One-dimensional Kondo lattice model as a Tomonaga-Luttinger liquid

Naokazu Shibata
Institute for Solid State Physics, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan

Alexei Tsvelik
Department of Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, United Kingdom

Kazuo Ueda
Institute for Solid State Physics, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan
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Arguments are presented that in the one-dimensional Kondo lattice model f-electron spins participate in filling of the Fermi sea. It is shown that in its paramagnetic phase this model belongs to the spin-1/2 Tomonaga-Luttinger liquid universality class. The ratio of the spin and charge velocities v_σ/v_ρ and K_ρ are estimated to be of the order of $(T_K/\epsilon_F)^{1/2}$. [S0163-1829(97)03225-6]

I. INTRODUCTION

One can use a one-dimensional Kondo lattice (KL) model as a toy model to study the long-standing problem of whether localized electrons determine the volume of the Fermi surface. Recent numerical results show that in the paramagnetic metallic phase, the KL model belongs to a universality class of spin-1/2 Tomonaga-Luttinger (TL) liquid.[1–3] In particular it has been shown that the Friedel oscillations are characterized by the large Fermi vector.[1] So it seems that the f electrons do participate in the Fermi surface formation. On the other hand, the conclusions of the bosonization studies are controversial. In the area of the paramagnetic metallic phase the TL liquid[4] with a large Fermi surface is obtained by Fujimoto and Kawakami[5] while the Luther-Emery liquid with a spin gap is also predicted by White and Affleck.[6] Recent analytical work based on the Lieb-Schultz-Mattis construction shows that there exists a gapless excitation away from half-filling.[7] Though its character is not yet clear, it seems to be consistent with the TL liquid with a large Fermi surface.

In this paper we undertake a further study of the TL phase of the KL model. Let the reader recall that the spin-1/2 TL liquid critical point is characterized by two parameters: the ratio of spin to charge density wave velocities v_σ/v_ρ and the number K_ρ which parametrizes scaling dimensions in the charge sector [the similar parameter in the spin sector is fixed by the SU(2) symmetry, $K_\sigma=1$]. The dynamical spin and charge susceptibilities at low (ω,q) are given by

$$\chi_\sigma(\omega_n,q)=\frac{2}{\pi}\frac{q^2}{q^2v_\sigma+\omega_n^2/v_\sigma}, \tag{1}$$

$$\chi_\rho(\omega_n,q)=\frac{2K_\rho}{\pi}\frac{q^2}{q^2v_\rho+\omega_n^2/v_\rho}. \tag{2}$$

Thus, if we shall manage to find these two parameters, the characterization of the low-energy sector of the KL model is complete.

II. LUTTINGER LIQUID PARAMETERS OBTAINED BY THE 1/N EXPANSION

The Hamiltonian of the one-dimensional KL model is

$$H=-t\sum_{i\sigma}(a_{i\sigma}^\dagger a_{i+1\sigma}+\text{H.c.})+J\sum_{i\mu}S_i^\mu s_i^\mu, \tag{3}$$

where $a_{i\sigma}^\dagger(a_{i\sigma})$ is the creation (annihilation) operator of a conduction electron at the ith site, and $s_i^\mu=(1/2)\Sigma_{\sigma\sigma'}a_{i\sigma}^\dagger\tau_{\sigma\sigma'}^\mu a_{i\sigma'}$, with $\tau_{\sigma\sigma'}^\mu$ $(\mu=x,y,z)$ being the Pauli matrices, are the spin density operators of the conduction electrons. The spin densities are coupled to the localized spins S_i^μ through an antiferromagnetic exchange coupling J.

In order to obtain analytical results we shall extend the symmetry of the KL model to the SU(N) and resort to the 1/N expansion (see Refs. 8 and 9). The corresponding Lagrangian density is

$$\mathcal{L}=a_j^*[\partial_\tau+\hat{\epsilon}(x)]a_j+f_j^*\partial_\tau f_j+i\lambda(f_j^*f_j-qN)-\frac{J}{N}(a_j^*f_j)(f_k^*a_k). \tag{4}$$

Here the dynamical field $\lambda(\tau,x)$ is introduced to enforce the local constraint of the fermion occupation number. The number q remains finite when $N\to\infty$.

