# Staggered liquid phases of the one-dimensional Kondo-Heisenberg lattice model

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We describe a family of one-dimensional (1D) liquids, which we call "staggered liquids," in the phase diagram of the 1D Kondo-Heisenberg model. It encompasses three distinct spin-gapped liquids and a Luttinger liquid (LL) phase. A staggered liquid is characterized by gapless modes with a large Fermi-sea signature in the charge-density wave (CDW) mode, and the superconducting order involves the near condensation of charge-2*e* Cooper pairs with finite center-of-mass momentum. In particular, the conventional gapless  $2k_F$  CDW and k = 0 pairing modes are absent. We analytically derive the phase transition from an intermediate-coupling spin-gap phase to the strong-coupling gapless LL phase of the Kondo-Heisenberg lattice model.

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# I. INTRODUCTION

Multicomponent one-dimensional electronic systems, of which the one-dimensional Kondo-Heisenberg model is a particular example, exhibit phases that were unanticipated in earlier studies of the one-dimensional electron gas (1DEG). The one-dimensional Kondo-Heisenberg model consists of a 1DEG interacting with a Heisenberg spin- $\frac{1}{2}$  chain via spin exchange interaction. In the present paper we characterize the stable fixed points of this model.

In particular limits of parameters, we obtain wellcontrolled analytical solutions that enable us to enumerate and characterize the quantum numbers of all gapless modes. Gapless modes are properties of the fixed point. Thus, our analysis lists the minimal set of stable fixed points in the global phase diagram of the Kondo-Heisenberg model. Surprisingly, we find that there is a common feature to all the fixed points in that charge-density wave (CDW) and pairing gapless modes are obtained with "unusual" wave numbers, and hence we give the name "staggered liquids" to the family of fixed points. In particular, whereas previously catalogued liquid phases of the 1DEG have a gapless charge-2epairing mode at k = 0, in a staggered liquid this mode appears at nonzero wave vector. Put differently, in a staggered liquid phase the dominant superconducting order involves the near condensation of Cooper pairs with finite center-of-mass momentum. Similarly, there is no gapless CDW mode at wave number  $2k_F$ . Our results are summarized in Tables I and II helow

In previous publications,<sup>1,2</sup> we have already characterized two distinct spin-gap phases (at weak coupling<sup>2</sup> and at a Toulouse point value of parameters). In the present paper we add a gapless Luttinger liquid (LL) phase (labeled "staggered LL") that is obtained by going away from the Toulouse point toward stronger coupling. Interestingly, although its mathematical form is similar to that of the commensurateincommensurate transition, we find the phase transition is first order. To our knowledge, this is the first analytical derivation of the phase transition from an intermediate-coupling spin-gap phase to the strong-coupling gapless LL phase in the Kondo lattice model. Moreover, a third distinct spin-gap phase is obtained by introducing weak attractive interactions to the staggered LL (and hence we name it the ''staggered BCS phase'').

We emphasize that in this paper we limit ourselves to cataloguing the stable fixed points. We do not discuss the range of their basins of attraction and the validity of the solutions away from the quantitatively controlled limits of parameters. In other words, we defer to a future publication the discussion of how exactly to construct the phase diagram as a function of Kondo interaction strength for a given discrete Kondo-Heisenberg lattice model at given incommensurate filling and with spin-rotation invariance.

The paper is organized as follows. In Sec. II, we define the model and the order parameters. Our results are summarized in Tables I and II. (The derivation of these results is presented in the ensuing sections.) In Sec. III, we review the weak-coupling limit  $(J_K \ll J_H)$  spin-gap fixed-point solution.<sup>2</sup> In Sec. IV, we review the Toulouse limit  $(J_H \ll J_K \sim E_F)$  spin-gap fixed-point solution, with some extended discussion of the unitary transformation. In Sec. V, we derive the phase transition to a gapless LL away from the Toulouse point toward stronger coupling  $(J_H \ll E_F \ll J_K)$ . In Sec. VI we make some additional concluding remarks. In order to facilitate the reading of the paper, a discussion and bosonization representation of the order parameters is given in an Appendix.

# II. KONDO-HEISENBERG MODEL AND ITS ZERO-TEMPERATURE FIXED POINTS

## A. The model

The Kondo-Heisenberg model (1) consists of two inequivalent interacting chains; one is a one-dimensional electron gas (described by the Hamiltonian<sup>3</sup>  $H^{1\text{DEG}}$ ), and the other an antiferromagnetic Heisenberg chain of localized spins  $\frac{1}{2}$ , { $\tau_j$ }. The chains interact via a spin exchange interaction with an antiferromagnetic coupling constant  $J_K > 0$ :

$$H = H^{1\text{DEG}} + H^{\text{Heis}} + H_K, \qquad (1)$$

$$H^{\text{Heis}} = J_H \sum_j \ \boldsymbol{\tau}_j \cdot \boldsymbol{\tau}_{j+1}, \qquad (2)$$



FIG. 1. Kondo-Heisenberg model.

$$H_K = 2J_K \sum_j \ \boldsymbol{\tau}_j \cdot \mathbf{s}(x_j), \tag{3}$$

where  $\mathbf{s}(x_j) = \psi_{\alpha}^{\mathsf{T}}(x_j)(\sigma_{\alpha\beta}/2)\psi_{\beta}(x_j)$  is the electron-gas spindensity operator at position  $x_j$  of the local spin  $\tau_j$  of the Heisenberg chain. We focus on the low-energy and longdistance behavior of the electron correlation functions by taking the continuum limit of the electron gas and linearizing the 1DEG dispersion relation about the Fermi points  $\pm k_F$ , with corresponding right- and left-going electron fields  $R_{\sigma}$ and  $L_{\sigma}$ :

$$\psi_{\sigma}(x) = R_{\sigma}(x)e^{+ik_Fx} + L_{\sigma}(x)e^{-ik_Fx},$$

where  $\sigma = \uparrow, \downarrow$  (see Fig. 1).

The effective Fermi wave numbers (in the sense of the generalized Luttinger theorem<sup>4</sup>) for the 1DEG and the spin chain are  $2k_F$  and  $2k_F^{\text{Heis}} = \pi/b$ , respectively (where  $b = x_{j+1} - x_j$  is the distance between the local spins of the Heisenberg chain). It is assumed that the two systems are mutually incommensurate, and that  $2k_F$  is incommensurate with any underlying ionic lattice. The continuum limit is taken for the 1DEG while the Heisenberg chain is initially left discrete (and remains so in some of the limit solution derivations). Therefore, the totality of our analysis is rigorously valid in the limit  $2k_F \ge \pi/b$  (i.e., where the number of electrons is much larger than the number of local spin- $\frac{1}{2}$  moments per unit length).

The 1DEG spin currents are decomposed into forwardand backscattering parts:

$$\mathbf{s}(x) = \psi_{\alpha}^{\dagger}(x_j) \frac{\boldsymbol{\sigma}_{\alpha\beta}}{2} \psi_{\beta}(x_j)$$
$$= \mathbf{J}_s(x) + \mathbf{n}_s(x),$$

where  $\mathbf{J}_{s(x)} = \mathbf{J}_{sR}(x) + \mathbf{J}_{sL}(x)$ ,  $\mathbf{J}_{sR} = \frac{1}{2} R_{\sigma}^{\dagger} \boldsymbol{\sigma}_{\sigma\sigma'} R_{\sigma'}$ , and  $\mathbf{J}_{sL} = \frac{1}{2} L_{\sigma}^{\dagger} \boldsymbol{\sigma}_{\sigma\sigma'} L_{\sigma'}$  are the ferromagnetic (q=0) spin currents of right- and left-moving electrons, respectively, and

$$\mathbf{n}_s(x) = e^{-i2k_F x_j} \mathbf{n}_R(x) + e^{+i2k_F x_j} \mathbf{n}_L(x),$$

where  $\mathbf{n}_R = R_{\sigma}^{\dagger}(\boldsymbol{\sigma}_{\sigma,\sigma'}/2)L_{\sigma'}$  and  $\mathbf{n}_L = L_{\sigma}^{\dagger}(\boldsymbol{\sigma}_{\sigma,\sigma'}/2)R_{\sigma'}$  are the staggered magnetization  $(q = 2k_F)$  components of the 1DEG.

