Regular and singular Fermi-liquid fixed points in quantum impurity models

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We show that the traditional classification of quantum inpurity models based on thermodynamics is insufficient to probe the nature of their low-energy dynamics. We propose an analysis based on scattering theory, dividing Fermi liquids into regular Fermi liquids and singular Fermi liquids. In both cases electrons at the Fermi energy scatter elastically off the impurity, but in the case of regular Fermi liquids the scattering has analytical properties in the vicinity of the Fermi energy, while for singular Fermi liquids it does not, resulting in a breakdown of Nozières' Fermi-liquid picture and singular thermodynamic behavior. Using the Bethe ansatz and numerical renormalization group, we show that the ordinary Kondo model is a regular Fermi liquid whereas the underscreened Kondo model is a a singular Fermi liquid. Conventional regular Fermi liquid behavior is reestablished in an external magnetic field H, but with a density of states which diverges as $1/H$. Our results may be relevant for the recently observed field-tuned quantum criticality in heavy electron materials.

I. INTRODUCTION

Quantum impurity models have been classified, conventionally, into one of two categories, Fermi liquid[1] (FL) and non-Fermi-liquid (NFL) depending on their low-temperature specific-heat behavior. In particular, systems with singular dependence on temperature are usually called NFLs. In this paper, we show that thermodynamics is insufficient to probe the nature of the low-energy dynamics and a more subtle analysis based on electron-impurity scattering theory is required. We illustrate our ideas using recent as well as established results on the underscreened Kondo model (UKM).

In a Fermi liquid, electrons at the Fermi level scatter elastically off the impurity, i.e., both the ingoing and outgoing states consist of a single electron with momentum k.[2] By an electron we mean an eigenstate of the noninteracting Hamiltonian H_0, to be distingushed from quasi-particles, the eigenstates of the fully interacting Hamiltonian H. In a generic non-Fermi liquid impurity system, this is not the case. Even when the incoming electrons are on the Fermi surface they can scatter inelastically: an incoming electron state does not scatter into a single outgoing electron state, but instead, excites a large variety of collective modes including particle-hole excitations. In the extreme case of the two-channel Kondo model, e.g., the out-going scattering state does not include any single electron component after scattering with the impurity.[3]

This difference between Fermi liquids and non-Fermi-liquids is clearly captured through the energy- and magnetic field-dependent properties of the single particle matrix elements of the many-body S matrix. For the sake of simplicity, let us consider a nondegenerate interacting ground state and postpone the discussion of degenerate interacting ground states to Sec. II. In the nondegenarate case the single particle matrix elements of the S matrix are defined as $\langle k\mu,\text{in}|\hat{S}|k'\mu',\text{in}\rangle$, where k and k' denote the momenta of incoming and outgoing electrons with respect to the Fermi momentum and μ, μ' denote the rest of their quantum numbers (spin, flavor, angular momentum, etc.). The matrix elements depend only on $\omega=k=k'$ where ω denotes the energy of incoming particle measured with respect the Fermi energy $(v_F=\hbar=1)$, and the S matrix simplifies to $\langle k\mu,\text{in}|\hat{S}|k'\mu',\text{in}\rangle=2\pi\delta(k-k')S^{\mu\mu'}(\omega)$. In the absence of magnetic field, symmetry guarantees that $S^{\mu\mu'}(\omega)=\delta^{\mu\mu'}S(\omega)$, where unitarity requires $S(\omega)$ to be a complex number with modulus less than or equal to 1.

We shall call a system a "Fermi liquid" if $|S(\omega=0)|=1$, the condition implying that at the Fermi level the inelastic scattering cross section vanishes and hence single particle scattering is completely characterized by phase shifts. Electrons on the Fermi are in this case well defined quasi-particles. On the other hand, we shall call a model non-Fermi-liquid if $|S(\omega=0)|<1$. NFLs have a nonvanishing many particle scattering rate and a finite inelastic scattering cross section at the Fermi surface. As a result conduction electrons are not well-defined quasiparticles even on the Fermi level.