Next we decouple the interaction by the Hubbard-Stratonovich transformation:

$$-\frac{J}{N}(a_j^*f_j)(f_k^*a_k)\to N\frac{V^*V}{J}+V(a_j^*f_j)+V^*(f_j^*a_j). \tag{5}$$

The resulting partition function is gauge invariant:

$$f_j(\tau,x)\to f_j(\tau,x)e^{i\phi(\tau,x)},$$

$$V(\tau,x)\to V(\tau,x)e^{-i\phi(\tau,x)},$$

$$\lambda(\tau,x)\to\lambda(\tau,x)-\partial_\tau\phi(\tau,x). \tag{6}$$

It is convenient to choose the gauge where the field V is real. We choose the following parametrizations:

$$V(\tau,x)=V_0\sqrt{1+[r(\tau,x)/V_0\sqrt{N}]}, \tag{7}$$

$$i\lambda=T_K+iu/\sqrt{N}, \tag{8}$$

where V_0 is the saddle point value of V which we shall determine later and r is a new field chosen in such a way that its measure of integration is trivial.

We shall expand the partition function around its saddle point:

$$V=V_0, \quad i\lambda=T_K. \tag{9}$$

Expanding to the second order in r we get

$$\mathcal{L}=\mathcal{L}_0+\mathcal{L}_{\rm int},$$

$$\mathcal{L}_0=a_j^*[\partial_\tau+\hat{\epsilon}(x)]a_j+f_j^*(\partial_\tau+T_K)f_j+V_0(a_j^*f_j+\text{c.c.}), \tag{10}$$

$$\mathcal{L}_{\rm int}=\frac{r^2}{4J}+\frac{r}{2\sqrt{N}}(:a_j^*f_j+\text{c.c.}:)+\frac{iu}{\sqrt{N}}:f_j^*f_j:, \tag{11}$$

where the dots mean that the average is substructed, $:A:\equiv A-\langle A\rangle$, and the r^2 term comes from the expansion of the square root in the expression for V, Eq. (7). The saddle point parameters V_0 and T_K are determined self-consistently by the vanishing of the terms linear in r and u:

$$\frac{1}{N}\sum_{j=1}^{N}\langle f_j^\dagger(n)f_j(n)\rangle=q, \tag{12}$$

$$\frac{1}{N}\sum_{j=1}^{N}[\langle a_j^\dagger(n)f_j(n)\rangle+\langle f_j^\dagger(n)a_j(n)\rangle]=-\frac{2V_0}{J}. \tag{13}$$

In the leading order in $1/N$ the spectrum is determined by the saddle point. This gives us a great advantage because the saddle point describes the large Fermi surface. The single-electron spectrum has the following well-familiar form:

$$E_\pm(p)=[\epsilon(p)+T_K]/2\pm\sqrt{[\epsilon(p)-T_K]^2/4+V_0^2}. \tag{14}$$

Substituting the saddle point Green's functions into Eqs. (12) and (13) we get

$$q=\rho(0)V_0^2/T_K, \quad T_K=D\exp[-1/\rho(0)J], \tag{15}$$

where $\rho(0)$ is the bare density of states per one channel, and D is the bandwidth. The expression for the new Fermi vector is

$$k_F=k_F^{(0)}+\pi q. \tag{16}$$

It follows from this equation that the charge susceptibility remains unaffected by the presence of the spins.

Only the mode $E_-(p)$ crosses the chemical potential. Near the Fermi points the spectrum can be linearized:

$$E_-(p)\approx\pm v^*(p\mp p_F), \quad v^*=v_F\rho(0)T_Kq. \tag{17}$$

Now one can calculate the spin and charge density response functions (2) directly. The calculation of the spin-spin correlation function is straightforward: In the leading order in $1/N$ the only contribution comes from the polarization loop of two $G_f=\langle\langle ff^+\rangle\rangle$ functions. The result reproduces Eq. (1) with $v_\sigma=v^*$.