Due to the incommensurate electron filling, backscattering interaction terms are irrelevant in the renormalization group (RG) sense, and for our purposes may be dropped from the Hamiltonian that describes the fixed points. As a result, the spin and charge sectors decouple,

$$H = \int dx [\mathcal{H}_c + \mathcal{H}_{\rm spin}].$$

The charge sector is described by a Gaussian model<sup>3</sup>

$$\mathcal{H}_c = \frac{1}{2} \left[ K_c \Pi_c^2(x) + \frac{1}{K_c} v_c (\partial_z \Phi_c)^2 \right].$$

Since in this paper we are not interested in the effects of anomalous 1D exponents ( $K_c \neq 1$ ), we will set  $K_c = 1$ , unless otherwise explicitly stated. The subsequent analysis and manipulations deal only with the spin sector fields. The Kondo exchange interaction reduces to

$$H_K = J_K \sum_j \ \boldsymbol{\tau}_j \cdot \mathbf{J}(x_j). \tag{4}$$

#### B. Order parameters and staggered correlations

Study of the different stable phases of the Kondo-Heisenberg array begins with an analysis of the gapless excitations of the decoupled fixed point. From there, as usual, we sort the phases by determining which of these excitations become gapped and which remain gapless in the presence of the (Kondo) couplings between the 1DEG and the Heisenberg chain. Since our ultimate goal is to study the coupled system, we need also to consider the character of gapless excitations constructed of composite operators from the two subsystems. An extensive exposition of the order parameters is given in the Appendix. Below, we note only the modes that are relevant for a spin-gap system.

In the spin-gap phases, only spin-0 modes may be gapless. Thus, we focus our investigation on singlet pairing modes (charge 2e, spin 0) and CDW modes (charge 0, spin 0). The corresponding usual 1DEG order parameters are

$$O_{\rm SP} = \frac{1}{\sqrt{2}} \left( R^{\dagger}_{\uparrow} L^{\dagger}_{\downarrow} + L^{\dagger}_{\uparrow} R^{\dagger}_{\downarrow} \right), \tag{5}$$

$$O_{\rm CDW} = \frac{1}{2} [(R^{\dagger}_{\uparrow}L_{\uparrow} + R^{\dagger}_{\downarrow}L_{\downarrow}) + \text{H.c.}].$$
(6)

Modes of composite nature are a composite odd-parity singlet pairing

$$O_{c-\text{SP}} = -i[R^{\dagger}_{\alpha}(\boldsymbol{\sigma}\boldsymbol{\sigma}_{z})_{\alpha\beta}L^{\dagger}_{\beta}]\cdot\boldsymbol{\tau}, \qquad (7)$$

and a composite particle-hole mode  $O_{c-\text{CDW}}$ , which will play a central role in the ensuing discussion,

$$O_{c-\text{CDW}} = \mathbf{n}_{1\text{DEG}} \cdot \boldsymbol{\tau}.$$
 (8)

Upon evaluating the corresponding correlation functions  $\chi_i(x,x') = \langle O_i(x)O_i(x') \rangle$ , we find gapless modes with power-law correlations of the form

$$\chi_i(x_j - x_{j'}) = (-1)^{(j-j')} \chi_0(x_j - x_{j'}), \qquad (9)$$

where  $\chi_0 \sim x^{-\alpha_i}$ . The staggering factor  $(-1)^j$  in the correlation functions (9) effectively modulates the usual powerlaw correlations by the reciprocal lattice vector  $\pi/b$  of the spin chain  $\{\tau_j\}$ . As a result, the gapless modes are found in unusual finite momentum values: The singlet pairings have momentum  $\pi/b$  (and there is no k=0 singlet pairing with charge 2*e*), and the gapless CDW modes are at momentum

$$2k_F^* = 2k_F + \frac{\pi}{b} \tag{10}$$

(and not at  $2k_F$  like the CDW in a free 1DEG). These are the defining characteristics of a "staggered liquid."

Insight into the gapless mode properties is gained by considering the so-called  $\eta$ -pairing modes at momentum  $\pm 2k_F$ ,

$$\eta_R = R_{\uparrow}^{\dagger} R_{\downarrow}^{\dagger},$$
  
$$\eta_L = L_{\uparrow}^{\dagger} L_{\downarrow}^{\dagger}, \qquad (11)$$

corresponding to right- and left-going singlet pairs. In a bosonization representation (see the Appendix) it is easy to see that the  $\eta$ -pairing operators depend only on the 1DEG charge sector fields. The charge sector is unaffected by the relevant part of the Kondo and Heisenberg interactions at all the zero-temperature fixed points. Therefore, the gapless  $\eta$ -pairing modes always exist and carry momentum  $2k_F$  as in the free 1DEG. It is instructive to define operators

$$\eta^{\text{even}} \equiv \frac{1}{\sqrt{2}} (\eta_R + \eta_L),$$
$$\eta^{\text{odd}} \equiv \frac{1}{\sqrt{2}} (\eta_R - \eta_L) \tag{12}$$

(though in themselves they do not carry a well-defined momentum quantum number). We found that an interdependence of the gapless modes is established by the following operator identities:

$$[O_{\rm CDW}, \eta^{\rm even}] = O_{\rm SP}, \tag{13}$$

$$[O_{\rm CDW}, \eta^{\rm odd}] = 0, \qquad (14)$$

$$[O_{c-\text{CDW}}, \eta^{\text{even}}] = 0, \qquad (15)$$

$$[O_{c-\text{CDW}}, \eta^{\text{odd}}] = O_{c-\text{SP}}.$$
(16)

Hence, the gapless wave numbers of CDW and pairing operators are always connected by momentum  $2k_F$ .

## C. Main results: Staggered liquid fixed points

For the purpose of characterizing fixed points, the issue of counting gapless modes requires clarification. Since the  $\eta$ -pairing modes are gapless in all cases where the charge sector is gapless (i.e., at all the fixed points of the Kondo-Heisenberg lattice model at incommensurate filling), the interdependence of modes [given in Eqs. (13) and (16)] implies that formally only the CDW modes need to be counted, while the pairing modes  $O_{\rm SP}$  and  $O_{c-\rm SP}$  are redundantly derived from combinations of CDW and  $\eta$ -pairing operators. In spite of that, since common discussions in the literature are done in terms of the usual pairing order parameters  $O_{\rm SP}$  and  $O_{c-\rm SP}$ , we will list them in our tables below.

We have found four distinct fixed points associated with different parameter values.

TABLE I. Spin-gap phases.

	$O_{\rm CDW}$	$O_{\rm SP}$	$O_{c-\mathrm{CDW}}$	$O_{c-SP}$
Weak coupling	X	X	$2k_F^*$	$\frac{\pi}{h}$
Toulouse point	$2k_F^*$	$\frac{\pi}{b}$	$2k_F^*$	$\frac{b}{\pi}$
Staggered BCS	$2k_F^*$	$\frac{b}{\pi}{b}$	X	D X

(1)  $J_K \ll J_H \ll E_F$ : A spin-gap phase at weak-intermediate coupling.<sup>2</sup>

(2)  $J_K \gtrsim E_F \gg J_H$ : A spin-gap Toulouse point phase<sup>1</sup> at intermediate coupling.

(3)  $J_K \gg E_F \gg J_H$ : A gapless *staggered* Luttinger liquid phase at strong coupling.

(4)  $J_K \gg E_F \gg J_H$ : A spin-gap *staggered* BCS phase at strong coupling, with additional weak attractive charge interactions.