However, even when a quantum impurity is a Fermi liquid in the sense described above one may still find singular thermodynamic behavior. This would occur when the eigenvalues of the S matrix for electron impurity scattering approach

Fermi Liquid | Singular Fermi Liquid | Non–Fermi Liquid

$|S(\omega = 0)| = 1$

$S(\omega)$ analytic around $\omega = 0$

$\sigma_{\text{inel}}(\omega \sim 0) = 0 + \text{terms analytic in } \omega$

$|S(\omega = 0)| = 1$

$S(\omega)$ singular around $\omega = 0$

$\sigma_{\text{inel}}(\omega \sim 0) = 0 + \text{terms singular in } \omega$

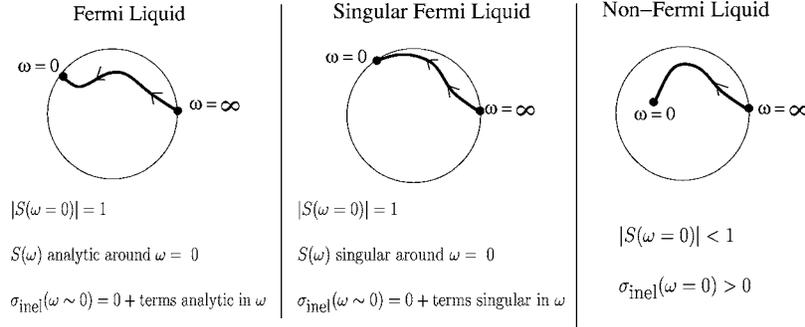$|S(\omega = 0)| < 1$

$\sigma_{\text{inel}}(\omega = 0) > 0$

FIG. 1. Sketch of the renormalization group flows of the eigenvalues of the single particle S matrix in the simplest case of nondegenerate interacting ground states. The eigenvalues are within the unit circle. Particles at high enough energies ($\omega \rightarrow \infty$) do not see the impurity, therefore $S \rightarrow 0$ in this limit. Inelastic scattering processes are allowed whenever $|S(\omega)| < 1$. In Fermi liquids at the Fermi energy $|S(\omega=0)| = 1$, implying the absence of inelastic scattering of electrons. For non-Fermi-liquids $|S(\omega=0)| < 1$, while for singular Fermi liquids $S(\omega)$ approaches the unit circle nonanalytically as $\omega \rightarrow 0$.

the unit circle nonanalytically as the electron energy ω approaches the Fermi level. This would lead to a singular density of states and therefore impact thermodynamics. For this reason, we propose to divide Fermi liquids into two types: regular Fermi liquids (RFLs) and singular Fermi liquids (SFLs). In the former, the eigenvalues of the single particle S matrix approach the unit circle analytically, whereas in the latter, they approach it singularly. For both types of fixed points, the single particle S matrix is unitary at the Fermi energy, implying that an incoming electron at the Fermi surface scatters elastically off the impurity. However, the two types of FLs exhibit very different phenomenological properties. A regular Fermi liquid exhibits the usual properties associated with FLs, and hence, by an abuse of notation, we shall often omit the term "regular" when referring to this class of fixed points. On the other hand, SFLs exhibit a wide variety of behavior not ordinarily associated with Fermi liquids such as extreme sensitivity to applied fields and a divergent specific heat. This classification scheme and the main properties of the three impurity classes are summarized in Fig. 1.

An example is provided by the striking difference in the low-temperature physics of the ordinary Kondo model (KM) and the underscreened Kondo model (UKM) (see Ref. 4, and references therein). The UKM describes the antiferromagnetic interaction of a magnetic impurity of spin $S > 1/2$ with a sea of conduction electrons. At low temperatures, the impurity spin is partially screened from spin S to spin $S^* = S - 1/2$. What distinguishes the UKM from the ordinary Kondo model is the residual magnetic moment that remains even after screening. This residual moment couples ferromagnetically to the remaining conductionte electrons. Though the ferromagnetic coupling is irrelevant, it tends to zero very slowly. As a result, there is a subtle interplay between the residual moment and the electron fluid that leads to radically different physics from the ordinary KM at the strong-coupling fixed point of the UKM.