The calculation of the charge response function is more complicated. We chose the following approach: First we shall integrate out the high-energy degrees of freedom in the partition function and obtain the effective action for the low-energy sector; then we shall bosonize this action and obtain the parameters of the TL liquid. To do the integration it is convenient to diagonilize the saddle point Hamiltonian and to express the fermionic operators in terms of the new annihilation operators $A_{\pm,j}(k)$ corresponding to excitations with the dispersion $E_\pm(k)$ (since the transformation is diagonal in the flavor indices, we shall omit them):

$$a(k)=\sqrt{\alpha_k}A_+(k)+\sqrt{\beta_k}A_-(k),$$

$$f(k)=-\sqrt{\beta_k}A_+(k)+\sqrt{\alpha_k}A_-(k), \tag{18}$$

where

$$\alpha_k+\beta_k=1, \quad \beta_k=\frac{1}{2}\left\{1-\frac{[\epsilon(k)-T_K]}{\sqrt{[\epsilon(k)-T_K]^2+4V_0^2}}\right\}. \tag{19}$$

Substituting these expressions into Eq. (11) and omitting the terms containing only A_+ we get

$$\int dx\mathcal{L}_{\rm int}=L_1+L_2, \tag{20}$$

$$L_1=\sum_q\frac{r(-q)r(q)}{4J}+\frac{1}{2\sqrt{N}}\sum_{k,q}[r(q)(\sqrt{\alpha_{k+q}\alpha_k}-\sqrt{\beta_{k+q}\beta_k})$$
$$-2iu(q)\sqrt{\beta_{k+q}\alpha_k}][A_{+,j}^*(k+q)A_{-,j}(k)+\text{c. c.}], \tag{21}$$

$$L_2=\frac{1}{\sqrt{N}}\sum_{k,q}[A_{-,j}^*(k+q)A_{-,j}(k)][\sqrt{\alpha_F\beta_F}r(q)+i\alpha_Fu(q)], \tag{22}$$

where α_F and β_F are taken at the Fermi surface: $\alpha_F\approx1$ and $\beta_F\sim T_K/D$.

Integrating over A_+ we get in the leading order in $1/N$ the following action for the fields r and u:

$$S_{\rm eff}=\frac{1}{2}\sum_{\omega,q}\Pi(\omega,q)[4r(-\omega,-q)r(\omega,q)$$
$$+u(-\omega,-q)u(\omega,q)]. \tag{23}$$

To get the effective action for the low-lying excitations we need to know the function $\Pi(\omega,q)$ for the area around $q=0$ and for $q=2k_F$. The result is $\Pi(0,0)=\rho(0)$.

