Kondo spin liquid and magnetically long-range ordered states in the Kondo necklace model

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A simplified version of the symmetric Kondo lattice model, the Kondo necklace model, is studied by using a representation of impurity and conduction electron spins in terms of local Kondo singlet and triplet operators. Within a mean-field theory, a spin gap always appears in the spin triplet excitation spectrum in one dimension (1D), leading to a Kondo spin liquid state for any finite values of coupling strength t/J (with t as hopping and J as exchange); in 2D and 3D cubic lattices the spin gaps are found to vanish continuously around $(t/J)_c \approx 0.70$ and $(t/J)_c \approx 0.38$, respectively, where quantum phase transitions occur and the Kondo spin liquid state changes into an antiferromagnetically long-range ordered state. These results are in agreement with variational Monte Carlo, higher-order series expansion, and recent quantum Monte Carlo calculations for the symmetric Kondo lattice model.

Since the discovery of the class of stoichiometric insulating compounds known as Kondo insulators,¹ there has been revived interest in the symmetric Kondo lattice Hamiltonian

$$H = -t \sum_{\langle i,j \rangle} \left(C_{i,\sigma}^{\dagger} C_{j,\sigma} + \text{H.c.} \right) + J \sum_{i} \mathbf{S}_{i} \cdot C_{i,\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} C_{i,\beta}$$
(1)

as a model of concentrated magnetic impurity spins coupled to conduction electrons. One of the important issues is the interplay between the Kondo screening and the magnetic interactions among localized spins mediated by the conduction electrons. The former effect favors a nonmagnetic Kondo spin liquid (singlet) state, while the latter interactions tend to stabilize an antiferromagnetically (AF) long-range ordered state. The character of such a transition between these two distinct phases has been a long-standing issue since it was pointed out by Doniach.² There have been a lot of investigations for the symmetric one-dimensional (1D) model, showing that its ground state is a disordered Kondo spin liquid state for *any* finite values of the coupling strength t/J.³ For two- and three-dimensional models, however, various approximate approaches, such as variational Monte Carlo calculations,⁵ higher-order series expansions,⁴ quantum Monte Carlo simulations,^{6,7} and infinite dimensional calculations,⁸ suggest that the Kondo spin liquid state may change into an AF long-range ordered state at certain value of the coupling strength at low temperatures.

Since there are a lot of difficulties in directly attacking the symmetric Kondo lattice model even in the 1D case, a simplified version called the Kondo necklace model was introduced by Doniach,²

$$H = t \sum_{\langle i,j \rangle} \left(\tau_i^x \tau_j^x + \tau_i^y \tau_j^y \right) + J \sum_i \mathbf{S}_i \cdot \boldsymbol{\tau}_i, \qquad (2)$$

where both τ_i and \mathbf{S}_i are spin-1/2 Pauli operators, denoting the conduction electron spin and impurity spin operators, respectively, and $\langle i,j \rangle$ means summation over the nearestneighbor conduction electron sites. Actually this simplified model is meaningful in general *D* dimensions (D=1,2,3) in its own right. Due to the suppression of charge fluctuations in the symmetric model, the charge degrees of freedom are frozen out, so the first term of Eq. (2) represents the spin degrees of freedom imitating the propagation of the conduction electrons. This can be clearly seen in the 1D case, where the first term is equivalent after a Jordan-Wigner transformation to a band of spinless fermions, which interact with localized spins via an AF spin-spin exchange coupling.²

