Gap-formation mechanism of the Kondo-necklace model

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We investigate a gap-formation mechanism of the one-dimensional Kondo-necklace model at zero temperature. An analytic treatment using the bosonization method shows that the model undergoes the Kosterlitz-Thouless transition at the critical coupling $J_c=0$, which is described by the quantum sine-Gordon model. This result is contrary to the previous investigations on the ground-state phase transition, where some finite critical coupling values have been predicted. To clarify the validity of our analytic calculation result, we estimate the singlet-triplet gap by employing White's density matrix renormalization group method; the numerical calculation is carried out for the systems up to 200 sites with open boundary condition. As a result, we find that the excitation gap observed in the large J region becomes smaller quickly with the decrease of J. However, the data show the existence of a small gap for $J\geqslant 0.25$, which seems to support $J_c=0$.

So far, the intensive studies on the valence fluctuation and heavy fermion systems have been performed using both analytic and numerical approaches, where the periodic Anderson model is generally considered to be a canonical one for describing a variety of properties observed in the Ce and actinide compounds.[1] In the model, there are two kinds of electrons: the well-localized f electrons and the propagating Bloch electrons; we have expected that the quite different physical phases observed in such compounds should be understood consistently in the context of the interaction effects between these two kinds of electrons.

When the energy level of f orbits lies deep in the Fermi sea and at the same time the Coulomb repulsion force strongly suppresses the double occupancy of f orbits (i.e., in the Kondo limit), the f-electron charge degrees of freedom are quenched. Then, the system is described by the Kondo lattice model

$$H_{\mathrm{KL}}=-t\sum_{\langle l,m\rangle\sigma}(c_{l\sigma}^{\dagger}c_{m\sigma}+\text{ H.c. })+J\sum_{l}\mathbf{S}_l\cdot\mathbf{s}_l, \qquad (1)$$

where the f electrons are reduced to the magnetic moments $\mathbf{S}_l$ and they are coupled with the spin components of conduction electrons $\mathbf{s}_l$. The Kondo lattice model is also a standard one for the compounds in the Kondo regime: there has been a great amount of investigations, where the $1/N$ expansion and the slave boson methods or Gutzwiller-type variational approaches are often employed.[2–6] Moreover, for one-dimensional systems, numerical techniques such as the quantum Monte Carlo simulation and exact diagonalization methods are also powerful tools and allow us to investigate the models without any approximations.[7–10]

Focusing on the magnetic aspect. Doniach[11] has pointed out that the model at the half-filling possesses a competition between the antiferromagnetically ordered state arising from the Ruderman-Kittel-Kasuya-Yoshida interaction and the nonmagnetic Kondo singlet state. Further, for the aim of investigating the competition problem, they have carried out a drastic simplification of the Kondo lattice model by neglecting conduction electron charge degrees of freedom and introduced so-called Doniach Kondo-necklace model

$$H_{\mathrm{KN}}=W\sum_{\langle l,m\rangle}(\tau_l^x\tau_m^x+\tau_l^y\tau_m^y)+J\sum_{l}\mathbf{S}_l\cdot\boldsymbol{\tau}_l, \qquad (2)$$

where $\boldsymbol{\tau}_l$ and $\mathbf{S}_l$ are the quantum spin operators of length $1/2$.[11] The XY-coupling term imitates the usual band energy of the conduction electrons, and the second term represents the Kondo exchange coupling. In the following, we use the nearest-neighbor hopping amplitude W as the unit of energy, and thus the Kondo coupling J is only the model parameter.

In this paper, we will discuss the ground-state properties of the one-dimensional Kondo-necklace; the gap formation is mainly argued using both the bosonization method[12] and White's density-matrix renormalization-group (DMRG) calculation technique.[13] The former analytic method has been successfully applied to one-dimensional quantum systems. Following the standard procedure, we construct the phase Hamiltonian of the Kondo necklace, and then we calculate the excitation gap, using the self-consistent harmonic approximation method.[14] On the other hand, the DMRG method, which was recently proposed by White, has achieved great improvements in the efficiency of the numerical renormalization-group calculation by utilizing the information of the reduced density matrix for a physical system combined with a proper environment.[13] As a result, the convergency of the data against the number of states (m) kept in the DMRG transformation is remarkably accelerated; a ground state and lower excited states are accurately investigated. In the latter part of this paper, we shall show the DMRG calculation data on the singlet-triplet gap, which should be properly reflecting the gap formation of the Kondo necklace: $G(J,N)=E(J,N;1)-E(J,N;0)$ [$E(J,N;M)$ is the ground-state energy in the sector of a given total $S^z=M$] and argue the validity of our prediction from the bosonization calculation.