We bosonize the fermionic operators,

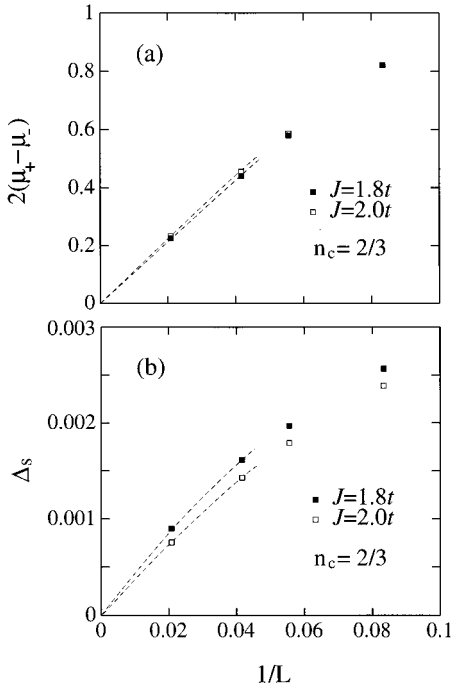

FIG. 1. (a) Size dependence of the difference of the chemical potentials, $\mu_+-\mu_-$, in the one-dimensional Kondo lattice model. $2\mu_+(L)=E_g(n_c=n_c^0+2/L,L)-E_g(n_c=n_c^0,L)$. $2\mu_-(L)=E_g(n_c=n_c^0,L)-E_g(n_c=n_c^0-2/L,L)$. $E_g(n_c,L)$ is the ground-state energy at the carrier density n_c in the system of length L. $n_c^0=2/3$. (b) Size dependence of the spin gap $\Delta_s(L)=E_g(S_z^{\rm tot}=1,L)-E_g(S_z^{\rm tot}=0,L)$. $E_g(S_z^{\rm tot},L)$ is the lowest energy in the Hilbert space of total spin $S_z^{\rm tot}$. $n_c=2/3$. The energy unit is t. Typical truncation errors in the DMRG calculations are 10^{-4}.

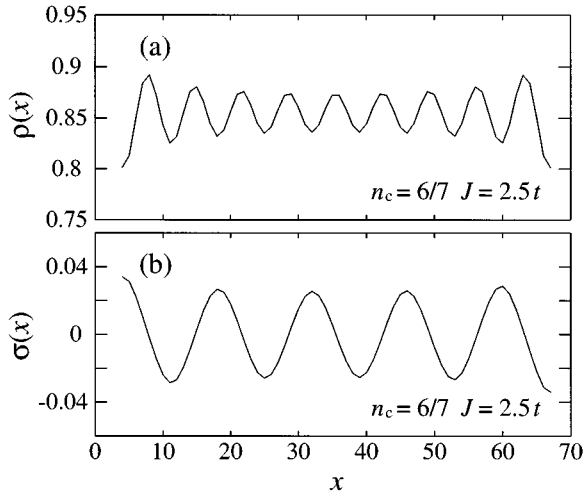

FIG. 2. (a) Charge density Friedel oscillations induced by the open boundary conditions. The system size is 70 sites. (b) Spin density Friedel oscillations induced by applying local magnetic fields at the both ends. The strength of the local magnetic fields is $0.2t$. Typical truncation errors in the DMRG calculations are 1×10^{-6} for $J=2.5t$.

$$\sum_{k,j} A^*_{-,j}(k+q)A_{-,j}(k)=i\sqrt{N/\pi}q\Phi_\rho(q) \quad (|q|\ll k_F), \tag{24}$$

where Φ_ρ is the charge field, and integrate over u and r. Since β_F is so small, the largest contribution to the effective action comes from the fluctuations of the u field. The bosonized version of the effective action in the charge sector is given by

$$S_{\rm eff}=\int d\tau dx\left[\frac{1}{2v^*}(\partial_\tau\Phi_\rho)^2+\frac{1}{2\pi\rho(0)}(\partial_x\Phi_\rho)^2\right]. \tag{25}$$

From this action one can derive the canonical expression for the charge susceptibility and K_ρ. At least in the leading order in $1/N$ the result does not depend on N:

$$v_\rho=\sqrt{v^*/\pi\rho(0)} \tag{26}$$

and

$$K_\rho=\sqrt{\pi\rho(0)v^*}. \tag{27}$$

III. DENSITY MATRIX RENORMALIZATION GROUP STUDY

In order to check the validity of the large-N results for the $N=2$ case we numerically estimate the TL liquid parameters, making use of the density matrix renormalization group (DMRG).[10] This method is the most suitable for studying long-range and low-energy properties since it allows one to study long chains, iteratively enlarging the system size, and to obtain the ground-state wave function with only small systematic errors, which can be estimated from the eigenvalues of the density matrix. The obtained results are consistent with the above arguments and indicate $K_\rho\ll1/2$ in the weak-coupling limit ($J\to0$).