Although the simplified model has only U(1) spin symmetry, lower than SU(2) for the Kondo lattice model, the essential feature of these two models is kept. Thus, one would expect that the main physical properties of the original symmetric Kondo lattice model should be maintained in the Kondo necklace model. However, most approaches used to treat the 1D Kondo necklace model, including the variational mean-field calculation,² approximate real-space renormalization group theory,⁹ and recent finite-size scaling analysis,¹⁰ have found a finite critical value of the coupling strength $(J/t)_c \sim 0.24 - 0.38$, below which an AF quasi-long-range order state appears, *in contrast to* $J_c = 0$, the result of quantum Monte Carlo simulations for the 1D Kondo necklace model¹¹ and the numerical result for the 1D symmetric Kondo lattice model.^{12,13} It is thus controversial whether the simplified spin model can be used to approximate the original symmetric Kondo lattice model. In this paper, we try to resolve this issue, starting from the Kondo necklace model, using the Kondo spin singlet and triplet representations, to reproduce correct ground states of the symmetric Kondo lattice model. In the 1D case, the system is found to be in a Kondo spin liquid state with a finite spin gap for any finite t/J, while on 2D and 3D cubic lattices a quantum phase transition occurs around $(t/J)_c \sim 0.70$ and $(t/J)_c \sim 0.38$, respectively, where the Kondo spin liquid state changes into an AF long-range ordered state, in excellent agreement with the variational Monte Carlo calculation,⁵ higher-order series expansion,⁴ and recent quantum Monte Carlo simulations,⁶ on the corresponding symmetric Kondo lattice model.

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Our starting point is the strong coupling limit t=0, where the lowest-energy state of the model Hamiltonian, Eq. (2), reduces to a sum over contributions from independent local Kondo spin singlet states at each lattice site. When $t\neq 0$, interactions between these independent local Kondo spin singlets are switched on. It will be seen later that this leads to very reasonable results even for $t \ge J$, which is of interest here. Usually, for two s=1/2 spins τ_i and \mathbf{S}_i placed on a lattice site, the local Hilbert space is spanned by four states consisting of one singlet and three triplet states defined as being created out of the vacuum $|0\rangle$ by the singlet and triplet creation operators: $|s\rangle = s^{\dagger}|0\rangle$ and $|t_{\alpha}\rangle = t_{\alpha}^{\dagger}|0\rangle$ ($\alpha = x, y, z$). A representation of the impurity spins and conduction electron spins in terms of these singlet and triplet operators is given by

$$S_{n,\alpha} = \frac{1}{2} \left(s_n^{\dagger} t_{n,\alpha} + t_{n,\alpha}^{\dagger} s_n - i \epsilon_{\alpha\beta\gamma} t_{n,\beta}^{\dagger} t_{n,\gamma} \right),$$

$$\tau_{n,\alpha} = \frac{1}{2} \left(-s_n^{\dagger} t_{n,\alpha} - t_{n,\alpha}^{\dagger} s_n - i \epsilon_{\alpha\beta\gamma} t_{n,\beta}^{\dagger} t_{n,\gamma} \right), \tag{3}$$

where α , β , and γ represent components along the *x*, *y*, and *z* axes, respectively, and ϵ is the antisymmetric Levi-Cività tensor. This type of spin representation in terms of singlet and triplet (bond) operators was first proposed by Sachdev and Bhatt to study the properties of dimerized phases¹⁴ and then it was successfully used to consider spin ladders¹⁵ and s=1 antiferromagnetic Heisenberg spin chains.¹⁶ As shown later, this representation faithfully describes the low-temperature physics in the symmetric Kondo lattice model. In order to restrict the physical states to either singlets or triplets, a local constraint is introduced: $s_n^{\dagger}s_n + \sum_{\alpha} t_{n,\alpha}^{\dagger}t_{n,\alpha} = 1$. Taking the singlet and triple operators at each site to satisfy the bosonic commutation relations $[s_n, s_n^{\dagger}]=1$, $[t_{n,\alpha}, t_{n,\beta}^{\dagger}] = \delta_{\alpha,\beta}$, and $[s_n, t_{n,\alpha}^{\dagger}] = 0$, the SU(2) algebra of the spins τ_n and **S**_n can be reproduced:

$$[S_{n,\alpha}, S_{n,\beta}] = i \epsilon_{\alpha\beta\gamma} S_{n,\gamma}, \quad [\tau_{n,\alpha}, \tau_{n,\beta}] = i \epsilon_{\alpha\beta\gamma} \tau_{n,\gamma},$$
$$[S_{n,\alpha}, \tau_{n,\beta}] = 0, \quad \mathbf{S}_n^2 = \tau_n^2 = \frac{3}{4}. \tag{4}$$

