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Large Fermi surface of the one-dimensional Kondo lattice model

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A Luttinger-liquid fixed point is obtained in the strong-coupling limit of the one-dimensional Kondo-lattice model with a frustrating next-nearest-neighbor hopping. The Luttinger-liquid phase has a large Fermi surface whose area is determined by the total number of conduction electrons and localized spins. A numerical study for finite systems shows that the paramagnetic ground state of the finite Kondo lattice model away from half-filling is adiabatically connected with this fixed point.

The Kondo lattice model (KLM) is one of the canonical models for the heavy-fermion systems. Although the model has been studied intensively, it was only recently that the ground-state phase diagram in one dimension was determined for the model with nearest-neighbor hopping.[1] It consists of three phases. The first is a ferromagnetic (FM) metallic phase, which includes the low-density limit[2] and the strong-coupling limit.[3,4] The second phase is a paramagnetic (PM) metallic phase which is obtained in the weak-coupling limit away from either half-filling or the low-density limit. The third phase is an insulating spin-liquid phase at half-filling.[5,6]

Among the three phases, properties of the PM metallic phase are not well understood compared with the other two. In one dimension many interacting electron systems belong to the class of Luttinger liquids.[7] In fact, numerical studies for the KLM by exact diagonalization[1] or Monte Carlo simulation[4] show that the spin and charge correlations have a dominant structure at $2k_{Fc}$ corresponding to the Fermi surface (FS) which is determined only by the density of *conduction electrons* without counting localized f electrons. On the other hand, the KLM in the weak-coupling limit can be regarded as an effective model for the periodic Anderson model (PAM) in the limit of strong electron correlation. For the latter it may be natural to guess that its PM phase has a large FS, containing both the *conduction electrons and f electrons*.[8]

The fact that KLM is an effective model of the PAM does not necessarily mean that the KLM also has the large FS. For the PAM, f electrons are always mixed with conduction electrons $\langle f_i^\dagger c_i\rangle=\langle c_i^\dagger f_i\rangle^*\neq 0$, which means that the f electrons have some finite weights at the Fermi energy. On the other hand, in the KLM charge degrees of freedom of the f electrons are completely suppressed [local $U(1)$ gauge symmetries], leading to the absence of the mixing, $\langle f_i^\dagger c_i\rangle=\langle c_i^\dagger f_i\rangle^*=0$. From this point of view, it would be even surprising if the f electrons participate in the FS sum rule. A variational Monte Carlo study by using the Gutzwiller projected hybridization form supports the large FS for the KLM.[9] However, in the variational treatment it is hard to decide whether the large FS is a consequence of the choice of the trial wave function, or the real property of the system. Therefore, even though the PM state of the KLM may belong to the universality class of Luttinger liquids, such a basic question as the large or small FS is not settled yet.

In this paper we study the Kondo lattice model with both nearest-, $-t$, and next-nearest-neighbor hoppings, $-t'$. First, it is shown that for a negative t' there appears a region of the PM ground state in the strong-coupling limit in addition to that in the weak-coupling region. In the strong-coupling regime we will show that the FS is *large*. This is the first unambiguous example that localized electrons described purely by spin degrees of freedom participate in the FS sum rule. Next we show that for finite systems there is an adiabatic path connecting the two PM regions in the strong- and weak-coupling regimes. Although this is a suggestion that the KLM in one dimension generally has a *large* FS in PM phase, at present it is premature to draw a definitive conclusion for infinite systems.

The Hamiltonian of the one-dimensional KLM studied in this paper is written as

$$\mathscr{H}=-t\sum_{j\sigma}(c_{j\sigma}^\dagger c_{j+1\sigma}+\text{H.c.})-t'\sum_{j\sigma}(c_{j\sigma}^\dagger c_{j+2\sigma}+\text{H.c.})+J\sum_j \mathbf{S}_{cj}\cdot\mathbf{S}_{fj}, \tag{1}$$

where $\mathbf{S}_{cj}\equiv\Sigma_{\tau\tau'}c_{j\tau}^\dagger(\frac{1}{2}\boldsymbol{\sigma})_{\tau\tau'}c_{j\tau'}$ and $\mathbf{S}_{fj}$ is a localized spin with $S=\frac{1}{2}$. In the following the KLM with only t is referred to as t-KLM and the KLM with both t and t' as t-t'-KLM, if distinction is necessary. Because of the electron-hole symmetry for the conduction electrons, it is sufficient to consider electron concentrations less than half-filling ($0<\rho=N/L<1$).