Now we shall describe results of the numerical analysis of the model (3). The paramagnetic metallic state of this model, which is expected to be a TL liquid, is realized only in the region of rather weak exchange coupling away from both half-filling ($n_c=1$) and the low carrier density limit ($n_c\to0$). The ground state is always insulating at half-filling and ferromagnetic both in the strong-coupling limit ($J\to\infty$) for general carrier densities ($n_c\neq1$) and in the low-carrier-density limit.[11]

We first calculate spin excitation gap Δ_s and difference of chemical potentials $\mu_+-\mu_-$ as a function of the system size L. As expected, both Δ_s and $\mu_+-\mu_-$ [Figs. 1(a) and 1(b) for the case of $n_c=2/3$ and $J=1.8t,2.0t$] vanish in the bulk limit ($L\to\infty$), which confirms that the paramagnetic phase of the KL model is a TL liquid.

The finite-size corrections of $\mu_+-\mu_-$ and Δ_s in Fig. 1 are related to the charge susceptibility and the spin velocity, respectively. Since we have used open boundary conditions, $\Delta_s(L)=v_\sigma\Delta k(L)=v_\sigma\pi/L$ and $\mu_+(L)-\mu_-(L)=\Delta n_c(L)/\chi_\rho=2/(\chi_\rho L)$. The obtained values are shown in Table I. Once we have obtained v_σ, then we can calculate χ_σ through the relation $K_\sigma=\pi v_\sigma\chi_\sigma/2$; see Eq. (1). Because the SU(2) symmetry in the spin space guarantees $K_\sigma=1$, a rather large χ_σ is obtained as is shown in Table I. This large χ_σ is naturally expected because there is a macroscopic number of almost free spins in both weak- and strong-coupling regions. The f spins are almost but not exactly independent with each other: In the weak-coupling region, L almost-free f spins, and in the strong-coupling region, $L(1-n_c)$ f spins unpaired with conduction electrons.

TABLE I. Luttinger liquid parameters of the one-dimensional Kondo lattice model. The carrier density n_c is 2/3. The energy unit is t. The errors are estimated from the ambiguity of the power law decay of the charge density Friedel oscillations.

	K_ρ	v_σ	χ_σ	v_ρ	χ_ρ
$J=0$	1	-	-	1.73	0.37
$J=1.5t$	0.19 ± 0.03			0.30 ± 0.06	0.42
$J=1.8t$	0.24 ± 0.02	0.014	46	0.41 ± 0.06	0.38
$J=2.0t$	0.27 ± 0.02	0.011	56	0.48 ± 0.06	0.36

Now we discuss the charge susceptibility. In the strong-coupling limit it tends to the value for the free spinless fermions: $\chi_\rho^{-1}=\pi t\sin(\pi-\pi n_c)$. On the other hand, in the weak-coupling limit we expect a J-independent charge susceptibility as is predicted by the Gutzwiller-type variational calculations:[12] $\chi_\rho^{-1}=\pi t\sin(\pi n_c/2)$. The density $n_c=2/3$ is rather special in the sense that the values expected for the strong-coupling limit and weak-coupling limits are the same. Thus we expect that χ_ρ depends only weakly on J. In general, in the weak-coupling limit we have an asymptotic form of the charge velocity which is proportional to K_ρ as

$$v_\rho=2K_\rho t\sin(\pi n_c/2) \tag{28}$$

from the relation $K_\rho=\pi v_\rho\chi_\rho/2$, Eq. (2). However, we have to be careful close to half-filling where the charge susceptibility tends to diverge owing to the charge gap at half-filling.

The estimation of the correlation exponent is one of the most difficult calculations even by the DMRG method. In order to estimate K_ρ we need to see the long-range behaviors of the system with sufficient accuracy. In the present study we use asymptotic form of the Friedel oscillations because they are numerically more reliable than long-range off-diagonal correlations.

The Friedel oscillations are density oscillations induced by a local perturbation. In a TL liquid, power law anomalies in correlation functions naturally reflect themselves in the Friedel oscillations; the Friedel oscillations induced by an impurity potential are

$$\delta\rho(x)\sim C_1\cos(2k_Fx)x^{(-1-K_\rho)/2}+C_2\cos(4k_Fx)x^{-2K_\rho}, \tag{29}$$

as a function of the distance x from the impurity,[13–15] and analogously, spin density oscillations induced by a local magnetic field behave as

$$\sigma(x)\sim D_1\cos(2k_Fx)x^{-K_\rho}. \tag{30}$$

Thus, we can determine K_ρ from the asymptotic form of the oscillations.