Substituting the operator representation of the impurity and conduction electron spins, we obtain the following form of the model Hamiltonian:

$$\begin{split} H &= H_0 + H_1 + H_2 + H_3, \\ H_0 &= \frac{J}{4} \sum_i \left(-3s_i^{\dagger}s_i + \sum_{\alpha} t_{i,\alpha}^{\dagger}t_{i,\alpha} \right) \\ &+ \sum_i \mu_i \left(s_i^{\dagger}s_i + \sum_{\alpha} t_{i,\alpha}^{\dagger}t_{i,\alpha} - 1 \right), \\ H_1 &= \frac{t}{4} \sum_{\langle ij \rangle} \left[s_i^{\dagger}s_j^{\dagger}(t_{i,x}t_{j,x} + t_{i,y}t_{j,y}) + s_i^{\dagger}s_j(t_{i,x}t_{j,x}^{\dagger} + t_{i,y}t_{j,y}^{\dagger}) + \text{H.c.} \right], \end{split}$$

$$H_{2} = -\frac{t}{4} \sum_{\langle ij \rangle} \left[t_{i,z}^{\dagger} t_{j,z}^{\dagger} (t_{i,x} t_{j,x} + t_{i,y} t_{j,y}) - t_{i,z}^{\dagger} t_{j,z} (t_{i,x} t_{j,x}^{\dagger} + t_{i,y} t_{j,y}^{\dagger}) + \text{H.c.} \right],$$

$$H_{2} = \frac{it}{2} \sum_{i} \sum_{j \in \mathcal{I}} \left[s_{i,z}^{\dagger} t_{i,z} t_{j,x}^{\dagger} + t_{i,y} t_{j,y}^{\dagger} + t_{i,y} t_{j,y}^{\dagger} + t_{i,y} t_{j,y}^{\dagger} \right]$$

$$H_{3} = \frac{1}{4} \sum_{\langle ij \rangle} \sum_{\alpha,\beta,\gamma} \epsilon_{\alpha\beta\gamma} [s_{i}^{+} t_{i,\alpha} t_{j,\beta}^{+} t_{j,\gamma} + s_{j}^{+} t_{j,\alpha} t_{i,\beta}^{+} t_{i,\gamma} + \text{H.c.}],$$
(5)

where a site-dependent chemical potential μ_i has been introduced to impose the local constraint. Here the local spin triplet states are split into two parallel spin states with $m_s = \pm 1$ and an antiparallel spin state with $m_s = 0$. H_1 describes the couplings between the singlet state and the parallel spin triplet states, while H_2 corresponds to the couplings of the parallel spin and the antiparallel spin triplet states. H_3 describes an interaction of one singlet boson and three different components of triplet bosons.

The above Hamiltonian can be solved by a mean-field decoupling of the quartic terms. It yields an effective Hamiltonian H_{mf} with only quadratic operators. We take $\langle s_i^{\dagger} \rangle = \langle s_i \rangle = \overline{s}$, which corresponds to a *condensation of the local Kondo spin singlets on each site* in accordance with the configuration of the ground state in the strong coupling limit, and the local chemical potential is replaced by a global one. We will consider here only the terms H_0 and H_1 , as it can be shown that inclusion of H_2 changes the results only slightly^{15,17} and all the decouplings of H_3 identically vanish within the present mean-field theory. After performing a Fourier transformation of the boson operators, $t_{i,\alpha} = (1/\sqrt{N}) \Sigma_{\mathbf{k}} t_{\mathbf{k},\alpha} e^{-i\mathbf{k}\cdot\mathbf{r}_i}$, the mean-field effective Hamiltonian is given by

$$H_{mf} = N \left(-\frac{3}{4} J \overline{s}^{2} + \mu \overline{s}^{2} - \mu \right) + \left(\frac{J}{4} + \mu \right) \sum_{\mathbf{k}} t^{\dagger}_{\mathbf{k},z} t_{\mathbf{k},z} + \sum_{\mathbf{k},\beta=x,y} \left[\Lambda_{\mathbf{k}} t^{\dagger}_{\mathbf{k},\beta} t_{\mathbf{k},\beta} + \Delta_{\mathbf{k}} (t^{\dagger}_{\mathbf{k},\beta} t^{\dagger}_{-\mathbf{k},\beta} + t_{\mathbf{k},\beta} t_{-\mathbf{k},\beta}) \right], \quad (6)$$

