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Fermi surface of the one-dimensional Kondo-lattice model

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We show a strong indication of the existence of a large Fermi surface in the one-dimensional Kondo-lattice model. The characteristic wave vector of the model is found to be $k_F=(1+\rho)\pi/2$, ρ being the density of the conduction electrons. This result is at first obtained for a variant of the model that includes an antiferromagnetic Heisenberg interaction J_H between the local moments. It is then directly observed in the conventional Kondo lattice ($J_H=0$), in the narrow range of Kondo couplings where the long distance properties of the model are numerically accessible. [S0163-1829(96)00841-7]

I. INTRODUCTION

Many experiments tell us that one of the low temperature states of the heavy fermion materials is a Fermi liquid whose quasiparticle masses are 10^2 to 10^3 larger than those of the normal metals.[1] It is commonly believed that the heavy Fermi liquid state is one of the possible ground states of the Kondo-lattice model (KLM). The most popular description of the heavy fermion state is that below a characteristic temperature $T_{\rm coh}$ ($T_{\rm coh}\lesssim 10$ K), the conduction electrons (c electrons) and the local moments (f electrons) have common excitations. This picture leads to the important fact that the localized spins also participate in the Fermi surface (FS). Thus, the FS has a large area. De Haas–Van Alphen measurements[2] of some heavy fermion compounds have shown that the FS has an f character. *Ab initio* local density approximation (LDA)[3] computations of the band structure of heavy fermions also predict a large FS, although these calculations fail to reproduce heavy masses. These results are indeed expected from the Luttinger theorem which states that the volume of the FS is unchanged by the electron-electron interaction. Intuitively, however, it is not straigthforward to understand in the framework of the KLM, how the f electrons can be included in the FS since there is no explicit hybridization between the c electrons and them. LDA computations have shown the existence of a narrow f bandwith which is due to hybridization.[4] The KLM itself is an effective model of the periodic Anderson lattice (PAM) in the limit of nearly integral valence and of strong Coulomb correlation. One may thus wonder whether or not the residual f electron's itinerant character present in the strong coupling limit of the PAM plays a crucial role in the formation of the heavy Fermi liquid state.

Analytical[5,6] and numerical[7–9] studies have focused on the FS of the one-dimensional (1D) KLM. Their results remain very controversial. In the following, we will study the 1D KLM numerically. A numerical study of the 1D KLM presents two essential difficulties. The first one arises from the very low energy scale of the Kondo physics which requires the investigation of lattices of very large sizes. In real materials, the heavy masses involve a very small value of the quasiparticle weight. For the 1D model, in the physical range of parameters ($J_K\ll 1$), the size of the expected singularity in the electron momentum distribution $n_c(k)$ is likely to be very small. The second problem is the occurrence of a ground-state phase transition from a paramagnetic (PM) state at weak couplings to a ferromagnetic (FM) state at strong couplings.[7,9] Therefore, the results of the strong coupling regime where the model converges more rapidly to the thermodynamic limit cannot be extrapolated to the weak coupling region where size effects are still significant even in very long chains. We will show that the study of a KLM [Eq. (1)] in which the strong coupling regime is smoothly connected to the weak coupling one can give insight of the existence of a large FS for the usual KLM. Then, a careful analysis of the usual KLM will be made. A large FS means that the Fermi wave vector is located at $k_F=k_{F_c}+\pi/2$, k_{F_c} being the Fermi wave vector of the c electrons only. We will consider the following KLM:

$$H=-t\sum_{is}(c_{is}^{+}c_{i+1s}+\text{H.c.})+J_K\sum_i \mathbf{S}_{ic}\cdot\mathbf{S}_{if}+J_H\sum_i \mathbf{S}_{if}\cdot\mathbf{S}_{i+1f}, \tag{1}$$