Figure 2 shows induced charge and spin density Friedel oscillations of the KL model obtained by the DMRG for $J=2.5t$ at $n_c=6/7$. The Fourier components of spin density Friedel oscillations for $J=1.8t,2.5t,2.5t$ at $n_c=2/3,4/5,6/7$, respectively, are also shown in Fig. 3. The charge density Friedel oscillations are induced naturally by the open boundary conditions of the system and the spin density oscillations are introduced by applying local magnetic fields at the both ends. As is already shown for $n_c=4/5$ in the previous work,[1] the period of the oscillations is explained by the assumption

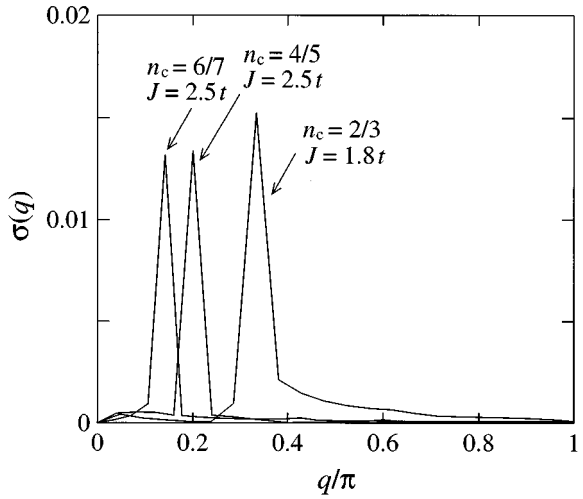

FIG. 3. Fourier components of the spin density Friedel oscillations.

of the spin-1/2 TL liquid with a large Fermi surface, $k_F=\pi(1+n_c)/2$, which includes f spin densities as well as the density of conduction electrons.

Now we calculate the correlation exponent K_ρ. In order to obtain K_ρ, we simply use the slope of the envelope function of the charge density oscillations, assuming that its decay is proportional to x^{-2K_ρ}, because the dominant component of the oscillations is the $4k_F$ component even for the case of $J=1.5t$. In Fig. 4, the obtained K_ρ for the exchange coupling from $J=4.0t$ to $1.5t$ at $n_c=2/3$ are presented. Since the $2k_F$ spin density oscillations decay much slower than the charge density oscillations, it is not possible to determine K_ρ from the spin density oscillations in the present system size. However, the slower decay of the spin density oscillations is consistent with the TL liquid prediction, Eq. (30), which gives a smaller exponent, x^{-K_ρ}.

As is clearly seen in Fig. 4, K_ρ is always smaller than 1/2 and monotonically decreases with decreasing J. In the

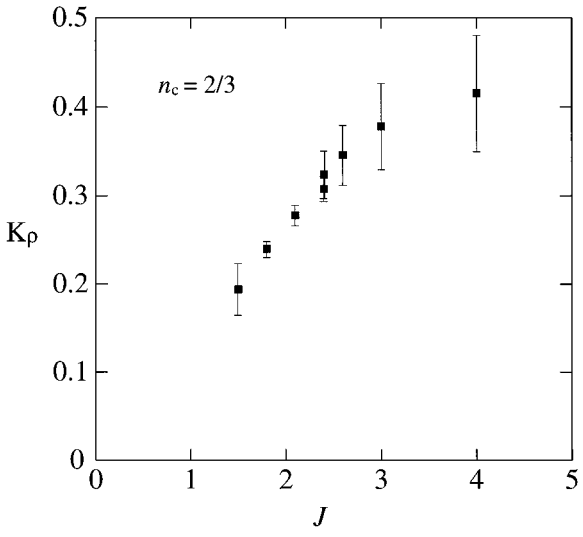

FIG. 4. Correlation exponent K_ρ estimated from the decay rate of the charge density Friedel oscillations. The error bars are determined from the ambiguity of the power law fitting. $n_c=2/3$. J is in units of t.

