing of spin configurations, and exotic spin liquid states without any apparent symmetry breaking. Another interesting possibility is the so-called partial order (or partial disorder) where the frustration is relieved by a long-ranged magnetic ordering with leaving spins on a subsystem in the paramagnetic state. For instance, on a frustrated lattice consisting of triangles, it is conceivable that the system exhibits a three-sublattice ordering of spin-up, down, and paramagnetic sublattices. The paramagnetic spins are almost disconnected from the ordered sublattices because of a cancellation of magnetic interactions, and therefore, behave like free spins, which leads to a Curie-type contribution in the magnetic susceptibility.

In Kondo systems, localized spins interact with each other through the RKKY interaction mediated by conduction electrons in addition to the usual superexchange interaction, and hence, the magnetism and the electronic state of conduction electrons are strongly correlated. A keen competition between Kondo singlet formation and magnetic ordering has been studied to clarify the quantum critical phenomena and non Fermi liquid state [1]. When the lattice structure is geometrically frustrated in the Kondo problems, a fascinating mechanism of relieving frustration can be expected in analogy with the partial order phenomena: The frustration can be relieved by forming Kondo singlet state on a subsystem embedded in magnetically ordered one. In this case, the partial ‘disordered’ sites are nonmagnetic due to the Kondo singlet formation, not Curie-like
paramagnetic. This is a novel, intriguing competition between Kondo singlet formation and the magnetic ordering emerging due to geometrical frustration, in which some peculiar behaviors can be expected in both magnetic and charge sectors.

In fact, such interesting phenomena have been found in some f-electron materials. An example is CePdAl in which localized Ce moments form a 2D distorted Kagome lattice. It was shown that this material exhibits a partial magnetic order of a collinear stripe type at low temperatures [2] where the remaining nonmagnetic sites are considered to be in the Kondo-singlet state [3]. Another example is found in UNi$_4$B, where U moments constitute the 2D triangular lattice. This compound also shows a partial Kondo-singlet formation at low temperatures accompanied by a peculiar noncollinear magnetic ordering [4].

On the other hand, there have been few theoretical studies on the geometrically frustrated Kondo systems. A mean-field study was performed for an effective Blume-Emery-Griffiths type model, and phase diagrams including a partial Kondo-singlet phase were obtained [5]. The effective model was derived from the Kondo lattice model by integrating out the conduction electrons, and therefore, it does not capture feedback effects between conduction electrons and localized moments, which will play a significant role in the partial Kondo-singlet formation. A similar phenomenon was studied for a three-impurity Kondo problem by the numerical renormalization group [6], however, it is still unclear what happens when the frustration exists at all the lattice sites and a macroscopic degeneracy is expected.

In the present contribution, we theoretically investigate the partial Kondo-singlet formation in geometrically-frustrated Kondo systems. As a first step, here we study the so-called Kondo necklace model which has been studied as a good variant of the Kondo lattice model at half filling [1]. We investigate the ground state of the model by employing the Lanczos exact diagonalization and the bond-operator mean-field approximation [7]. We discuss how the models show a tendency toward the partial Kondo-singlet formation.

2. Model and method

Our model is the Kondo necklace model which is a simplified version of the Kondo lattice model at half filling (one conduction electron per site on average). It has been studied for a long time to clarify the peculiar properties of f electron compounds [1]. The Hamiltonian is given by

$$\mathcal{H} = W \sum_{\langle ij \rangle} (\vec{\tau}_i^x \tau_j^x + \tau_i^y \vec{\tau}_j^y) + J \sum_i \vec{\tau}_i \cdot \vec{S}_i,$$

where both $\vec{\tau}$ and $\vec{S}$ are $S = 1/2$ Pauli operators at $i$th site; $\vec{\tau}$ spins effectively describes conduction electron degrees of freedom, and $\vec{S}$ spins represent the localized moment in the Kondo lattice model. The summation on $\langle ij \rangle$ is taken for nearest-neighbor pairs. The coupling between $\vec{\tau}$ spins, $W$, corresponds to the hopping integral of conduction electrons, and $J$ describes the $s$-d coupling leading to the Kondo singlet formation. We take $J$ as an energy unit hereafter.

We investigate the ground state of the model (1) on frustrated lattices, the one-dimensional (1D) delta chain [the inset of Fig. 1(a)] and the two-dimensional (2D) Kagome lattice [Fig. 2(a)]. We study the ground state of the models by the Lanczos exact diagonalization of small clusters and the bond-operator mean-field approximation. The latter approximation has been applied to the Kondo necklace model in the absence of frustration, and known to describe successfully both magnetic and Kondo singlet states as well as the phase transition between them [7].