where $\mathbf{S}_{ic}^{\alpha}=\frac{1}{2}\Sigma_{s,s'}c_{is}^{+}\sigma_{ss'}^{\alpha}c_{is'}$ and $\mathbf{S}_{if}^{\alpha}$ is a localized spin. The hopping integral t is set to 1. A direct Heisenberg exchange term between local moments J_H is introduced here. We have recently argued[9] that the occurrence of a ferromagnetic phase transition in the KLM in the strong coupling region is due to the fact that the RKKY interaction becomes ineffective. One would thus expect that a sufficiently strong antiferromagnetic Heisenberg coupling between the local moments can stabilize a PM ground state. In the conventional KLM, this term is usually omitted because typical lattice parameters in the heavy fermion compound are 3.5−4 Å while the ionic radii of the f ions are less than 1 Å, so that the overlap between the f orbitals is negligible. It should be noted that the strong J_K regime of the Hamiltonian (1) is relevant in the study of high-T_c materials. In this case, J_H is the superexchange interaction between copper ions. The double occupancy in the c electron band is naturally suppressed by J_K, so that one need not include an explicit repulsion term between these electrons. We have investigated Hamiltonian (1) using the density matrix renormalization group (DMRG) method.[10]

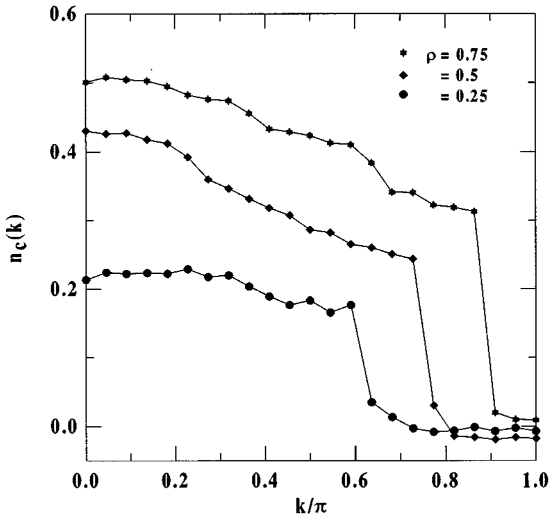

FIG. 1. The electron momentum distribution $n_c(k)$ for $\rho=0.75$, 0.5, and 0.25 at $J_K=10$ and $J_H=0.5$.

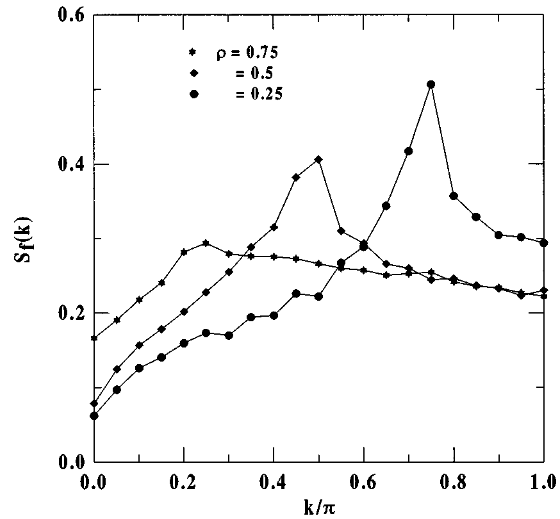

FIG. 2. The magnetic structure factor $S_f(k)$ for $\rho=0.75$, 0.5, and 0.25 at $J_K=10$ and $J_H=0.5$.

We have chosen an algorithm with open boundary conditions. We keep between 64 and 150 states in the two external blocks. These states are labeled by the z component of the total spin S_T^z The ground state corresponds to the lowest state with $S_T^z=0$. The maximum truncation error is in the order of 10^{-4}. Although we have reached $N=60$ sites, the longest distance in the calculation of the correlation function is $L=22$. Because we have first built lattices of 20 sites before we start to calculate the correlation functions. This way, we minimize the end effects and density fluctuations that are larger in the early steps of the algorithm.