A Bethe ansatz and a large N analysis of the underscreened Kondo model show that at zero field, this system exhibits singular behavior, with a divergent specific heat coefficient C_v/T at zero field.[5,6] In a finite field, the linear spe-

cific heat coefficient is found to diverge as $1/|H|\ln^2(T_K/|H|)$. To decide wheter this singular behavior corresponds to a NFL or a SFL we need study the scattering properties of the model. We reexamine it using Bethe-ansatz and numerical renormalization group (NRG) methods. From the Bethe-ansatz solution, we find that at zero magnetic field the sacttering matrix elements tend to the unitary limit, albeit in a singular manner,

$$\delta_s(\omega, H = 0) = \frac{\pi}{2} + \left(S - \frac{1}{2}\right)\frac{\pi}{2 \ln \frac{T_k}{\omega}} + \cdots. \quad (1)$$

At finite field it becomes analytic, yet showing a singular behavior as the magnetic field scales to zero:

$$\delta_s(\omega = 0, H) = \frac{\pi}{2} + \left(S - \frac{1}{2}\right)\frac{\pi}{2 \ln \frac{T_k}{H}} + \cdots. \quad (2)$$

The singular nature of the phase shifts energy dependence results in the breakdown of Nozières' picture of the strong coupling fixed point and indicates that the physics of the UKM and the ordinary Kondo model are quite different. These results are confirmed using the numerical renormalization group (NRG) calculations on a $S=1$ UKM, where we can directly compute the phase shift of spin 1/2 electron excitations from the finite size spectrum. Such a calculation has been carried out earlier in the absence of the magnetic field by Cragg *et al.*,[7] who found that the NRG spectrum can be described in terms of phase shifts $\pi/2$ (apart from the presence of a decoupled residual spin S^*). Here we also determine the phase shifts for a $S=1$ model in the presence of a local magnetic field H and confirm that they scale as $\delta_\pm \approx \pi/2 \pm \pi/[4 \ln(T_K/|H|)]$ for small magnetic fields, in agreement with the Bethe ansatz results. Thus the fixed point finite size spectrum of the UKM is that of a Fermi liquid, i.e., scattering at the Fermi energy can be simply characterized in terms of phase shifts.

The analysis we present here may also be relevant to heavy fermion systems: application of the behavior of Re-

cent experimental studies on heavy electron materials fine-tuned away from an antiferromagnetic quantum critical point (QCP) using a magnetic field[8,9] revealed that parameters of the heavy Fermi liquid can be field-tuned. In particular, the temperature-dependent properties of the system near the QCP were shown to depend only on the ratio $T/(B-B_c)$. This behavior is strikingly reminiscent of the field tuned change in behavior of the UKM.

The paper is structured as follows. In Sec. II, we discuss the general classification of regular and singular Fermi liquids and the application of this classification scheme for Kondo models in more detail. In Sec. III, we use the Bethe ansatz to calculate the DOS and find that it is singular in the absence of a magnetic field. In Sec. IV, we present numerical renormalization group calculations confirming our Bethe-ansatz results. In Sec. V, we discuss the breakdown of Nozières Fermi-liquid picture for the UKM. Some details of the Bethe-ansatz calculations are given in a longer version of this draft.

II. SINGULAR FERMI LIQUIDS AND NON-FERMI-LIQUIDS

The nature of the low-temperature dynamics and thermo-dynamics of a quntum impurity system can be most easily captured, as mentioned above, through the many-body S matrix, which we shall discuss in detail in this section. We shall analyze a general quantum impurity problem described by the following Hamiltonian:

$$H = -i\sum_\mu \int dx : \psi_\mu^\dagger(x,t)\partial_x\psi_\mu(x,t): + H_{\text{int}}. \qquad (3)$$

Here the fields ψ_μ are chiral one-dimensional fermions, and usually represent radial excitations in some three-dimensional angular momentum channel coupled to the impurity. The label μ represents those discrete internal degrees of freedom (spin, flavor, crystal field, angular momentum indices, etc.) that may couple to the impurity. The precise form of the impurity-fermion interaction, H_{int} is of no importance for the purpose of our discussion below.