3. Results

3.1. 1D delta chain

Let us start with the case of the delta chain. This lattice structure has two nonequivalent sites which we call here the apical and chain sites as shown in the inset of Fig. 1(a). We calculate
the ratio of the expectation values of $\langle \vec{\tau}_i \cdot \vec{S}_i \rangle$ at a chain site to that at an apical site, which measures the disproportionation of the Kondo singlet. The results are plotted in Fig. 1(a) for the system sizes $L = 4$ and 6 (the number of sites is $2L$) under the periodic boundary condition along the chain. The ratio shows a minimum at $W \sim 4$, where the Kondo singlet at apical sites becomes dominant compared to that at chain sites. At the same time, as shown in Fig. 1(b), the antiferromagnetic correlation grows among the chain sites. This is a symptom of the partial Kondo-singlet state composed of the antiferromagnetic chain sites and the Kondo-singlet apical sites, though the symmetry is intrinsically broken due to the lattice geometry in this case.

In Fig. 1(a), we also plot the result obtained by the bond-operator mean-field approximation for the two-sites unit cell of neighboring apical and chain sites. It also has a minimum, and agrees well with the results of the exact diagonalization except for large $W$ region, even in this frustrated 1D case.

![Figure 1](image.png)

**Figure 1.** (a) Ratio of $\langle \vec{\tau}_i \cdot \vec{S}_i \rangle$ at a chain site to that at an apical site. Inset shows the lattice structure of the delta chain. (b) Spin correlation $\langle \vec{\tau}_i \cdot \vec{\tau}_j \rangle$ among the chain sites.

### 3.2. 2D Kagome lattice

Next, we discuss the case of the Kagome lattice whose structure is shown in Fig. 2(a). In this lattice, all the sites are equivalent, and therefore, we cannot expect any symmetry breaking in finite size systems. Here, considering a chain-type partial Kondo-singlet state similar to the 1D delta chain case, we apply an infinitesimally small symmetry-breaking field corresponding to the chain-type pattern as shown in the inset of Fig. 2(b), and calculate the energy gain by the perturbation (see the caption for details). Shown in Fig. 2(b) are the exact-diagonalization results for 9 and 12-sites clusters under periodic boundary conditions. For both sizes, the energy gain becomes largest for an intermediate value of $W \sim 2 - 3$. This indicates a possibility of such partial Kondo-singlet formation in that intermediate region.

On the basis of these results for small clusters, we examine a spontaneous symmetry-breaking of three-sublattice ordering in the thermodynamic limit by the bond-operator mean-field approximation. Unfortunately, we do not see any signature of a partial Kondo-singlet formation: The obtained ground states are always uniform in our model. The results for the spin gap is shown in Fig. 2(c). The spin gap opens for all $W$, but interestingly, it shows a minimum for an intermediate $W \sim 1 - 2$. This minimum coincides with those seen in Fig. 2(b), suggesting that the system retains an instability to the partial Kondo-singlet formation.

### 4. Discussion and concluding remarks

The good agreement between the results by the exact diagonalization and by the bond-operator mean-field approximation in Sec. 3.1 suggests that the mean-field theory can capture an essential
Figure 2. (a) Kagome lattice structure. The shaded areas show the 9 and 12-sites clusters used in the exact diagonalization. (b) Energy change due to the chain-type symmetry-breaking field obtained by the exact diagonalization. The results are normalized by the unperturbed energy. The symmetry-breaking fields are introduced by modulating the Kondo coupling $J$ as $J - \Delta J/2$ for open and $J + \Delta J$ for closed-symbol sites in the inset, and the results are for $\Delta J = 0.01 J$. (c) Spin gap to the first triplet excitation calculated by the bond-operator mean-field approximation.

effect of spin fluctuations including Kondo singlet formation even in geometrically frustrated cases. In the 2D Kagome case, although a symptom of the partial Kondo-singlet formation appears in the results by both methods, the mean-field result does not show a spontaneous symmetry breaking, and instead, it predicts the uniform spin-gap state. The result implies that it is not easy to stabilize a partial Kondo-singlet state on the 2D Kagome lattice within our model. Considering the partial Kondo-singlet states observed in real materials, a possible route to reproduce them is to include additional effects in our model such as further-neighbor interactions, strong anisotropy of the localized moments due to the crystal field, and interlayer couplings. The results will be discussed elsewhere.

Calculations for other frustrated lattices as well as by another theoretical tools such as a variational method and a cluster extension of the dynamical mean-field theory are under way. Moreover, extensions of our work to the Kondo lattice model including conduction electrons explicitly are also in progress.

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