II. RESULTS FOR THE KONDO-HEISENBERG CASE ($J_H \neq 0$)

The Hamiltonian (1) has *a PM ground state with a Luttinger Fermi surface* when $J_H=0.5$ in the strong J_K regime. We have chosen our value for the Heisenberg coupling on the grounds that it is necessary that J_H exceeds the effective FM coupling $J_{\rm eff}^{\rm max}$ between the f electrons to stabilize the PM ground state for all J_K. Our first choice was $J_H=0.1$. For this value, we found that the ground state is PM in the weak J_K region, FM for intermediate couplings, then PM for strong J_K. We can estimate $J_{\rm eff}$ by using the results of the strong coupling expansion.[11] $J_{\rm eff}J_K/t^2$ is approximatively 0.05, 0.2, and 0.25, respectively, for the partial band fillings ρ=0.25, 0.5, and 0.75. Then, knowing that the strong coupling region starts for J_K of order 1, one obtains the upper bound, $J_{\rm eff}^{\rm max}\simeq 0.25$ for $t=1$. Our value of 0.5 thus includes a security factor. In Fig. 1, we show $n_c(k)$ (the Fourier transform of $\langle c_{i\sigma}^{+}c_{j\sigma}\rangle$) for the band-fillings ρ=0.25, 0.5, and 0.75 for $J_K=10$. $n_c(k)$ at 0.25 and 0.75 are affected by density fluctuations, since the band filling is not constant during the DMRG iterations. Nevertheless, clean singularities are observed at $k_F=0.625\pi$, 0.75π, and 0.875π. The magnetic structure factor of the localized electrons $S_f(k)$ (the Fourier transform of $\langle S_{if}^z S_{jf}^z\rangle$), shown in Fig. 2, presents a maximum at $2k_F$=0.75π, 0.5π, and 0.25π, respectively. These values correspond to $2\pi-2k_F$, since $2k_F$ is greater than π. Clearly, neither the bare c electron nor the bare f electron signatures are detected. There are instead unique compound particles propagating with a characteristic wave vector at k_F. An analogy can be made with the Hubbard model.[12] At half-filling, in the $J_K=\infty$ limit, all the conduction electrons form on-site singlets with the localized spins, so that the overall system is in a singlet state. The nonhalf-filled cases correspond to the introduction of holes in the system. These holes which can hop from site to site are associated with the $N-N_c$ unpaired f electrons, N_c being the number of c electrons. Obviously, double occupancy of holes is forbidden: one has a $U=\infty$ Hubbard model of $\rho_h=1-\rho$ hole density. Depletion effects[13] are also observed in Fig. 2: the reduction of the conduction electron density increases the tendency to magnetism. The maximum of $S_f(k)$ increases when ρ decreases.

Now we wish to discuss how the system evolves when J_K is reduced. We show in Fig. 3 $n_c(k)$ at $\rho=0.5$ for $J_K=10,8,6,4,3,2.5$, and 2. The height of the singularity at

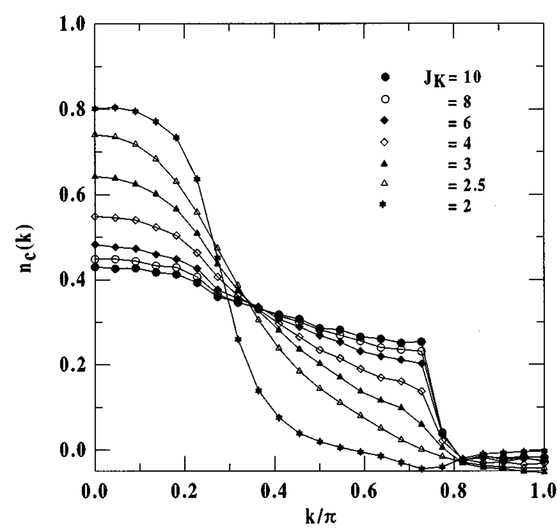

FIG. 3. $n_c(k)$ for various values of J_K at $\rho=0.5$ and $J_H=0.5$.

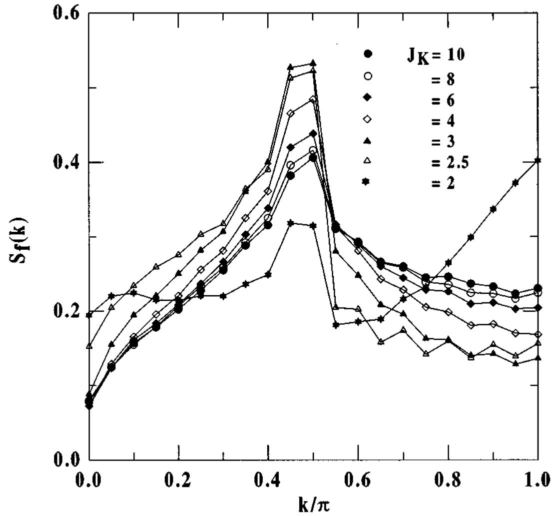

FIG. 4. $S_f(k)$ for various values of J_K at $\rho=0.5$ and $J_H=0.5$.