We comment that all the fixed-point Hamiltonians (associated with the above noted phases) that we derived are in fact spin-rotation invariant, even though the bare interaction parameters were in some cases breaking spin-rotation invariance. It is an example of the possibility that the ultimate zero-temperature fixed point can possess higher symmetry than the original microscopic model. Yet we emphasize again that such issues do not affect the validity of our analysis for cataloging the fixed points of the most general microscopic Kondo-Heisenberg model (with or without spinrotation invariance).

In Tables I and II below, we characterize the above noted fixed points in terms of the momentum quantum number of their gapless CDW and pairing modes (X signifies that the particular mode is gapped). Obviously, the gapless LL is characterized by having also gapless spin-density-wave (SDW) modes and triplet pairing modes.

Whereas previously cataloged liquid phases of the 1DEG have a gapless charge-2*e* pairing mode at k=0, in all of the above noted phases this mode appears at nonzero wave vector. Similarly, there is no gapless CDW mode at wave number  $2k_F$ .

# III. WEAK-COUPLING LIMIT $(J_K \ll J_H)$ SPIN-GAP FIXED POINT

In the weak-interchain-coupling limit

$$J_K \ll J_H, E_F.$$

It is allowed to make further approximation by taking the continuum limit also for the Heisenberg spin chain (such an approximation is not valid in the opposite limit  $J_K \gg J_H$ , which is discussed in Sec. IV). The local spin-chain field is

TABLE II. Gapless Luttinger liquid phase.

	$O_{\rm CDW}$	$O_{\rm SP}$	$O_{c-\mathrm{CDW}}$	$O_{c-SP}$
Staggered LL	$2k_F^*$	$\frac{\pi}{b}$	$2k_F^*$	$\frac{\pi}{b}$

then also decomposed into the smooth (ferromagnetic) and staggered (antiferromagnetic) components:

$$\boldsymbol{\tau}_{j} = [\mathbf{J}_{R}^{\tau}(x_{j}) + \mathbf{J}_{L}^{\tau}(x_{j})] + (-1)^{j} \mathbf{n}_{\tau}(x_{j}).$$
(17)

(Note that we will consistently use the subscripts  $\tau$  and *s* to distinguish the spin-chain fields from the 1DEG fields.)

In order to distinguish contributions coming from various interaction terms, we introduce distinct Kondo coupling coefficients for forward scattering  $(J_f)$  and mixed interactions  $(J_m)$ :

$$H_K = J_f (\mathbf{J}_R^{\tau} + \mathbf{J}_L^{\tau}) \cdot (\mathbf{J}_R^s + \mathbf{J}_L^s) + J_m (-1)^j \mathbf{n}_{\tau} \cdot (\mathbf{J}_R^s + \mathbf{J}_L^s).$$
(18)

The mixed interaction, of the ferromagnetic 1DEG component with the staggered impurity component [i.e., the  $J_m(-1)^j \mathbf{n}_{\tau} \cdot (\mathbf{J}_R + \mathbf{J}_L)$  term] has naive scaling dimension  $\frac{3}{2}$ , but the oscillating  $(-1)^j$  factor, which acts as an effective extra derivative factor  $(\partial_x)$ , renders this term perturbatively irrelevant in the renormalization group sense with respect to the free Hamiltonian  $H_0^s$ . The forward current-current interaction  $J_f(\mathbf{J}_{\tau R} + \mathbf{J}_{\tau L}) \cdot (\mathbf{J}_R + \mathbf{J}_L)$  has scaling dimension 2, is marginally relevant, and leads to the opening of a spin gap.<sup>2,5</sup> (The  $J_m$  term will prove to be essential for understanding the Toulouse limit solution in Sec. IV.) Therefore, at incommensurate filling in the weak-coupling limit, the Kondo-Heisenberg Hamiltonian (1) reduces to

$$H_{\text{weak}} = \mathcal{H}^{c} + \mathcal{H}_{0}^{s} + J_{f} \int dx (\mathbf{J}_{R}^{\tau} + \mathbf{J}_{L}^{\tau}) \cdot (\mathbf{J}_{R}^{s} + \mathbf{J}_{L}^{s}),$$
$$\mathcal{H}^{c} = \frac{1}{2} \bigg[ K \Pi_{c}^{2}(x) + \frac{1}{K} \upsilon_{c} (\partial_{x} \Phi_{c})^{2} \bigg], \qquad (19)$$
$$\mathcal{H}_{0}^{s} = \sum_{\mu = s, \tau} \frac{2 \pi \upsilon_{\mu}}{3} (: \mathbf{J}_{R}^{\mu} \mathbf{J}_{R}^{\mu} : + : \mathbf{J}_{L}^{\mu} \mathbf{J}_{L}^{\mu} :),$$

where  $v_{\tau}$  and  $v_s$  are the spin-wave velocities of the Heisenberg chain and 1DEG, respectively ( $v_{\tau} = \pi J_H/2$ ). For a detailed derivation of the gapless modes of model (19), we refer the reader to Ref. 2. The end results are quoted in the first line of Table I. It is remarkable that only composite modes are gapless.

## IV. TOULOUSE LIMIT $(J_H \ll J_K \sim E_F)$ SPIN-GAP FIXED POINT

In the limit

$$J_H \ll J_K \sim E_F$$

the intrachain interaction  $J_H$  is small compared with the interchain interaction  $J_K$ , and it is incorrect to take the continuum limit for the spin chain prior to accounting for the effect of the interaction  $J_K$ . For simplicity, since  $J_H \ll J_K$ , we will first take the limit  $J_H = 0$ . (We shall find that bringing back  $J_H \ll J_K$  is an irrelevant perturbation, in the renormalization group sense, due to the spin gap of the Toulouse fixed point phase.) Thus, we model the local spins as initially independent, and leave the Kondo interaction in its discrete form:

$$H = H_0^{1\text{DEG}} + 2J_K \sum_j \tau_j \cdot \psi_\alpha^{\dagger}(x_j) \frac{\sigma_{\alpha\beta}}{2} \psi_\beta(x_j).$$
(20)

In this limit, effective interaction and coherence between the local spins will come about explicitly mediated by the itinerant 1DEG (i.e., in a kind of Rudelman-Kittel-Kasuya-Yoshida interaction which is not introduced by hand to the models as  $J_H$ ).

Below, we review and discuss the Toulouse point derivation and results of Ref. 1. For the purpose of calculating correlation functions, we bosonize the 1DEG fermionic fields,<sup>3</sup>

$$L_{\sigma}(x) = \frac{F_{\sigma}}{\sqrt{2\pi a}} e^{-i\sqrt{\pi}[\theta_{\sigma}(x) + \phi_{\sigma}(x)]},$$

$$R_{\sigma}(x) = \frac{F_{\sigma}}{\sqrt{2\pi a}} e^{-i\sqrt{\pi} \left[\theta_{\sigma(x)} - \phi_{\sigma}(x)\right]},$$

where  $\theta_{\sigma}(x) = \int_{-\infty}^{x} dx' \Pi_{\sigma}(x')$ , and  $[\Pi_{\sigma}(x'), \phi_{\sigma}(x)] = -i\delta(x'-x), \sigma = \uparrow, \downarrow$ . The anticommuting Klein factors  $\{F_{\sigma}, F_{\sigma'}\} = \delta_{\sigma, \sigma'}$  are needed for the proper anticommutation of fermions with different spin. As is commonly done, we reexpress the operators in terms of bosonic spin fields  $\phi_s(x) = (1/\sqrt{2})[\phi_{\uparrow} - \phi_{\downarrow}]$  and charge fields  $\phi_c(x) = (1/\sqrt{2})[\phi_{\uparrow} + \phi_{\downarrow}]$ , and correspondingly defined momenta  $\Pi_s$  and  $\Pi_c$ .