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In the limit of $J=\infty$, the degrees of freedom per site are reduced from eight to three: a local singlet composed of one conduction electron and an f spin, and an unpaired f spin (up or down). By identifying these local singlets as vacant sites, the $J=\infty$ KLM is mapped to the $U=\infty$ Hubbard model with $\tilde{N}\equiv L-N$ particles, which are referred to as $\tilde{f}$ electrons in the following.[3,10] Since a hopping matrix element for the $\tilde{f}$ electrons is reduced to half, the effective Hamiltonian in this limit is given by

$$\mathscr{H}_{t\text{-}t'}=+\frac{t}{2}\sum_{j\sigma}(\tilde{f}^{\dagger}_{j\sigma}\tilde{f}_{j+1\sigma}+\text{H.c.})+\frac{t'}{2}\sum_{j\sigma}(\tilde{f}^{\dagger}_{j\sigma}\tilde{f}_{j+2\sigma}+\text{H.c.}), \tag{2}$$

where the double occupancy of the $\tilde{f}$ electrons is forbidden (t-t' model). The change in the sign of the hopping matrix elements comes from the fermionic sign of the original f electron which is a component of the local singlet.

When $t'=0$, the ground state of the t-t' model has a complete $2^{\tilde{N}}$-fold spin degeneracy, because the nearest-neighbor hopping does not change the spin configuration. The wave functions in the ground-state multiplet are[11]

$$|\Psi\{\sigma_j\}\rangle=\sum_{j_i<j_2<\cdots<j_{\tilde{N}}}\det|\phi_\alpha(j)|\tilde{f}^{\dagger}_{j_1\sigma_1}\cdots\tilde{f}^{\dagger}_{j_{\tilde{N}}\sigma_{\tilde{N}}}|0\rangle, \tag{3}$$

where the one-particle eigenfunctions $\{\phi_\alpha\}$ are chosen to be the lowest $\tilde{N}$ levels of the nearest-neighbor hopping terms.

A finite but small t' is sufficient to lift the spin degeneracy, since it introduces spin exchange processes. For a small t', the effective spin interaction in the ground-state multiplet may be calculated, keeping the charge configuration fixed:

$$\begin{aligned}&\langle\Psi(\sigma'_1\cdots\sigma'_{\tilde{N}})|\mathscr{H}_{t\text{-}t'}|\Psi(\sigma_1\cdots\sigma_{\tilde{N}})\rangle\\&\quad=\left\langle\sigma'_1\cdots\sigma'_{\tilde{N}}|J_{\text{eff}}\sum_j\mathbf{S}_j\cdot\mathbf{S}_{j+1}|\sigma_1\cdots\sigma_{\tilde{N}}\right\rangle+\text{const},\\&J_{\text{eff}}=-\frac{t'}{2\pi}\left(\frac{2}{\pi\tilde{\rho}}\sin^2\pi\tilde{\rho}-\sin2\pi\tilde{\rho}\right),\end{aligned} \tag{4}$$

where $\tilde{\rho}=1-\rho$. The effective Heisenberg coupling is ferromagnetic for $t'>0$ and antiferromagnetic for $t'<0$. For a large but finite J, the second-order processes in t produce a coupling of the same form with t' replaced by t^2/J.[3] Therefore, when $t'>0$ there is no frustration in the t-t'-KLM and the ground state in the strong-coupling limit is ferromagnetic for all $0<\rho<1$. On the other hand for a frustrated t-t'-KLM ($t'<0$), the ground state is singlet in the strong-coupling limit for any $0<\rho<1$.

We performed numerical exact diagonalization for the frustrated t-t'-KLM with the open boundary conditions to determine the region of ferromagnetism. Figure 1 shows the phase diagram of the frustrated t-t'-KLM with $t'=-0.1$ ($t=1$) determined by the systems from $L=4$ to $L=9$. Finite-size effects are very small in the present case, similarly to the results of the t-KLM.[1] In addition to the PM region in the weak-coupling regime, a new PM region opens from the side of low electron concentration to the strong-coupling limit. It is seen that the zeroth-order estimation for the FM and PM boundary, $J\sim t^2/|t'|$, fits fairly well. It should also be mentioned that the theorem of ferromagnetism for the KLM with one conduction electron[2] does not apply to the present case, because of the frustration introduced by the negative t'.