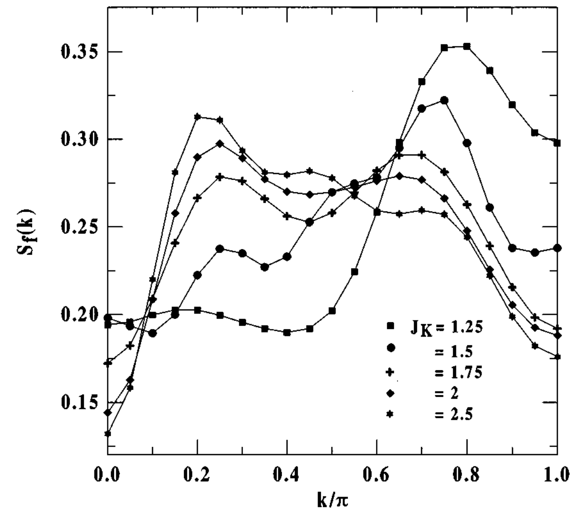

FIG. 5. $S_f(k)$ for $J_K=1.25$, 1.5, 1.75, 2, and 2.5 at $\rho=0.75$ and $J_H=0$.

k_F decreases as J_K is reduced. Concurrently the drop at k_{F_c} which, was negligibly small in the strong J_K case, increases. The c electron character is progressively enhanced. The local spin-spin correlation which is $\langle S_{ic}S_{if}\rangle=-0.3748\simeq-\frac{3}{4}\rho$ at $J_K=100$, is equal to -0.366 at $J_K=10$ and -0.183 at $J_K=2$. The deviation of this quantity from the perfect on-site singlet value $-\frac{3}{4}\rho$ means that the singlet clouds have a spatial extension at lower J_K. At $J_K=2$, short-range effects coexist along with the long-range behavior of the system. Clearly, it becomes hard to define the exact position of the FS. This can be better illustrated in $S_f(k)$ (Fig. 4) at $\rho=0.5$. A new peak appears at $k=\pi$ at small J_K, signaling short-range antiferromagnetic correlations. At $J_K=1.5$ (not shown here), the peak at $2k_F$ is not seen. We can no longer observe the long-distance behavior of the model because of the finite-size effects (long correlation length; see the discussion below). Since there is no phase transition in the system, the weak and the strong J_K regimes are continuously connected. We thus believe that *the FS is large even at smaller* J_K. The above discussion is similar to the one made by Kotliar in the framework of the PAM.[14] The local singlets of the strong-coupling limit are obtained as the Kondo resonances are pulled out of the c electron band by increasing J_K. The FS is conserved during this process.