A. Nondegenerate ground state

Let us first discuss the simplest case, when the interacting ground state of Eq. (3) is nondegenerate. The central quantity we are interested in is the many-body S matrix $\hat{S}$ defined in terms of incoming and outgoing scattering states $|a\rangle_{\text{in}}$ and $|b\rangle_{\text{out}}$ as (see, e.g., Ref. 10)

$$\langle b,\text{out}|a,\text{in}\rangle \equiv \langle b,\text{in}|\hat{S}|a,\text{in}\rangle. \qquad (4)$$

The "in" and "out" states are eigenstates of the total Hamiltonian, Eq. (3), satisfying the boundary conditions that they tend to plane waves (more precisely, to the eigenstate of H_0, $c_{k,\mu}^\dagger|G\rangle = \int \exp(ikx)\psi_\mu^\dagger(x,t)|G\rangle)$ in the $t\to-\infty$ and $t\to\infty$ limits, respectively. In the interaction representation, the explicit form of the S matrix is given by the well-known expression $\hat{S}=T\exp\{-i\int_{-\infty}^{\infty}H_{\text{int}}(t)dt\}$, where T is the time ordering opera-

tor, and the interaction $H_{\text{int}}(t)$ is adiabatically turned on and off during the time evolution.

The unitarity of the S matrix poses severe constraints on the single particle matrix elements of the S matrix (see above),

$$\langle k\mu,\text{in}|\hat{S}|k'\mu',\text{in}\rangle = 2\pi\delta(k-k')\mathcal{S}_{\mu\mu'}(\omega). \qquad (5)$$

Indeed, the eigenvalues of of $\mathcal{S}$,

$$s_\lambda(\omega) \equiv r_\lambda(\omega)e^{i2\delta_\lambda(\omega)} \qquad (6)$$

must be within the unit circle

$$|s_\lambda(\omega)| = r_\lambda(\omega) \leqslant 1. \qquad (7)$$

The phase shift $\delta_\lambda(\omega)$ above corresponds to the phase shift picked up by elastically scattered particles of energy ω, and is relevant for interference effects. In the case of the single channel Kondo model, e.g., $r_\lambda(\omega) \approx 1 - C\omega^2/T_K^2$, but $\delta_\lambda(\omega) \approx \pi/2 + \tilde{C}\omega/T_K$ for small energies, with C and $\tilde{C}$ constants of order unity.

To distinguish between eleastic and inelastic processes it is convenient to consider the T matrix defined through,

$$\hat{S} = \hat{1} + i\hat{T}.$$

We can then define the on-shell T matrix $\mathcal{T}(\omega)_{\mu\mu'}$ analogous to Eq. (5), and the corresponding eigenvalues are simply given by

$$\tau_\lambda(\omega) = -i[s_\lambda(\omega) - 1]. \qquad (8)$$

As discussed in Ref. 13, the knowledge of the single particle matrix elements of the many-body T matrix enables us to compute the total scattering cross section off the impurity in the original three-dimensional impurity problem through the optical theorem as

$$\sigma_{\text{tot}} = \sigma_0 \sum_\lambda 2|\varphi_\lambda(\omega)|^2 \,\text{Im}\{\tau_\lambda(\omega)\}, \qquad (9)$$

where $\sigma_0 = \pi/k_F^2$ with k_F the Fermi momentum, and $\varphi_\lambda(\omega)$ denotes the wave function amplitude of the incoming electron in scattering channel λ. Elastic scattering off the impurity can be defined as single particle scattering processes where the outgoing state consists of a single outgoing electron. The elastic scattering cross section is simply proportional to the square of the elements of the T matrix, and is given by

$$\sigma_{\text{el}} = \sigma_0 \sum_\lambda |\varphi_\lambda(\omega)|^2 |\tau_\lambda(\omega)|^2. \qquad (10)$$

Having determined both σ_{tot} and σ_{el}, we can define the *inelastic* scattering cross section off the impurity as the difference of these cross sections[26] $\sigma_{\text{inel}} = \sigma_{\text{tot}} - \sigma_{\text{el}}$, which simplifies to

$$\sigma_{\text{inel}} = \sigma_0 \sum_\lambda |\varphi_\lambda(\omega)|^2 [1 - r_\lambda(\omega)^2]. \qquad (11)$$

It is clear from this expression that if $\mathcal{S}$ has an eigenvalue that is *not* on the unit circle, this implies that one can construct an incoming single particle state which with some

probability scatters *inelastically* into a multiparticle outgoing state.