The crucial step that we introduced in Ref. 1 is to make a unitary transformation of the fields,

$$U = \exp\left[-i\sqrt{2\pi}\sum_{j} \tau_{j}^{z}\theta_{s}(x_{j})\right], \qquad (21)$$

$$U\sqrt{2\pi}(\partial_x\phi_s)U^{\dagger} = \sqrt{2\pi}(\partial_x\phi_s) - 2\pi\sum_l \tau_l^z \delta(x_l - x),$$
(22)

$$U\tau^+ e^{-i\sqrt{2\pi}\theta_s} U^\dagger = \tau^+, \qquad (23)$$

$$U\cos[\sqrt{2\pi}\phi_s(j)]U^{\dagger} = (-1)^j\cos[\sqrt{2\pi}\phi_s(j)]. \quad (24)$$

In words, going across an impurity, the spin phase  $\sqrt{2 \pi \phi_s}$  is shifted by  $\pm \pi$ , i.e., transformed fields with opposite spins acquire a phase shift of  $\delta_{\sigma} = \pm \pi/2$ . It is reminiscent of the unitarity limit scattering we expect from the low-energy physics of the single-impurity Kondo effect.<sup>6</sup> Therefore we interpret the unitary transformation as going to a Kondo strong-coupling basis.

The resulting transformed Kondo lattice Hamiltonian is given by

$$U^{\dagger}HU = \tilde{H}_{0} + \Delta J_{z} \sqrt{\frac{2}{\pi}} \sum_{j} \tau_{j}^{z} \partial_{x} \phi_{s}(x_{j})$$
  
+  $\frac{J_{\perp}}{\pi a} \sum_{j} \tau_{j}^{x} (-1)^{j} \cos[\sqrt{2\pi} \phi_{s}(j)], \quad (25)$ 

$$\tilde{H}_{0} = H_{0}^{s} + H_{0}^{c} - (J_{z} + \Delta J_{z}) \frac{1}{b} \sum_{j} (\tau_{j}^{z})^{2}, \qquad (26)$$

where  $H_0^s = (v_s/2) \int dx [\Pi_s^2 + (\partial_x \phi_s)^2]$ , and

$$\Delta J_z = J_z - \pi v_F. \tag{27}$$

In Eq. (25) we have introduced independent interaction coefficients  $J_z$  and  $J_{\perp}$  for the Ising and spin-flip parts of the Kondo exchange interaction  $J_K$ . Hence, formally we are here examining a generalization of the Kondo-Heisenberg model (1) to non-spin-rotation-invariant interactions.

The transformed fields constitute the low-energy spectrum of  $\tilde{H}_0$ , into which part of the interaction energy has been incorporated. The transformed fields are taking advantage of the Ising part of the magnetic Kondo interaction at the cost of kinetic energy [due to twisting of the spin field  $\phi_s(x)$ ]. These are originally high-energy states of the bare free 1DEG Hamiltonian  $H^{1\text{DEG}}$ . For the transformed fields to become low-energy states due to interactions, it is clear that the Kondo interaction strength needs to be on the order of the 1DEG bandwidth. To this effect, note the shift of the groundstate energy per impurity (irrespective of the existence of a spin gap) in Eq. (26):

$$\begin{split} \Delta E_{j} &= -(J_{z} + \Delta J_{z}) \frac{1}{b} \sum_{j} (\tau_{j}^{z})^{2} \\ &= 8 - (2J_{z} - \pi v_{F}) \frac{1}{4b} \,. \end{split} \tag{28}$$

It represents the absorption of a part of the Kondo interaction energy  $-2J_z/4b$  (equal to the gain from forming an Ising singlet) into the transformed free-field Hamiltonian (26), at the cost of kinetic energy  $+\pi v_F/4b$ . Hence, for strong enough interactions the transformed free fields have lower energy than the bare 1DEG free fields, and therefore determine the low-frequency correlations of various order parameters. Thus, the Toulouse point solution is an outcome of finite "strong enough" interactions and cannot be reached by perturbative methods about the noninteracting basis.

For a special value of the coupling constants,

$$J_z = \pi v_F \Longrightarrow \Delta J_z = 0 \tag{29}$$

(the Toulouse point), we are left with an exactly solvable fixed-point Hamiltonian,  $^{1}$ 

$$\tilde{H}^{*} = H_{0}^{c} + H_{0}^{s} + \frac{J_{\perp}^{f}}{\pi a} \sum_{j} \tau_{j}^{x} (-1)^{j} \cos[\sqrt{2\pi}\phi_{s}(j)].$$
(30)

The spin part of the fixed-point Hamiltonian has a discrete sine-Gordon form, and therefore a spin gap. The transformed spin fields which develop an expectation value are  $\langle \tau_j^x(-1)^j \rangle \neq 0$  and  $\langle \cos[\sqrt{2\pi}\phi_s(j)] \rangle \neq 0$ . In calculating correlation functions, it is important to remember the effect of the unitary transformations, which lead to

$$\langle \cos[\sqrt{2\pi}\phi_s(x)]\cos[\sqrt{2\pi}\phi_s(x')]\rangle \sim (-1)^{j-j'}$$

[j(x) is defined as the *j* impurity site to the left of position *x*]. The bare impurity correlations  $\langle \tau_j^x \tau_j^{x'} \rangle$  decay exponentially. However, the transformed impurity spins  $\tilde{\tau}_j^x = U^{\dagger} \tau_j^x U$  exhibit staggered long-range order at T=0,  $\langle \tilde{\tau}_j^x \tilde{\tau}_j^x \rangle = \text{const} \times (-1)^{(j-j')}$ ; this nonlocal order parameter characterizes the coherent ground state. That is all the information needed for deducing the correlation functions of all order parameters, and thus determining the gapless modes as was done in Ref. 1 and summarized in the second line of Table I.

We take this opportunity to elaborate on the significance of the field transformation. The  $\pi$  phase shift of the field  $\sqrt{2\pi}\phi_s$  across an impurity site (22) gives rise to a staggered coefficient  $(-1)^j$  in the Hamiltonian (30) since

$$\exp\left[i2\,\pi\sum_{l=1}^{j}\,\tau_{l}^{z}\right] = (-1)^{j}.$$

Note that the factor  $(-1)^j$  is effectively "counting" impurities, and is obtained irrespective of the order of the bare  $\{\tau_l^z\}$  themselves (imagine an Ising chain of  $\{\tau_l^z\}$ ; there is a factor  $e^{\pm i\pi} = -1$  per impurity). Indeed, the correlation function  $\langle \tau_i^z \tau_{i'}^z \rangle$  is short range.

It is interesting to trace back the relevant interaction in the Toulouse fixed-point Hamiltonian in terms of the continuum limit of the Heisenberg spin chain (18). Due to the additional  $(-1)^{j}$  phase factor, in the transformed basis, the relevant slowly varying interaction is now  $J_m \mathbf{n}_{\tau} \cdot (\mathbf{J}_R + \mathbf{J}_L)$ , while the interaction  $J_f(-1)^j (\mathbf{J}_{\tau R} + \mathbf{J}_{\tau L}) \cdot (\mathbf{J}_R + \mathbf{J}_L)$  is now also rapidly oscillating and irrelevant. Thus, Toulouse fixed-point physics originates from the interaction  $J_m$  that couples the conduction electrons to the staggered component of the impurity array, an interaction that is relevant only with respect to the transformed fixed-point Hamiltonian  $\tilde{H}_0$ , and was irrelevant in the untransformed basis. This possibility would be missed in the continuum limit if we had dropped the  $J_m(-1)^j \mathbf{n}_{\tau} \cdot (\mathbf{J}_R + \mathbf{J}_L)$  term at the outset (as is usually done, e.g., in Ref. 5). The perturbative relevance of various interaction terms is changed after a transformation to the "proper" strong-coupling basis of fields about which perturbative RG analysis is performed. The notation  $J_m$  is not accidental, and it is exactly the one that is responsible for the nontrivial fixed point of the two-impurity Kondo problem.<sup>7</sup>

## V. STRONGER-COUPLING $(J_H \ll E_F \ll J_K)$ STAGGERED LUTTINGER LIQUID FIXED POINT

## A. Phase transition away from the Toulouse limit

In a previous paper,<sup>1</sup> we analyzed the commensurateincommensurate (*C-I*) transition in the charge sector at the Toulouse point, as a function of the filling factor, and found a phase transition from an insulating phase (with both charge and spin gaps) to a conducting phase with only a spin gap. Here, we are interested only in the case of incommensurate filling (for which there is no charge gap). In this section, we analyze the phase transitions in the spin sector by varying the parameter values away from the Toulouse point, while maintaining the same incommensurate charge filling factor.