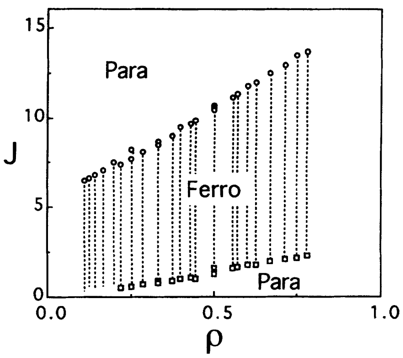

FIG. 1. The ground-state phase diagram of the frustrated t-t'-KLM with $t'=-0.1$.

Now we turn to the momentum distribution of the conduction electrons. In the strong-coupling limit, the momentum distribution per spin in the t-t'-KLM is obtained from that of the t-t' model through the relation

$$n^c_k=\tfrac{1}{2}(1-\tfrac{1}{2}\tilde{\rho}-n^{\tilde{f}}_k), \tag{5}$$

where a PM phase is assumed for simplicity.

As we discussed already, in the strong-coupling limit, the ground-state wave function for the t-t' model with a sufficiently small $-t'$ is given by a product of the Slater determinant and the spin wave function for the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model. This wave function is precisely the same as that of the $U=\infty$ Hubbard model studied by Ogata and Shiba.[11] Note here that the single-particle energy of the t-t' model, $t\cos k+t'\cos 2k$, takes the minimum value at $k=\pi$, if $0<-t'<0.25$. Thus the Fermi points of the t-t' model are at $\pm\pi(1-\tilde{\rho}/2)$. It means that for the $J=\infty$ t-t'-KLM, the Fermi wave vector is also $k_F=\pi(1-\tilde{\rho}/2)=\pi(1+\rho)/2$ and n^c_k is larger in between $\pm k_F$ than outside. Therefore it is concluded that the ground state of the frustrated t-t'-KLM is a Luttinger liquid with the large FS in the strong-coupling limit.

A Luttinger liquid is characterized by the critical exponent of the momentum distribution defined by

$$n^c_k=n^c_{k_F}-\text{const}\times\text{sgn}(|k|-k_F)||k|-k_F|^{\alpha}. \tag{6}$$

For the $U=\infty$ Hubbard model, and therefore in the limit of small $-t'$ of the $J=\infty$ t-t'-KLM, α has been determined to be $\frac{1}{8}$ by the combination of the conformal field theory and the Bethe ansatz solution.[12] Ogata and Shiba[11] have shown that $n_{k_F}=\frac{1}{2}$ gives the best fits for the $U=\infty$ Hubbard model independent of the electron concentration, which means $n^c_{k_F}=\rho/4$ for the $J=\infty$ t-t'-KLM.

Figure 2 shows n^c_k of the $J=\infty$ t-t'-KLM ($t'=-0.1$) at quarter-filling ($\rho=\frac{1}{2}$) and third-filling ($\rho=\frac{2}{3}$). It shows clearly that the FS is large. The arrows in the figure show the

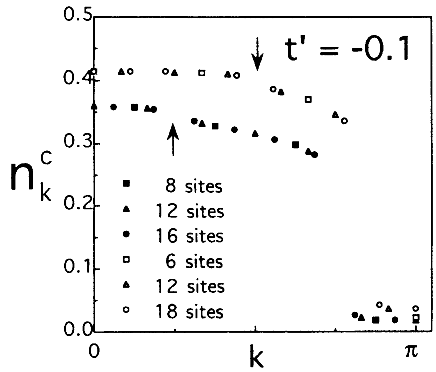

FIG. 2. The momentum distribution of the $J=\infty$ t-t'-KLM with ($t'=-0.1$) at quarter-filling (filled symbols) and third-filling (open symbols). The arrows indicate the singularities at $3k_F$ where $k_F=\pi(1+\rho)$.