with $\Lambda_{\mathbf{k}} = (J/4 + \mu) + \frac{1}{2}t\overline{s^2}\lambda(\mathbf{k})$, $\Delta_{\mathbf{k}} = \frac{1}{4}t\overline{s^2}\lambda(\mathbf{k})$, and $\lambda(\mathbf{k}) = \sum_{a=1}^{d} \cos k_a$. The lattice spacing has been taken to be unity. This mean-field Hamiltonian can be diagonalized by a Bogoliubov transformation into new boson operators: $\tilde{t}_{\mathbf{k},\beta} = u_{\mathbf{k}}t_{\mathbf{k},\beta} + v_{\mathbf{k}}t_{-\mathbf{k},\beta}^{\dagger}$, where the coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are even functions of \mathbf{k} , and are determined to be $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = \cosh 2\theta_{\mathbf{k}} = \Lambda_{\mathbf{k}}/[\sqrt{\Lambda_{\mathbf{k}}^2 - (2\Delta_{\mathbf{k}})^2}]$ and $2u_{\mathbf{k}}v_{\mathbf{k}} = \sinh 2\theta_{\mathbf{k}} = -2\Delta_{\mathbf{k}}/[\sqrt{\Lambda_{\mathbf{k}}^2 - (2\Delta_{\mathbf{k}})^2}]$. Then we obtain

$$H_{mf} = \omega_0 \sum_{\mathbf{k}} t^{\dagger}_{\mathbf{k},z} t_{\mathbf{k},z} + \sum_{\mathbf{k},\beta=x,y} \omega_{\mathbf{k}} \tilde{t}^{\dagger}_{\mathbf{k},\beta} \tilde{t}_{\mathbf{k},\beta} + E_g, \qquad (7)$$

where $\omega_0 = (J/4 + \mu)$ is the dispersionless energy level of the antiparallel spin triplet excited state, $\omega_{\mathbf{k}} = \sqrt{\Lambda_{\mathbf{k}}^2 - (2\Delta_{\mathbf{k}})^2}$ corresponds to the excitation spectrum of the parallel spin triplet excited states, and the ground state energy of the system is $E_g = N(-\frac{3}{4}J\overline{s}^2 + \mu\overline{s}^2 - \mu) + \Sigma_{\mathbf{k}}(\omega_{\mathbf{k}} - \Lambda_{\mathbf{k}})$. By minimizing the ground-state energy with respect to μ and \overline{s} , we derive the following saddle-point equations:



FIG. 1. The variation of the spin gap upon increasing of the coupling parameter t/J of the 1D model at T=0.

$$\frac{1}{N} \sum_{\mathbf{k}} \frac{\Lambda_{\mathbf{k}}}{\sqrt{\Lambda_{\mathbf{k}}^2 - (2\Delta_{\mathbf{k}})^2}} = (2 - \overline{s}^2),$$

$$\frac{t}{N} \sum_{\mathbf{k}} \sqrt{\frac{\Lambda_{\mathbf{k}} - 2\Delta_{\mathbf{k}}}{\Lambda_{\mathbf{k}} + 2\Delta_{\mathbf{k}}}} \lambda(\mathbf{k}) = 2J \left(\frac{3}{4} - \frac{\mu}{J}\right). \tag{8}$$

When a dimensionless parameter

$$d = \frac{t}{J} \frac{\overline{s}^2}{\left(\frac{1}{4} + u/J\right)}$$

is introduced, a self-consistent equation for d can be obtained,

$$d = \frac{2t}{J} \left[1 - \frac{1}{2N} \sum_{\mathbf{k}} \frac{1}{\sqrt{1 + d\lambda(\mathbf{k})}} \right],\tag{9}$$

to determine the variational parameters \overline{s} and μ and the spin triplet excitation spectra: $\omega_0 = J(\frac{1}{4} + \mu/J)$ and $\omega_k = J(\frac{1}{4} + \mu/J)\sqrt{1 + d\lambda(\mathbf{k})}$. There is a minimum spin gap in the parallel spin triplet spectrum at the AF reciprocal vector momentum $\mathbf{k} = \mathbf{Q}$: $\Delta_{sp} = J(\frac{1}{4} + \mu/J)\sqrt{1 - Zd/2}$, where Z is the total number of the nearest neighbors on the cubic lattice.