We investigate the phase transitions within the transformed field Hamiltonian (25). The local stability of the Toulouse limit fixed point  $(J_z^* = \pi v_F)$  is ensured by the existence of a spin gap. This is all that can be deduced from perturbative renormalization group calculations. Thus, the phase transition can be established only via nonperturbative methods. Below, we determine analytically the finite parameter space region characterized by the Toulouse fixed-point solution, i.e., the zero-temperature stability of the spin gap to finite deviations  $\Delta J_z = (J_z - \pi v_F) > 0$  away from the Toulouse line toward stronger coupling. We find an electronic gapless phase beyond a finite distance from the Toulouse point.

Treating the transformed impurity spins in self-consistent mean-field approximation, we replace them by their expectation values in the transformed Hamiltonian,

$$U^{\dagger}HU \rightarrow H_{0}^{s} + H_{0}^{c} + \Delta J_{z} \sqrt{2/\pi} \sum_{j} \langle \tau_{j}^{z} \rangle \partial_{x} \phi_{s}(x_{j})$$
$$+ \frac{J_{\perp}}{\pi a} \sum_{j} \langle (-1)^{j} \tau_{j}^{x} \rangle \cos[\sqrt{2\pi} \phi_{s}(j)]. \quad (31)$$

The spin sector of the Hamiltonian (31) has a form familiar from the study of commensurate-incommensurate transitions,

$$\frac{\tilde{H}^s}{v_s} = \frac{1}{2} \int dx [\Pi_s^2 + (\partial_x \phi_s - \delta)^2] + h \int dx \cos[\beta \phi_s(x)],$$
(32)

where  $\beta = \sqrt{2\pi}$ ,

$$\delta = \delta_0 \sin(\gamma) = \Delta J_z \frac{c}{a} \sqrt{2/\pi} \langle \tau_j^z \rangle,$$
  
$$h = h_0 \cos(\gamma) = J_\perp |\langle \tau_j^x \rangle| \frac{c}{2\pi a^2 v_s},$$
(33)

c = b/a, and

$$\langle (-1)^{j} \tau_{j}^{\chi} \rangle = \frac{1}{2} \cos(\gamma),$$
$$\langle \tau_{j}^{\chi} \rangle = \frac{1}{2} \sin(\gamma). \tag{34}$$

The general character of the phase transition in the Hamiltonian (32) is well known:<sup>8</sup> The system remains commensurate until  $|\delta|$  exceeds a finite critical value  $\delta^c$ . Therefore, the Toulouse limit is proved to be stable over a finite range of parameter space  $\Delta J_z \neq 0$ .

Yet care should be taken to identify the exact nature of the transition and the character of the ensuing gapless phase. The ground state of Eq. (32) is determined by the field configuration that minimizes the energy. As we shall see, the *C-I* 

transition in our Hamiltonian (31) is unusual because the parameters  $\delta$  and *h* are themselves not constants, but instead are dynamic fields that need to be determined self-consistently by an additional mean-field minimization condition on  $\langle \tau_j^z \rangle$  and  $\langle \tau_j^x \rangle$ . There are, in principle, three possible ground-state solutions for the Hamiltonian (32).

*Phase 1*: A uniform spin-gap phase, identical to the Toulouse point solution, with no finite gradients of  $\partial_x \phi_s(x_j)$ , i.e.,  $\langle \cos[\sqrt{2\pi}\phi_s(j)] \rangle \neq 0$ ,  $\langle (-1)^j \tau_j^x \rangle \neq 0$ ,  $\langle \partial_x \phi_s \rangle = 0$ , and hence also  $\langle \tau_j^z \rangle = 0$ .

*Phase* 2: A gapless incommensurate spin "soliton lattice" ground state with periodic steplike kinks in the  $\phi_s(x_j)$ field. In such a phase,  $\langle \partial_x \phi_s \rangle \neq 0$ , but still  $\langle \cos[\sqrt{2\pi}\phi_s(j)] \rangle \neq 0$ , and both  $\langle (-1)^j \tau_j^x \rangle \neq 0$  and  $\langle \tau_j^z \rangle \neq 0$ . *Phase* 3: A free gapless SDW phase,  $\langle \partial_x \phi_s \rangle \neq 0$ ,  $\langle \cos[\sqrt{2\pi}\phi_s(j)] \rangle = 0$ . In that phase  $\langle \tau_j^z \rangle = 0$  and  $\langle \tau_j^z \rangle \neq 0$ .

The name "soliton lattice" comes from the classical solution, which has long-range periodic order. Quantum fluctuations turn the long-range order into power-law correlations, and thus the quantum ground state should properly be termed a soliton liquid. Nevertheless, this does not change the qualitative distinctions (in terms of nonzero expectation values) between the various phases. For simplicity, I will discuss the phases in classical terms.

To find the transition points between the phases we need to compare, for a given  $\Delta J_z = (J_z - \pi v_F) \neq 0$ , the groundstate energy of the spin-gap phase (phase 1) with those of the gapless phases. The usual result for commensurateincommensurate transitions, where the parameters *h* and  $\delta$ are constant, is that the soliton lattice solution (phase 2) has lower energy than the SDW solution, and the transition is second order. This is not the case here, due to the fact that the parameters *h* and  $\delta$  are themselves interdependent dynamic variables. Thus, we need to minimized the ground state energy with respect to both the soliton spacing *l* (as usually done) and also the mean-field parameter  $\gamma$ .

The resulting commensurate-incommensurate transition in the transformed 1D Kondo lattice Hamiltonian (32) is first order. The argument is the following. Remember that  $\tau_j^z$  and  $\tau_j^x$  are noncommuting. Therefore, if there is a second-order transition to the soliton lattice phase, at the transition point  $\delta \approx (4/\pi) \sqrt{h_0}$  both  $\delta \sim \langle \tau_j^z \rangle \neq 0$  and  $h \sim |\langle \tau_j^x \rangle| \neq 0$  are less by a finite amount than their respective maximum values  $\delta_0$  and  $h_0$ . The energy of the soliton lattice at the second-order transition is equal to the energy of the commensurate phase with the same value of h, which is always less than the maximum energy of the commensurate phase 1 (for which  $h = h_0$  and  $\delta = 0$ ). Thus we establish that the commensurateincommensurate transition is necessarily first order.

But what is the incommensurate phase? There is no closed expression for the soliton lattice energy away from the dilute limit (i.e., far from the putative second-order transition). Yet we can analyze the competition between phase 2 and phase 3 in the dense soliton lattice limit (when the distance between soliton centers is less than a single soliton width). In that limit, the commensurate energy contribution (due to  $h \neq 0$ ) is exponentially small, while the  $\partial_x \phi_s$  term contribution is approximately linear in  $\delta < \delta_0$ . Thus (again in

contrast with the usual case of constant coefficients  $\delta, h \neq 0$ ), the dense soliton lattice energy is less favorable than the SDW phase 3 (in which h=0 and  $\delta = \delta_0$ ).