We start with constructing the phase Hamiltonian of the Kondo necklace, which may present some significant insight into the gap formation mechanism. For this aim, we use Schulz's method by which the one-dimensional $S=1$ Heisenberg system was transformed to the model described by two kinds of bosonic fields.[15] Actually, in the recent study on the $S=1/2$ quantum Heisenberg ladder with which the necklace model possesses a similar structure, the ground-state phase diagram was discussed on the basis of the Wilson's renormalization-group treatment of the phase Hamiltonian.[16] Here, we only outline the procedure to obtain the phase Hamiltonian; for a more detailed explanation, see Refs. 15 and 16. First of all, two kinds of spins $\{\mathbf{S},\boldsymbol{\tau}\}$ are transformed into fermion operators by the Jordan-Wigner transformation. Then, the continuum limit is taken and the dispersion is linearized at Fermi points. For each fermion, the left- and right-going branches are separated by introducing two kinds of fermion fields. And then, according to the bosonization procedure, the fermion system may be properly described by the density operators (bosons) of the fermion fields. Finally, taking the appropriate linear combination of the bosonic fields so as to get the decoupled form for the Kondo coupling part, we obtain the expression of the phase Hamiltonian, $H_{\rm ph}=H_{\rm QSG}+H_{\rm DSG}+H_{\rm cross}$ as follows:

$$H_{\rm QSG}=\frac{1}{2}\int dx\ C\Pi_1{}^2+D_1(\partial_x\Psi_1)^2+Y\cos\{\sqrt{8}\Psi_1\},\quad(3)$$

$$H_{\rm DSG}=\frac{1}{2}\int dx\ C\Pi_2{}^2+D_2(\partial_x\Psi_2)^2+Y\cos\{\sqrt{8}\Psi_2\}+Y\cos\{\sqrt{2}\pi X_2\},\quad(4)$$

and

$$H_{\rm cross}=\frac{1}{2}\int dx\ \pi a\Pi_1\Pi_2+\frac{a}{\pi}(\partial_x\Psi_1)(\partial_x\Psi_2),\quad(5)$$

where $\Pi_\alpha(x)\equiv\partial_x X_\alpha(x)$ and $[\Psi_\alpha(x),\Pi_\beta(y)]=i\delta_{\alpha,\beta}\delta(x-y)$. The coefficients in the Hamiltonian are determined by the Kondo coupling parameter J and the lattice constant a as $C=\pi a/2$, $D_{1,2}=(1/2\pm J/\pi)a/\pi$, and $Y=-J/a$. Here the field operators were shifted appropriately to keep the coefficient Y minus (cf. Ref. 16).

If the original Hamiltonian $H_{\rm KN}$ includes the nearest-neighbor XY coupling, i.e., $S_l^xS_{l+1}^x+S_l^yS_{l+1}^y$, the cross term $H_{\rm cross}$ does not appear and the former two parts, i.e., the quantum sine-Gordon (QSG) part and so-called the dual sine-Gordon (DSG) part, are completely decoupled each other. This implies that in the region where $H_{\rm QSG}$ and $H_{\rm DSG}$ are both massless, i.e., the Kondo coupling is irrelevant. $H_{\rm cross}$ is also irrelevant to the gap formation. In other regions, the irrelevancy of $H_{\rm cross}$ may become a subtle question. Nevertheless, as a simplest approximation, we neglect the cross term and treat the two remaining parts separately in the following calculations. We will discuss the point later.

The self-consistent harmonic approximation (SCHA) method is employed for the quantitative arguments on the phase Hamiltonian, which is based on the variational principle: We set the reference Hamiltonians

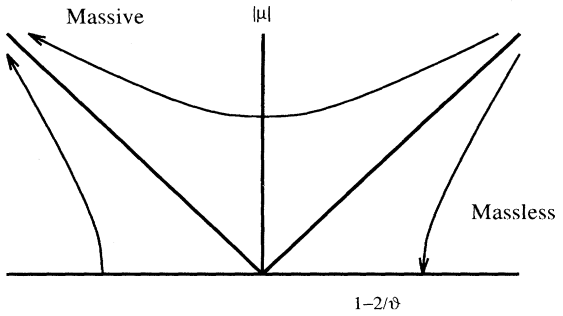

FIG. 1. Schematic phase diagram of the quantum sine-Gordon model obtained by Wilson's RG calculation. $|\mu|=\sqrt{CD_1}|Y|$. The Kondo-necklace model with $J=0$ is located to the original point; as the coupling takes a finite positive value, the system plunges into the massive phase.