strong-coupling limit, the conduction electrons and the localized f spins form local singlets, leading to a complete spin-charge separation. Since the charge part is described by the free spinless fermions, $K_\rho = 1/2$ is obtained in the strong-coupling limit as in the case of the infinite-U Hubbard model. With decreasing J from infinity the repulsive interaction between the neighboring spinless fermions is introduced in the leading order of t/J. Thus the situation is similar to the large-U Hubbard model with nearest-neighbor repulsions whose K_ρ is smaller than 1/2.[16,17]

In Fig. 4 we find a small discontinuity at $J = 2.4t$. This is due to the phase transition from the ferromagnetic state to the paramagnetic one. Since this transition is of first order accompanied by a jump in the total spin quantum number, from $S = L(1-n_c)/2$ to 0, or 1/2 with L being the number of the sites, it is natural that the K_ρ also shows a jump at the critical value J_c. In order to confirm the discontinuity we have calculated the K_ρ in both ferromagnetic and paramagnetic states at $J = 2.4t$ which is near but smaller than the critical point. The K_ρ in the ferromagnetic state is calculated by setting the total S_z as $L(1-n_c)/2$, which is the total spin in the ferromagnetic state.

In contrast to the slow decrease of K_ρ above the critical J_c, a rather sharp decrease is observed below J_c, and the K_ρ becomes smaller than 1/3 which means that the long range behavior of the charge-charge correlation is governed by $4k_F$ oscillations. The dominance of $4k_F$ oscillations is a characteristic feature of this new class of spin-1/2 TL liquid.

With further decreasing J, the K_ρ seems to cross the value $3-2\sqrt{2} \sim 0.17$. Since the exponent of the power law anomaly in the momentum distribution function, α, is given by $\alpha = (K_\rho + 1/K_\rho - 2)/4$, the power law anomaly is removed below this point and we cannot see a clear Fermi surface any more. It is very difficult to observe clear Friedel oscillations for K_ρ smaller than 0.17.

IV. CONCLUSIONS

In conclusion we have established that in the area of the phase diagram where the one-dimensional Kondo lattice is paramagnetic, it belongs to the universality class of spin-1/2 TL liquids. The f electrons do take part in the formation of the Fermi surface. According to the Luttinger theorem the volume of the Fermi sea is determined by those branches of the spectrum which cross the chemical potential. Despite the fact that most of the spectral weight of the f electrons is concentrated far from the chemical potential, they do have access to it via the Kondo resonance. We bring the attention of the reader to the fact that the Luttinger theorem does not require the existence of a pole in the single-electron Green's function and therefore can be applied outside the Fermi liquid domain. In particular, the system under consideration belongs to the spin-1/2 TL liquid universality class. It is a rather peculiar member of this class since K_ρ is small. How small is not entirely clear; the analytical calculations give $K_\rho = v_\sigma / v_\rho$ [see Eqs. (26) and (27)] which is one order of magnitude smaller than the values obtained numerically (see Table I). This may be due to the inaccuracy of the $1/N$ approximation; it is more likely, however, that the maximal system size available for the numerical calculations is not large enough to penetrate to the asymptotic region. Indeed we cannot analyze the numerical data in the weak-coupling region ($J/t < 1$) where the typical correlation length far exceeds the accessible system size. In small systems it is known that the dominant correlation is determined by the density of conduction electrons.[18] Thus the numerical values of K_ρ given in Table I should be considered as upper limits. This may appear unusual to those who consider the Hubbard model as a typical example of a TL liquid. The smallness of K_ρ clearly originates from the nonlocality of the effective interactions in space and time. In this sense the KL model is similar to charge density wave systems where the interactions are also retarded, being carried by low-energy optical phonons. In these systems $K_\rho \ll 1$.[19,20]

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