The above argument leads to two possible scenarios: Either there is a sequence of two first-order transitions (phase  $1 \rightarrow$  phase  $2 \rightarrow$  phase 3), or there is one first-order transition (phase  $1 \rightarrow$  phase 3). We conjecture that the second possibility is the correct one, and hence the phase transition occurs at  $\delta_0^{\text{critical}} = \sqrt{2h_0}$ , i.e.,

$$(\Delta J_z)_{\text{critical}} = \sqrt{J_\perp/2v_s a}.$$
(35)

In conclusion, at a finite deviation  $(\Delta J_z)_{\text{critical}}$  from the Toulouse point toward strong coupling, there is a first-order commensurate-incommensurate transition in the spin field  $\phi_s$ , in conjunction with a transformed impurity spin-flop transition from  $\{\langle \tau_j^x \rangle \neq 0, \langle \tau_j^z \rangle = 0\}$  to  $\{\langle \tau_j^x \rangle = 0, \langle \tau_j^z \rangle \neq 0\}$ . The transition is from the spin-gap phase 1 to the gapless SDW phase 3, with no soliton lattice region.

## B. Staggered Luttinger liquid: A strong-coupling phase

The transition in the spin sector to the gapless SDW phase leads to a state that we call the staggered Luttinger liquid. The staggered LL is expressed in terms of the transformed fermion fields, which have composite phase fields

$$\widetilde{R}_{\sigma}(x) \equiv U R_{\sigma}(x) U^{\dagger} = R_{\sigma}(x) \exp\left(+i2\pi \sum_{x_j < x} \tau_j^z \sigma\right),$$
(36)

$$\widetilde{L}_{\sigma}(x) \equiv U L_{\sigma}(x) U^{\dagger} = L_{\sigma}(x) \exp\left(-i2\pi \sum_{x_j \le x} \tau_j^z \sigma\right), \quad (37)$$

where  $\sigma = \pm \frac{1}{2}$  is the electron spin, and  $\tau^z$  is the impurity operator, which can take values  $\pm \frac{1}{2}$  (so  $2\pi\tau^z\sigma = \pm \pi/2$ ).

As for the Toulouse point, we calculate the correlation functions with respect to the spectrum of the transformed Hamiltonian. All the order parameters, which in bosonic form depend on the  $\phi_s$  field, have staggered correlation functions [as defined in Eq. (9)] irrespective of the impurity configuration  $\{\tau_{jl}^z\}$ . Since there is no spin gap, there are now also gapless spin-density-wave and triplet pairing modes. In the bosonization representation, both  $\cos(\sqrt{2\pi}\phi_s)$  and  $\sin(\sqrt{2\pi}\phi_s)$  have power-law decay of correlations [with an added staggered factor  $(-1)^{j-j'}$ ]

The  $\tau_j^z$  order of the transformed impurity array requires further clarification. The interimpurity interactions generated by integrating out the transformed 1 DEG degrees of freedom in the residual Kondo interaction,  $\Delta J_z^f \Sigma_j \tau_j^z \partial_{x_j} \phi_s$ , are long ranged (i.e., well beyond nearest-neighbor interaction). Honner and Gulacsi<sup>9</sup> suggest that the effective interaction is ferromagnetic, and thus at least conforms with strongcoupling calculations.<sup>10</sup>

#### C. Staggered BCS phase: A third spin-gap phase?

It is interesting to investigate what would be the form of a BCS pairing of a composite staggered LL, i.e., we introduce

a conventional weak attractive interaction U < 0 (e.g., due to phonons) to the 1 DEG Hamiltonian. The singlet pairing takes the form

$$\widetilde{O}_{\rm SP} = \frac{1}{\sqrt{2}} [\widetilde{L}_{\uparrow} \widetilde{R}_{\downarrow} + \widetilde{R}_{\uparrow} \widetilde{L}_{\downarrow}]$$
$$= (-1)^{j(x)} \frac{1}{\sqrt{2}} [L_{\uparrow} R_{\downarrow} + R_{\uparrow} L_{\downarrow}] = (-1)^{j(x)} O_{\rm SE}. \quad (38)$$

The resulting pair correlation function is staggered [as defined in Eq. (9)], with nodes at the Kondo impurity periodicity. It corresponds to a negative Josephson coupling across each Kondo impurity.<sup>11</sup> We stress that the node in the pair correlation function due to negative Josephson coupling is a node in the pair center-of-mass motion. It should not be confused with a node in the relative pair state.<sup>12</sup> There is no gapless k=0 pairing mode.

On the other hand, all the composite modes are now incoherent. In order to see this, note that in the gapless staggered LL phase the gapless composite pairing mode  $O_{c-SP}$ came from the component  $\sin(\sqrt{2\pi}\phi_s)\tau_j^z$  [see Eq. (A11) in the Appendix]. Due to the singlet pairing interaction  $\langle \cos(\sqrt{2\pi}\phi_s)\rangle \neq 0$ , and thus the correlation function  $\langle \sin[\sqrt{2\pi}\phi_s(x)]\sin[\sqrt{2\pi}\phi_s(x')]\rangle$ , is exponentially decaying. Moreover, as in the staggered LL,  $\langle \tau_j^z \rangle \neq 0$  and thus the part  $(R_{\uparrow}^{\dagger}L_{\uparrow}^{\dagger}\tau^- - R_{\downarrow}^{\dagger}L_{\downarrow}^{\dagger}\tau^+)$  of  $O_{c-SP}$  is also exponentially decaying. These results are summarized in line 3 of Table I.

Our analysis suggests a different possibility: An unconventional staggered BCS pairing phase may arise out of a two-step process, where the staggered LL is a precursor to the staggered BCS phase. First, at a temperature  $T_{hf}$  set by the renormalized Kondo interaction there is a crossover to a staggered LL phase, characterized by the unitarity limit phase shifts. Then, at a much lower temperature  $T_c$ , a conventional BCS pairing mechanism (e.g., phonons) leads to the unconventional finite momentum BCS pairing state. The above demonstrates the importance of considering the crossover effects, due to strong interactions, prior to the consideration of pairing mechanisms.

#### VI. CONCLUDING REMARKS

The main results of this paper are (1) the identification of the staggered liquid family of fixed points, as summarized in Tables I and II; (2) derivation of the phase transition from a spin-gap phase at intermediate coupling to a gapless staggered LL at strong coupling; (3) the commutation relations (13)-(16) that relate CDW and pairing modes. Below we make some additional comments on our results.

At weak coupling, the Kondo-Heisenberg model consists of a free-electron gas coupled to a spin-density-wave system. One would naturally expect a BCS mechanism leading to a state of k=0 BCS pairing of conduction electrons mediated by spin waves of the Heisenberg chain. We find it quite surprising that such a state does not materialize at any stable fixed point of the one-dimensional problem.

Previous numerical simulations in the strong-coupling

limit<sup>10</sup> have found that the "dominant" gapless CDW mode (in a gapless strong-coupling LL phase) has large Fermi-sea wave number  $2k_F^*$ . Pairing modes were never evaluated. Yet, from our commutation relations (13) and (16) it is clear that the pairing correlations must be staggered. We comment that, following the analysis in this paper, it is important that numerical simulations establish the existence of both  $O_{\rm CDW}$ and  $O_{c-{\rm CDW}}$  gapless CDW modes. The pairing modes then follow automatically as we explained.

The numerical simulations were performed in the extreme strong-coupling limit on a particular lattice structure for which our analytical methods are not rigorously valid. Therefore, it is important to establish whether the gapless strong-coupling LL phase in the numerical simulations is identical to the one we derived analytically by a phase transition from the Toulouse limit solution.<sup>2</sup>

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# APPENDIX: DISCUSSION OF ORDER PARAMETERS

The study of the different stable phases of the Kondo-Heisenberg array begins with an analysis of the gapless excitations of the decoupled fixed point. From there, as usual, we sort the phases by determining which of these excitations become gapped, and which remain gapless in the presence of the (Kondo) couplings between the 1DEG and the Heisenberg chain. In order to facilitate the readability of the paper, we give below the explicit expressions of various order parameters.