$$H_{\rm QSG}=\frac{1}{2}\int dx\ C\Pi_1{}^2+D_1(\partial_x\Psi_1)^2+B_{\Psi_1}\Psi_1^2,\quad(6)$$

$$H_{\rm DSG}=\frac{1}{2}\int dx\ C\Pi_2{}^2+D_2(\partial_x\Psi_2)^2+B_{\Psi_2}\Psi_2^2+B_{X_2}X_2^2,\quad(7)$$

where B_μ ($\mu=\Psi_1$, Ψ_2, and X_2) are the variational parameters. These are thus determined as to minimize the variational energies $\langle H_{\rm QSG}\rangle_1$ and $\langle H_{\rm DSG}\rangle_2$, where $\langle\cdots\rangle_1$ ($\langle\cdots\rangle_2$) denotes an expectation value evaluated from the ground state of the SCHA Hamiltonian $H_{\rm QSG}$ ($H_{\rm DSG}$). The harmonic potential terms in the reference Hamiltonians basically come from the expansions of the nonlinear cosine terms. By determining their curvatures self-consistently, we can effectively investigate at the low-energy region whether the mass-generating cosine terms are relevant or not. After some tedious calculations, it becomes clear that the Kondo necklace ($J>0$) is in the Ψ_1-massive, Ψ_2-massless, and X_2-massive phase (this corresponds to the Haldane phase for the Heisenberg ladder model as argued in Ref. 16). The J dependences of the mass gaps are then obtained as

$$G_{\rm QSG}\sim\left[\frac{2J}{\pi}\right]^{1/(2-\vartheta)},\quad G_{\rm DSG}\sim\left[\frac{(\pi-2J)J}{2\pi^2}\right]^{1/(2-1/\theta)},\quad(8)$$

where $\vartheta\equiv\sqrt{4\pi/(\pi+2J)}$ and $\theta\equiv\sqrt{4\pi/(\pi-2J)}$, respectively. From these expressions, we can find that, when $\delta\equiv 2J/\pi$ is small, $G_{\rm QSG}\sim\delta^{1/\delta}$ and $G_{\rm DSG}\sim\delta^{2/3}$ (thus $G_{\rm QSG}\ll G_{\rm DSG}$ holds), which enables us to conclude that the Kondo necklace in the small-J region is properly described by $H_{\rm QSG}$.

Now, we should mention the well-known result of the quantum sine-Gordon Hamiltonian: $H_{\rm QSG}$ shows the Kosterlitz-Thouless (KT) transition[17] and belongs to the $S=1/2$ XXZ universality class: The energy gap vanishes as the essential singularity form when the system approaches from the upper region to the transition point. Since parametrically the critical KT coupling J_c equals zero, the Kondo-necklace is always in the upper side of the KT phase (see Fig. 1), where the spin correlation functions decay exponentially in real space.

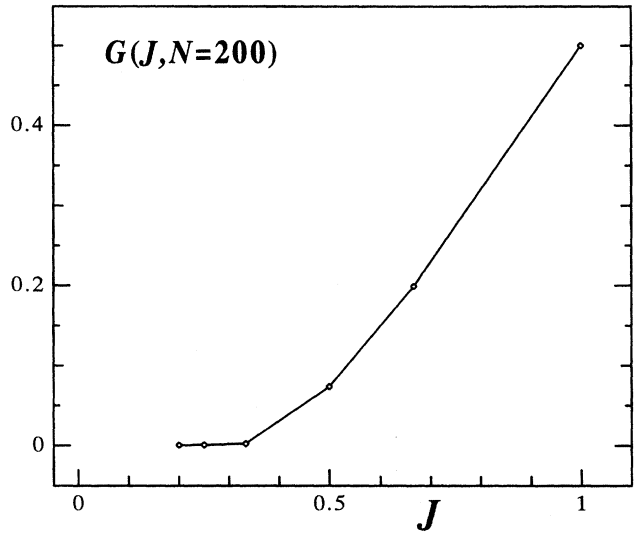

FIG. 2. J dependence of the gap for the 200-site Kondo necklace with an open boundary condition.