In the 1D case, we first numerically calculate the parameters d, $\overline{s^2}$, and μ/J for a range of the coupling strength 0 < t/J < 5, and the minimum spin gap $\Delta_{sp} = J(\frac{1}{4})$ $+\mu/J$) $\sqrt{1-d}$ is evaluated in the range of $0 \le t/J \le 5$, which has been delineated in Fig. 1. The dispersive band can also be parametrized by a spin density wave with a velocity given by $v_s = J(\frac{1}{4} + \mu/J)\sqrt{d/2}$. A linear drop of the spin gap is seen for small values of t/J. As t/J gets larger, the spin gap deviates considerably from the linear behavior and there is no indication at all suggesting a critical value for t/J where the gap would vanish. Since the excitation spectra are real and positive everywhere in the Brillouin zone, the system will be in a quantum disordered Kondo spin liquid state for *finite* values of the coupling strength t/J, and the spin-spin correlation function decays exponentially at large distances with a correlation length $\xi = v_s / \Delta_{sp}$. This is indeed consistent with both quantum Monte Carlo simulations for the 1D Kondo necklace¹¹ and numerical results for the 1D symmetric Kondo lattice model.^{12,13} Thus, starting from the limit t/J=0 with localized Kondo spin singlets on each site, we see



FIG. 2. The spin gap and the staggered magnetic moment at zero temperature of the 2D Kondo necklace model (bold line) in comparison with results of recent quantum Monte Carlo simulation (Ref. 6) for the 2D Kondo lattice model.

that any finite coupling strength delocalizes the local Kondo singlets, reducing the magnitude of the gap but not closing it completely.

Having secured the correct ground state for the 1D symmetric Kondo lattice model, we now turn to two- and threedimensional "Kondo necklace" models on a cubic lattice. In 2D, the variational parameters d, \overline{s}^2 , and μ/J can also be calculated from the saddle-point equations. The minimum spin gap appears in the parallel spin triplet excitation at k $=(\pi,\pi):\Delta_{sp}=J(\frac{1}{4}+\mu/J)\sqrt{1-2d}$, displayed in Fig. 2. The most important feature here is that as the coupling parameter t/J increases, the drop of the spin gap in the small values of t/J continues down to the point $(t/J)_c \approx 0.70$ where the spin gap actually vanishes. The critical coupling $(t/J)_c \approx 0.70$ corresponds to a quantum critical point for a phase transition from the quantum disordered Kondo spin liquid to a magnetically long-range ordered state. Surprisingly, the location of the critical point for the 2D Kondo necklace model is precisely the value obtained from the variational Monte Carlo calculation,⁵ the higher-order series expansion,⁴ and recent quantum Monte Carlo simulations,⁶ for the 2D symmetric Kondo lattice model. When a similar calculation is carried out in the 3D Kondo necklace model, the minimum spin gap appears at $\mathbf{k} = (\pi, \pi, \pi)$ and $\Delta_{sp} = J(\frac{1}{4})$ $(+\mu/J)\sqrt{1-3d}$, shown in Fig. 3. As t/J grows, the spin gap decreases and exhibits a critical value $(t/J)_c \approx 0.38$, where the spin gap disappears completely, showing a quantum



FIG. 3. The spin gap and the staggered magnetic moment at zero temperature for 3D Kondo necklace model.

phase transition from the quantum disordered Kondo spin liquid to a magnetically long-range ordered state as well. This transition point is in the same range as the higher-order series expansion⁴ for the 3D symmetric Kondo lattice model: $(t/J)_c \approx 0.50$.

Moreover, the present mean-field theory can also be applied to the magnetically long-range ordered phase in the 2D and 3D Kondo necklace models. If we assume that not only do the local Kondo spin singlets (*s* bosons) condense, but one of the local Kondo spin triplets ($t_{\mathbf{k},x}$ bosons) condenses as well on the AF reciprocal vector $t_{\mathbf{k},x} = \sqrt{Nt} \,\delta_{\mathbf{k},\mathbf{Q}} + \eta_{\mathbf{k},x}$, corresponding to *fixing the orientation of the localized spins along the x direction*, it will lead to another mean-field effective Hamiltonian