#### 1. Density-wave modes

The low-energy spin currents of the 1DEG,  $\mathbf{s}(x)$ , can be decomposed into two parts,

$$\mathbf{s}(x) = \mathbf{J}_s(x) + [\mathbf{n}_s(x)e^{i2k_F x} + \text{H.c.}], \quad (A1)$$

where

$$\mathbf{J}_{s} = \sum_{\lambda,\sigma,\sigma'} \psi^{\dagger}_{\lambda,\sigma} \frac{\boldsymbol{\sigma}_{\sigma,\sigma'}}{2} \psi_{\lambda,\sigma'}, \qquad (A2)$$

$$\mathbf{n}_{s} = \sum_{\sigma,\sigma'} R_{\sigma}^{\dagger} \frac{\boldsymbol{\sigma}_{\sigma,\sigma'}}{2} L_{\sigma'}$$
(A3)

are, respectively, the k=0 and the  $k=2k_F$  components of the SDW mode (charge 0, spin 1) of the 1DEG. (The index  $\lambda = R, L$  corresponds to right- and left-going electron fields.)

The Heisenberg chain spin current  $\tau_j$  may be similarly decomposed into a k=0 part  $\mathbf{J}_{\tau}$  and a finite momentum  $k = \pi/b$  part  $(-1)^j \mathbf{n}_{\tau}$  (where  $2\pi/b$  is the reciprocal lattice vector of the Heisenberg chain):

TABLE III. Gapless SDW excitations.

Operator	Wave number
<b>n</b> <sub>s</sub>	$2k_F$
$\mathbf{n}_{ au}$	$\frac{\pi}{b}$

For the density-wave excitations, we count only the number of finite momentum excitations. It follows by symmetry that, for finite momentum, if there is a gapless mode at momentum q then there is also a gapless mode with momentum -q. We count them as one mode. To summarize, the gapless spin-1 excitation of the 1DEG and the Heisenberg spin chain, and the operator whose correlation function is most directly sensitive to it, are listed in Table III.

The incommensurate 1DEG has one CDW excitation (charge 0 spin 0) with momentum,  $2k_F$ , created by the operator

$$\mathcal{O}_{\rm CDW} = \frac{1}{2} \sum_{\lambda,\sigma} \psi^{\dagger}_{\lambda,\sigma} \psi_{-\lambda,\sigma} \tag{A5}$$

$$\sim e^{+i[\sqrt{2\pi}\phi_c + 2k_F x]} \cos(\sqrt{2\pi}\phi_s). \tag{A6}$$

The generalized Luttinger theorem<sup>4</sup> asserts that there must be a gapless CDW mode at  $2k_F^* = 2k_F + \pi/b$ . It is realized by the existence of composite CDW order parameters<sup>13</sup> which are formed by combining a spin-1 SDW of the 1DEG with a spin-1 SDW of the Heisenberg chain into a composite singlet  $\hat{O}_{c-\text{CDW}}$ ,

$$O_{c-\text{CDW}} = \mathbf{s} \cdot \boldsymbol{\tau}$$
  
=  $\mathbf{n}_{R} \cdot \boldsymbol{\tau} = \frac{1}{2} \left( n^{+} \boldsymbol{\tau}_{j}^{-} + n^{-} \boldsymbol{\tau}_{j}^{+} \right) + n^{z} \boldsymbol{\tau}_{j}^{z}$  (A7)

$$= \mathbf{J}_{s} \cdot \mathbf{J}_{r} + \mathbf{J}_{s} \cdot \mathbf{n}_{r} (-1)^{j} + [e^{i2k_{F}x} \mathbf{n}_{s} \cdot \mathbf{J}_{\tau} + \text{H.c.}]$$
$$+ [e^{i2k_{F}x} \mathbf{n}_{s} \cdot \mathbf{n}_{\tau} + \text{H.c.}](-1)^{j}.$$
(A8)

To summarize, the noninteracting two-chain system of a Luttinger liquid and a Heisenberg spin chain has gapless finite momentum CDW modes at three wave vectors (Table IV). Note that the composite CDW excitations at wave vectors  $\pi/b$  and  $2k_F + \pi/b$  are not independent, since they can be related through a multiplication by the 1DEGO<sub>CDW</sub> (which has wave vector  $2k_F$ ). Thus, there are only three independent gapless CDW modes.

TABLE IV. Gapless CDW excitations.

Operator	Wave number
$\mathbf{n}_{s} \cdot \mathbf{n}_{ au}$	$2k_F + \frac{\pi}{k}$
$O_{\rm CDW}$	$2k_F^{b}$
$\mathbf{n}_{s} \cdot \mathbf{J}_{ au}$	$2k_F$
$\mathbf{J}_{s} \cdot \mathbf{n}_{ au}$	$\frac{\pi}{b}$

#### 2. Singlet pairing modes

The charge-2e singlet pairing modes also require careful consideration. In addition to the usual k=0 BCS even-parity singlet pairing,

$$O_{\rm SP} = \frac{1}{\sqrt{2}} \left[ L_{\uparrow}^{\dagger} R_{\downarrow}^{\dagger} + R_{\uparrow}^{\dagger} L_{\downarrow}^{\dagger} \right]$$
$$\sim e^{+i\sqrt{2\pi}\theta_c} \cos(\sqrt{2\pi}\phi_s), \tag{A9}$$

we note also the existence of an  $\eta$ -pairing mode at momentum  $\pm 2k_F$ ,

$$\eta_{R} = R_{\uparrow}^{\dagger} R_{\downarrow}^{\dagger} \sim e^{+i\sqrt{2\pi}\theta_{c}} e^{-i[\sqrt{2\pi}\phi_{c}+2k_{F}x]},$$
  
$$\eta_{L} = L_{\uparrow}^{\dagger} L_{\downarrow}^{\dagger} \sim e^{+i\sqrt{2\pi}\theta_{c}} e^{+i[\sqrt{2\pi}\phi_{c}+2k_{F}x]},$$
 (A10)

corresponding to right- and left-going singlet pairs.

As with the CDW modes, in addition to the singlet pairing modes of the 1DEG, it is necessary to consider the composite singlet pairing  $O_{c-SP}$  (a product of a triplet pairing in the 1DEG with a spin-1 mode of the Heisenberg chain) which turns out to be of odd parity<sup>14,15</sup>

$$O_{c-\text{SP}} = -i \frac{1}{2} (R^{\dagger} \boldsymbol{\sigma} \boldsymbol{\sigma}_{2} L^{\dagger}) \cdot \boldsymbol{\tau}$$

$$= \frac{1}{2} [(R^{\dagger}_{\uparrow} L^{\dagger}_{\uparrow} \tau^{-}_{j} - R^{\dagger}_{\downarrow} L^{\dagger}_{\downarrow} \tau^{+}_{j}) - (R^{\dagger}_{\uparrow} L^{\dagger}_{\downarrow} + R^{\dagger}_{\downarrow} L^{\dagger}_{\downarrow}) \tau^{z}_{j}]$$

$$\sim e^{+i\sqrt{2\pi}\theta_{c}} [e^{-i\sqrt{2\pi}\theta_{s}} \tau^{+}_{j(x)} + e^{+i\sqrt{2\pi}\theta_{s}} \tau^{-}_{j(x)}$$

$$+ 2i \sin(\sqrt{2\pi}\phi_{s}) \tau^{2}]. \qquad (A11)$$

(Note: If we do not take the Klein factors carefully into account than the bosonized form of the singlet and triplet composite pairing is erroneously exchanged.) It can be decomposed into two momentum components: a uniform k=0 composite singlet

$$\hat{O}_{c-\mathrm{SF}}^{k=0}(x) = -i \frac{1}{2} \left( R^{\dagger} \boldsymbol{\sigma} \boldsymbol{\sigma}_{2} L^{\dagger} \right) \cdot \mathbf{J}_{\tau}$$
(A12)

and a  $k = \pi/b$ , i.e., a staggered, composite singlet

$$\hat{O}_{c-\text{SP}}^{\text{stagger}}(x) = -i \frac{1}{2} \left( R^{\dagger} \boldsymbol{\sigma} \boldsymbol{\sigma}_{2} L^{\dagger} \right) \cdot \mathbf{n}_{\tau} (-1)^{j}.$$
(A13)

The commutation relations (13)–(16) relate to each gapless CDW mode a corresponding gapless pairing mode. Therefore, formally, only the  $\eta$ -pairing modes need to be counted. The concomitant "trivial" existence of the usual BCS pairing  $O_{\rm SP}$  and composite pairing  $O_{c-\rm SP}$  modes should be implicitly understood.