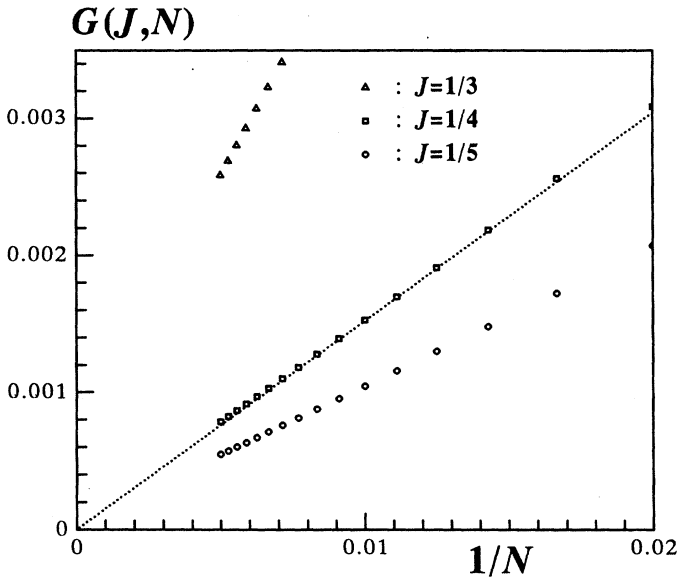

FIG. 3. System size dependence of the singlet-triplet excitation gap. The correspondence between the values of J and the symbol types are given in the figure. The dotted straight line is to guide the eyes.

Up to now, we have discussed the gap formation mechanism of the Kondo-necklace model within the bosonization treatment. However, in this procedure, some critical approximations are included; e.g., it is commonly recognized that the bosonization method may not keep the quantitatively reliable parametric relation between the original and the phase Hamiltonian. Further, the effects of the neglect of H_{cross} are still unclarified. On the other hand, some previous analytic and numerical investigations have concluded that the ground-state phase transition occurs at finite coupling values. For example, according to Doniach's mean-field calculation, the ground state changes from the antiferromagnetic state to the singlet one at $J=1$.[11] The result of the real-space renormalization-group calculation shows that the massless XY phase remains until a certain value of J ($\simeq 0.4$).[18] The quantum Monte Carlo simulation was also carried out for the systems up to $N=16$: The data seemingly exhibit the change of the correlation function behavior at $J\simeq 0.4$.[19] However, it may be quite difficult to deduce conclusions on the ground-state properties from the method. More recently, Santini and Sólyom have studied the excitation gap by the exact diagonalization method (up to $N=12$).[20] From a careful finite-size scaling analysis of the data, they have also concluded that the KT-like transition occurs at $J_c\simeq 0.24$, which is, however, considerably smaller than the above-mentioned values.

We now exhibit the numerical data calculated by the infinite system algorithm of the DMRG method: The singlet-triplet gap was estimated for systems up to 200 sites. Required from the standard DMRG method, the open boundary condition was employed. Each site contains two kinds of spins, i.e., $\{\tau_l, \mathbf{S}_l\}$; they were treated as one composite in our calculations.

We plot the J dependence of the gap for the largest site system in Fig. 2. The DMRG truncation error estimator[13] $Q(m,J)\equiv 1-P(m,J)$ strongly depends upon the number of states m and J: While at the $J=1$ case, $m\simeq 30$ is enough to realize $Q<10^{-9}$, the states up to $m=560$ are required to keep the same order of accuracy for the system with $J=1/5$. Note that it may be also possible to get $m\to\infty$ data using an appropriate extrapolation method. However, especially in the weaker-coupling region, the procedure becomes subtle so that the result may be significantly affected by a way of extrapolation. We thus plot the data with the largest m values. As shown in the figure, the magnitude of the gap becomes smaller quickly, but it is clearly visible for $J\geq 1/3$. In Fig. 3, the system size dependence of $G(J,N)$ is plotted for $J\leq 1/3$, where the low-energy region is magnified. Although the $1/N$ dependence of the data with $J=1/4$ is almost linear, we can recognize a weak downward convex tendency, which may indicate the existence of a finite excitation gap at $J=1/4$. (Its magnitude may be smaller than $\simeq 10^{-4}$ at $N\to\infty$.)

Unfortunately, to investigate a weaker-coupling region and thus to evaluate a smaller gap, we should estimate the ground-state energies more accurately, since almost all of convergent digits cancel each other. For this condition, we think that a proper finite-size scaling analysis technique should be employed, which remains as a future problem.

In conclusion, we have argued the gap formation mechanism of the one-dimensional Kondo-necklace model using both the bosonization method and White's DMRG method. The phase Hamiltonian was treated using the SCHA method, and the following results have been derived: Any small Kondo coupling brings a finite excitation gap, i.e., $J_c=0$, which is described by the quantum sine-Gordon model. This means simultaneously that the gap formation is described by the KT transition and belongs to the $S=1/2$ XXZ universality class. To clarify the validity of the bosonization result, we carried out the DMRG calculation of the Kondo necklace. Consequently, we have found that, although its magnitude

becomes quite small, the system possesses an excitation gap for $J \geqslant 1/4$. We however cannot rule out that the mass gap opens at a finite Kondo coupling value; it is also plausible that J_c takes a finite value due to the effect of the neglected cross term, which might become relevant in the massive phase. We thus hope that more accurate calculations may clarify the point.

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