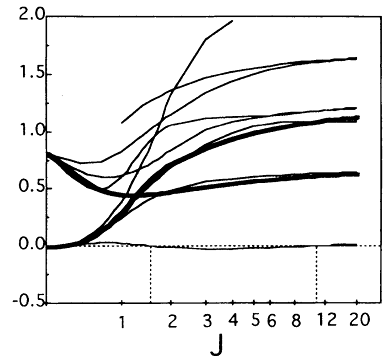

FIG. 3. Energy levels measured from the lowest singlet state for $L=4$. The thick lines are for other singlets. A level crossing with the lowest triplet occurs twice at $J=1.6$ and $J=10.7$, which are the boundaries of the FM region.

$3k_F$ singularities. The critical exponent is not universal and may depend on t'. At quarter-filling, from the numerical data it is estimated as $\alpha=0.13$ for $t'=-0.1$ and $\alpha=0.10$ for $t'=-0.25$ with $n^c_{k_F}=0.11$. For third-filling the best fits are obtained by $\alpha=0.14$ for $t'=-0.1$ and $\alpha=0.11$ for $t'=-0.25$ with $n^c_{k_F}=0.14$. These results are consistent with the previous discussions, if we consider the accuracy of the analysis, typically $\pm 0.01 \sim \pm 0.02$ for α. They also suggest that α becomes smaller than the limiting value $\frac{1}{8}$ as $-t'$ is increased.

In general the Fermi momentum, defined by the singularity in n^c_k may be a function of ρ and J. Now we know that the FS is large in the strong-coupling limit, $k_F(\rho,J)=\pi(\rho+1)/2$, independent of J. Suppose the KLM has a small FS in the weak-coupling region, $k_F(\rho,J)=\pi\rho/2$. This may be possible if this small FS region is separated from the large FS region by another phase like the FM phase or otherwise $k_F(\rho,J)$ must jump at some critical $J^*(\rho)$. Therefore, concerning the problem of the FS sum rule in the weak-coupling region, the first question is whether the PM phase in the weak-coupling region is connected to the one in the strong-coupling region through a narrow corridor besides the half-filling line or split into two parts (see Fig. 1). If it is connected continuously, it is probable that the FS is large everywhere.[13] However, it is difficult to determine the FM boundary in the region close to half-filling. As an alternative approach, we looked at the energy level scheme as a function of J at a fixed density (quarter-filling). For this purpose we calculated low-lying energy eigenvalues for finite systems ($L=4$ and 8) with the open boundary conditions. Figure 3 is the result for $L=4$. One can see that the singlet ground states in both limits are continuously connected. The same behavior is observed for $L=8$. This implies that the symmetry of the singlet state in the weak-coupling region is the same as that in the strong-coupling region and that there is an adiabatic path connecting the two regions.

The momentum distribution in the singlet state of the t-t'-KLM is shown in Fig. 4 for different values of J. In this figure, $L=8$ and $\rho=\frac{1}{2}$, and the open boundary conditions are used. With the open boundary condition, the "momenta" for a finite system k_i ($i=1,\ldots,L$) are defined through the relation, $\varepsilon_i=-2t\cos k_i-2t'\cos 2k_i$, where ε_i are the single-particle energies for the t-t'-KLM. By comparing Fig. 4(a) and Fig. 2, it is readily seen that for large J, n^c_k is similar to that of $J=\infty$ t-t'-KLM. The difference of n^c_k between the neighboring k points is the largest at the position corresponding to $k_{Fc}\equiv\pi\rho/2$ in the weak-coupling case. As J is increased, the largest difference occurs at the position corresponding to k_F [see Fig. 4(b)].

A straightforward interpretation of Fig. 4 would be that there is a transition from the large FS to the small one. Then, however, it is hard to understand the existence of the adia-