The operator  $O_{c-SP}$  is odd under spin-inversion operation  $(R_{\uparrow}^{\dagger} \leftrightarrow R_{\downarrow}^{\dagger}, \tau^{-} \leftrightarrow \tau^{+}, \tau^{z} \leftrightarrow -\tau^{z})$ , as expected for a singlet. Note that its spin-inversion parity is odd, even though the conduction electron part is in triplet pairing. In that sense the order parameter is a composite singlet. The operator is clearly odd under space-inversion operation *P* (exchanging *R* and *L*). The composite singlet operator  $O_{c-SP}$ , can be arrived at by taking the time derivative of the BCS singlet order parameter, <sup>14</sup>  $\partial O_{SP}/\partial t \propto [H_K, O_{SP}] = O_{c-SP}$  where  $H_K$  is the Kondo-Heisenberg Hamiltonian (20). Therefore,  $O_{c-SP}$  is odd under time reversal, or, alternatively, has only odd-w

dependence. The corresponding order parameter on a discrete lattice (e.g., on a zigzag ladder) is

$$O_{c-\mathrm{SP}} = -\frac{i}{2}(-1)^{j}(\psi_{j}^{\dagger}\boldsymbol{\sigma}\boldsymbol{\sigma}_{2}\psi_{j+1}^{\dagger})\cdot\boldsymbol{\tau}_{j}$$

[The factor  $(-1)^j$  is needed so that both odd and even *j* sites will conform in the continuum limit representation.]

There is a qualitative difference between the commutation relation (14) and previous commutation relations of  $O_{c-SP}$  in the literature. As elaborated below, we generated the composite singlet  $O_{c-SP}$  by a combination of  $2k_F^*$  composite particle-hole mode ( $\mathbf{n}_R \cdot \boldsymbol{\tau}$ ) and finite momentum  $k = 2k_F$  singlet ( $\eta_L$  pairing):

$$\mathbf{n}_{R} = \mathbf{O}_{2k_{F}\text{-}\text{SDW}} = R_{\alpha}^{\dagger} \frac{\sigma_{\alpha\beta}}{2} L_{\beta},$$

$$O_{c\text{-}\text{CDW}} = \mathbf{n}_{R} \cdot \boldsymbol{\tau} = \frac{1}{2} (n^{+} \tau_{j}^{-} + n^{-} \tau_{j}^{+}) + n^{z} \tau_{j}^{z}, \quad (A14)$$

$$O_{c\text{-}\text{SP}} = [\eta_{L}, O_{c\text{-}\text{CDW}}].$$

Note that the above generation of the composite singlet pairing is different from the usual way in which it is generated<sup>14</sup> using the  $\pi/b$  momentum composite particle-hole mode ( $\mathbf{J}_R \cdot \boldsymbol{\tau}$ ) and k=0 momentum singlet ( $O_{\text{SP}}$  pairing):

$$\mathbf{J}_{R} = R_{\alpha}^{\dagger} \frac{\boldsymbol{\sigma}_{\alpha\beta}}{2} R_{\beta},$$
$$\boldsymbol{O}_{\mathrm{SP}} = \frac{1}{\sqrt{2}} [R_{\uparrow}^{\dagger} L_{\downarrow}^{\dagger} - R_{\downarrow}^{\dagger} L_{\uparrow}^{\dagger}], \qquad (A15)$$

 $\mathbf{J}_R \cdot \boldsymbol{\tau}$  is an interaction term in the Hamiltonian, which develops a nonzero expectation value  $\langle \mathbf{J}_R \cdot \boldsymbol{\tau} \rangle \neq 0$  in the spin-gap phase of the Kondo lattice Hamiltonian. Thus, the relation  $O_{c-\text{SP}} = [O_{\text{SP}}, \mathbf{J}_R \cdot \boldsymbol{\tau}] = [O_{\text{SP}}, H]$  is important for establishing the time-reversal symmetry of  $O_{c-\text{SP}}$  as determined by the Hamiltonian. The  $(\mathbf{J}_R \cdot \boldsymbol{\tau})$  operator is not one of the gapless modes. In contrast,  $O_{c-\text{CDW}} = \mathbf{n}_R \cdot \boldsymbol{\tau}$  is a gapless mode in the spin-gap phase. Thus, our relation  $O_{c-\text{SP}} = [\eta_L, O_{c-\text{CDW}}]$  establishes the interdependence of gapless modes in the spin-gap phase.

 $O_{c-SP} = [O_{SP}, \mathbf{J}_{R} \cdot \boldsymbol{\tau}].$ 

The commutation relations (13)-(16) indicate that there must be some symmetry difference between the usual CDW( $O_{CDW}$ ) mode of the 1DEG and the composite CDW( $O_{c-CDW}$ ) mode, and that the composite CDW cannot be used in combination with  $\eta^{ever}$  to construct a BCS singlet mode  $\Delta$  (as can be done with the usual CDW). Clearly, there is no difference in the global symmetry properties of the two CDW modes (this would have been a violation of the generalized Luttinger theorem). The difference is in a relative internal symmetry of the two chain system; a  $\pi$  relative spin rotation around the z axis of the 1DEG with respect to the Heisenberg spin chain. This effect is best seen from the bosonized spin field dependence of the operators:

$$\Delta \sim \cos(\sqrt{2\pi\phi_{1s}}),$$

$$O_{\text{CDW}} \sim \cos(\sqrt{2\pi\phi_{1s}}),$$

$$O_{c\text{-CDW}} \sim \cos(\sqrt{2\pi}[\theta_{1s} - \theta_{2s}]]$$

(where subscripts 1 and 2 refer to the 1DEG and the impurity spin chain, respectively). A  $\pi$  relative spin rotation around the *z* axis is shifting  $\sqrt{2\pi} [\theta_{1s} - \theta_{2s}]$  by  $\pi$  and leaving  $\phi_{1s}$ unaffected. Thus under this operation, which we label  $\mathcal{R}_z^{\text{Srel}}(\pi)$ ,

$$\eta \rightarrow + \eta,$$

$$\Delta \rightarrow + \Delta,$$

$$O_{\rm CDW} \rightarrow + O_{\rm CDW},$$

$$O_{c-\rm CDW} \rightarrow - O_{c-\rm CDW}.$$
(A16)

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From these transformation properties (A16) it is clear that the composite CDW cannot be used in combination with  $\eta^{\text{even}}$  to construct a BCS singlet mode, since under  $\mathcal{R}_z^{S \text{ rel}}(\pi)\Delta \rightarrow +\Delta$ , while  $\eta^{\text{even}}O_{c-\text{CDW}} \rightarrow -\eta^{\text{even}}O_{c-\text{CDW}}$ . Hence, our final conclusion is that the Toulouse point phase and the weak-coupling limit spin-gap phase of the Kondo-Heisenberg model are distinct phases (as summarized in Table I).

There is a simple physical interpretation for the distinction made by the  $\mathcal{R}_z^{S \text{ rel}}(\pi)$  symmetry operation. The composite CDW( $O_{c-\text{CDW}}$ ) is actually constructed out of two spin-1 SDW modes which are coherently combined into a total spin singlet. Therefore, the mode is sensitive to the coherent relative phases of the spin fields between the 1DEG and the Heisenberg chain, which is probed by  $\mathcal{R}_z^{S \text{ rel}}(\pi)$ . In contrast, the "pure" CDW mode ( $O_{\text{CDW}}$ ) of the 1DEG is independent of any relative state of the Heisenberg chain.

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