III. RESULTS FOR THE CONVENTIONAL KLM ($J_H=0$)

We now discuss if the above conclusions can be extended to the PM phase of the conventional KLM. At first sight, one can argue that the conventional KLM is adiabatically reached by taking the limit $J_H\to 0$. Thus the conventional KLM may have a large FS in its PM phase. It should be noted from the above results and from the knowledge of the occurrence of a phase transition, that the range of J_K in which we can expect to detect a large FS with numerical methods in the conventional KLM is narrow. An estimation of this range can be obtained by examining the Kondo coherence length ξ_K of the one-impurity problem. $\xi_K=v_F/T_K$, where v_F is the Fermi velocity and T_K the Kondo temperature. The observation of the long-range properties of the model is only possible at distances $r\gg\xi_K$. For $r\lesssim\xi_K$ finite-size effects dominate, only short-range effects governed by the RKKY interaction will be observed. Sørensen and Affleck have recently made an accurate computation of ξ_K.[15] Some typical values are $\xi_K=1,2,4.85,8,$ and 23 for $J_K=2.5$, 2, 1.5, 1.25, and 1, respectively. Clearly, for $J_K\lesssim1.25$ the long-range behavior of the model is not attainable since the longest distance in our study is $L=22$. Moreover, the FM transition occurs at $J_K\simeq1.5$ for $\rho=0.5$ and $J_K\simeq2.75$ for $\rho=0.75$. At low band fillings, depletion effects enhance the FM instability. The PM phase boundary is shifted towards weak couplings where ξ_K becomes very large. Hence, at quarter-filling where there is no density fluctuations, this range is very narrow. Thus we have chosen to study the KLM at $\rho=0.75$ in the range $1.25\lesssim J_K\lesssim2.5$. In Ref. 9, we have found that $n_c(k)$ displays a sharp drop at k_{F_c} and $S_f(k)$ presents a maximum at $2k_{F_c}$ in the small J_K regime. As J_K was increased, these features vanished before the phase transition was reached. But we were unable to draw a firm conclusion about the location of the FS. A more careful analysis will now show that we had observed a short-range effect governed by the RKKY interaction. Furthermore, we will identify the true long-range properties of the model which are not easily observable. In Fig. 5, we display $S_f(k)$ at $\rho=0.75$ for $J_K=1.25,1.5,1.75,2,$ and 2.5. Starting from $J_K=1.25$, we can only detect the RKKY maximum at $2k_{F_c}=0.75\pi$. For $J_K=1.5$, the maximum of $S_f(k)$ is still located at the RKKY wave vector. But one can also observe a local maximum at the position of the large FS at $2k_F=0.25\pi$. At $J_K=1.75$ and 2, the height of the RKKY maximum decreases. At the same time, the height of the maximum at $2k_F$ increases. This trend is unambigously confirmed at $J_K=2.5$, where the maximum at $2k_F$ is now the highest. The height of these maxima however, is still smaller than the one at $2k_{F_c}$ for $J_K=0.5$ in Ref. 9, and are thus harder to detect. Finally, $n_c(k)$, shown in Fig. 6, corroborates the existence of the large FS in the KLM. $n_c(k)$ drops monotonously when $k<k_F=0.875\pi$, shows a small plateau just before $k=k_F$, and then drops abruptly at $k\simeq k_F$. The width

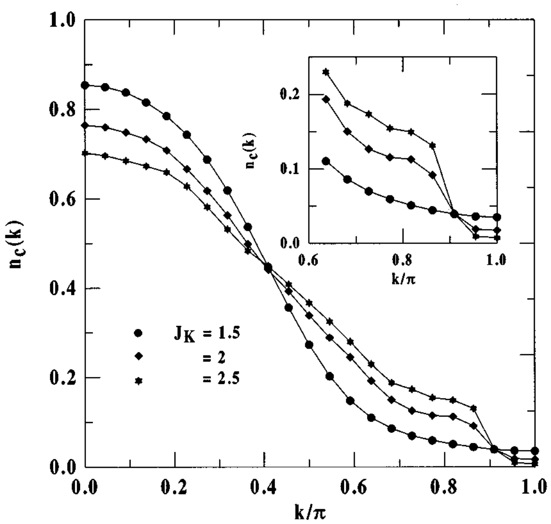

FIG. 6. $n_c(k)$ for $J_K=1.5$, 2, and 2.5 at $\rho=0.75$ and $J_H=0$.

of the plateau shrinks and then becomes undetectable when J_K is decreased. At the same time, the drop at k_{F_c} is enhanced indicating that the short-range effects are becoming dominant. This is consistent with the results for $S_f(k)$.

IV. CONCLUSION

In summary, we have shown that the KLM with a direct exchange Heisenberg coupling has a large FS in the strong Kondo coupling limit. We have shown that this phase is continously connected to the weak Kondo coupling regime. As a consequence, the latter model has a large FS in the small coupling regime. The conventional KLM can continously be reached by taking the limit of vanishing Heisenberg coupling. We have concluded from this that its FS should have a large area in its PM phase. Direct numerical computations made on the KLM support the existence of a large FS. Although these results are less conclusive, the paramagnetic phase of the coventional KLM presents strong finite-size effects. The height of the singularity in the electron momentum distribution decreases and becomes very small as the Kondo interaction goes towards the weak coupling region. This fact is consistent with the enhancement of the heavy quasiparticle mass observed in real materials. Finally, the nature of the heavy quasiparticles appear to be different from that proposed in the renormalized band structure studies.[16] In the renormalized band picture, the heavy quasiparticles result from the small hybridization between the conduction electrons and the renormalized f bands pinned at the Fermi level of the conduction electron sea. Our results suggest that these are instead loosely bound states made up of conduction electrons and f spin fluctuations. This is consistent with recent results from field theory[17] and exact diagonalization.[18]

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