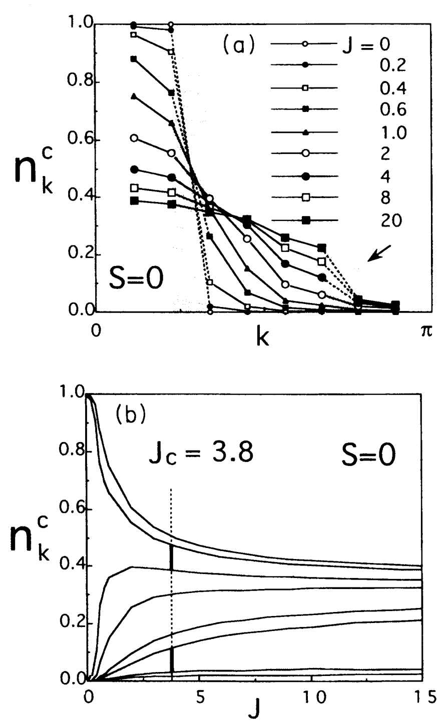

FIG. 4. The momentum distribution of the conduction electrons, n^c_k, for the frustrated t-t'-KLM with $t'=-0.1$: $L=8$ and $\rho=\frac{1}{2}$. (a) n^c_k vs k, compare with Fig. 2. (b) n^c_k vs J. From top to bottom, k is decreasing. J_c is the value for crossover between the large and small FS regimes.

batic path mentioned above, especially in the situation that there is no other singlet coming down. Another possible scenario is that the KLM in the PM phase shows the large FS in the thermodynamic limit but only at temperatures lower than a characteristic energy like T_K. For a finite system, there is a finite low-energy cutoff in the problem, which is determined by the discreteness of the energy levels for the conduction band. The results shown in Fig. 4 indicate that as the J is increased over the cutoff energy, the system shows a crossover from the small FS regime to the large FS regime.[14] The crossover coupling constant J_c may be defined as the J where the difference of n_k^c at $2k_{Fc}$ is equal to that at $2k_F$. If the infinite system shows the large FS behavior in sufficiently low-energy scale, J_c must decrease as the system size is increased, since the low-energy cutoff becomes smaller. From Fig. 4(b) we see that $J_c(L=8)\sim 3.8$, while for a smaller system $J_c(L=4)\sim 4.7$. Therefore we may conclude that the behavior of n_k^c as a function of J is consistent with the idea that the KLM has a large FS in the PM phase even in the small coupling region. However, it is also clear that a more systematic finite-size scaling is necessary to give a definite answer to the problem.

In conclusion, we found a Luttinger-liquid fixed point in the strong-coupling limit of the frustrated t-t'-KLM. The FS sum rule in this limit counts both the number of conduction electrons and the number of localized spins. The critical exponent for the momentum distribution is $\frac{1}{8}$ in the limit of small $-t'$.

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[13] Even if the PM region is continuously connected, it is difficult, strickly speaking, to rule out the possibility that there are two singularities at k_{Fc} and k_F.

[14] In the ground state of the FM region, n_k^c has a singularity at $2k_{Fc}$ for one spin direction, while none for the other spin direction [T. Nishino and K. Ueda (unpublished)]. This is consistent with the $4k_{Fc}$ structure found in the charge correlation function (Ref. 1).

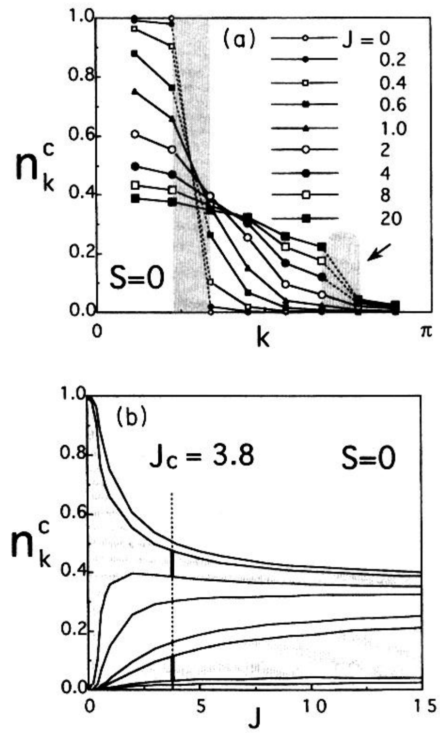

FIG. 4. The momentum distribution of the conduction electrons, n_k^c, for the frustrated t-t'-KLM with $t'=-0.1$: $L=8$ and $\rho=\frac{1}{2}$. (a) n_k^c vs k, compare with Fig. 2. (b) n_k^c vs J. From top to bottom, k is decreasing. J_c is the value for crossover between the large and small FS regimes.