$$H'_{mf} = E'_{g} + \omega_{0} \sum_{\mathbf{k}} t^{\dagger}_{\mathbf{k},z} t_{\mathbf{k},z} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} (\tilde{t}^{\dagger}_{\mathbf{k},y} \tilde{t}_{\mathbf{k},y} + \tilde{\eta}^{\dagger}_{\mathbf{k},x} \tilde{\eta}_{\mathbf{k},x}),$$

$$E'_{g} = N \left[-\frac{3}{4} J \overline{s}^{2} + \mu \overline{s}^{2} - \mu + \left(\frac{J}{4} + \mu - \frac{1}{2} Z t \overline{s}^{2} \right) \overline{t}^{2} \right]$$

$$+ \sum_{\mathbf{k}} (\omega_{\mathbf{k}} - \Lambda_{\mathbf{k}}), \qquad (10)$$

where ω_k has the same form as in the Kondo spin liquid case, and $\tilde{\eta}_{\mathbf{k},x}^{\dagger}$ and $\tilde{\eta}_{\mathbf{k},x}$ are the transverse spin triplet excitation modes. When the order parameter \overline{t} is nonzero, the saddle-point equation for \overline{t} yields $\mu = \frac{1}{2}Zt\overline{s}^2 - J/4$, which makes the parallel spin triplet excitation spectrum gapless: $\omega_{\mathbf{k}} = \frac{1}{2} Z t \overline{s^2} \sqrt{1 + 2\lambda(\mathbf{k})/Z}$. The ground state corresponds to a magnetically long-range ordering state with a maximum momentum $\mathbf{q} = \mathbf{Q}$, and the mean field \overline{t} represents the AF order parameter. A very appealing physical picture of forming AF long-range order in the Kondo necklace or the symmetric Kondo lattice models has been suggested: when t/J is small, the conduction electron spins are locked and the impurity spins are screened completely, and the ground state is a product of the local Kondo spin singlet quantum disordered phase.³ As t/J becomes larger and larger, the conduction electrons (the spin degrees of freedom) have more possibility to propagate to the nearest-neighbor sites, and the localized magnetic impurity spin is only *partially* screened $(\overline{s} \neq 0)$;

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then the remaining part of the magnetic impurities on different lattice sites starts to develop long-range correlations ($\bar{t} \neq 0$) mediated by the conduction electron spins.¹⁴ Such a magnetically long-range ordered state might be related to the ground states of the U-based heavy fermion compounds (URu₂Si₂ and UPt₃) with a very small magnitude of induced staggered magnetic moments. In order to determine the parameters \bar{s} and \bar{t} , we minimize the ground-state energy, derive the saddle-point equations, and finally obtain

$$\overline{s}^{2} = 1 + \frac{J}{Zt} - \frac{1}{2N} \sum_{\mathbf{k}} \sqrt{1 + 2\lambda(\mathbf{k})/Z},$$
$$\overline{t}^{2} = 1 - \frac{J}{Zt} - \frac{1}{2N} \sum_{\mathbf{k}} \frac{1}{\sqrt{1 + 2\lambda(\mathbf{k})/Z}}.$$
(11)

The AF order parameter is defined by $m_s = \overline{s} \cdot \overline{t}$, leading to the following expressions:

$$m_{s} = \sqrt{\left(0.35712 - \frac{J}{4t}\right) \left(0.52095 + \frac{J}{4t}\right)}, \text{ for 2D,}$$
$$m_{s} = \sqrt{\left(0.44234 - \frac{J}{6t}\right) \left(0.51263 + \frac{J}{6t}\right)}, \text{ for 3D.}$$

These results have also been displayed in Figs. 2 and 3, respectively. In Fig. 2, our results are also compared with the numerical results for the spin gap and staggered moment of the magnetic impurity spins in the recent quantum Monte Carlo simulation on the 2D symmetric Kondo lattice model at zero temperature.⁶

In summary, we have presented a mean-field theory for the Kondo necklace model in 1D, 2D, and 3D and have obtained their correct ground states corresponding to the respective Kondo lattice model. A long-standing controversial issue has been thus resolved regarding the relationship between these two models. As far as the spin part of the ground-state properties is concerned, the Kondo necklace model can reproduce the correct phase diagrams of the symmetric Kondo lattice model at zero temperature.

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