B. Degenerate gound states

The above discussions can be easily generalized to the case of an impurity model with a degenerate ground state. Let us denote a basis set within the ground state multiplet by $|G\rangle$, where $G = 1, \ldots, N_G$. The only difference in this case is that $\mathcal{S}$ aquires new indices

$$\mathcal{S}^{\mu\mu'} \to \mathcal{S}^{\mu\mu'}_{GG'}.$$

Let us consider a given state within the ground-state multiplet $|\alpha\rangle \equiv \Sigma_G \alpha_G |G\rangle$ and the corresponding single-particle S matrix

$$\mathcal{S}^{\mu\mu'}_\alpha \equiv \sum_{G,G'} \alpha^*_G \mathcal{S}^{\mu\mu'}_{GG'} \alpha'_G.$$

This scattering matrix measures the amplitude of those single particle processes, where the ground state has not been altered during the scattering process.

Starting from $\mathcal{S}^{\mu\mu'}_\alpha$ and following the lines of the previous subsection, we can trivially define $\mathcal{T}^{\mu\mu'}_\alpha(\omega)$ and the elastic and inelastic scattering amplitudes *provided* that the system is in ground state $|\alpha\rangle$ before the scattering. Note that even for degenerate ground states and non-Fermi-liquid systems, one can apply a small external perturbation H (tiny local magnetic field, e.g.) which selects a unique (usually Fermi liquid) ground state. One can then consider the $H \to 0$ limit by keeping ω finite.

C. Classification of fixed points

We are now ready to give a precise definition of a non-Fermi liquid: We define a quantum impurity model to be of non-Fermi-liquid type if there exist eigenvalues of the single particle S matrix $\mathcal{S}^{\mu\mu'}_\alpha(\omega)$, which are not on the unit circle in the $\omega \to 0$ limit for some state $|\alpha\rangle$ within the ground state multiplet. By Eq. (11) this immediately implies that non-Fermi-liquid models have the unusual property that even electrons at the Fermi energy can scatter off the impurity inelastically with a finite probability.

Typical examples of non-Fermi-liquid models are given by various versions of over-screened multichannel Kondo models. In the two channel Kondo model, e.g., it has been shown in Refs. 11 and 12 using bosonization methods that the single particle matrix elements of the S matrix identically vanish at the Fermi energy, immediately implying that $r_\lambda = 0$ and thus $\sigma_{el} = \sigma_{inel} = \sigma_{tot}/2$ at the Fermi energy.[13,14]

As opposed to non-Fermi-liquids, we define a model to be a Fermi liquid if all the eigenvalues of the single-particle S matrix $\mathcal{S}^{\mu\mu'}_\alpha(\omega)$ fall on the unit circle in the $\omega \to 0$ limit for *any* state $|\alpha\rangle$ within the ground-state multiplet. It is not too difficult to show, that this definition is equivalent to the requirement that

$$\mathcal{S}^{\mu\mu'}_{GG'}(\omega \to 0) \equiv \delta_{G,G'} \mathcal{S}^{\mu\mu'}_0, \tag{12}$$

with $\mathcal{S}^{\mu\mu'}_0$ a unitary matrix.

Inelastic scattering processes may, in particular, involve scattering within the interacting ground-state multiplet. Consider for example the ferromagnetic anisotropic Kondo model. It is not a Fermi-liquid model by this definition. This can be understood very easily as follows: For the ferromagnetic anisotropic Kondo model the fixed point Hamiltonian consists of a simple coupling of the z component of the spins

$$H^*_{int} = \frac{J^*_z}{2} S_z \sum_\sigma \psi^\dagger_\mu(0) \sigma^z_{\mu\mu'} \psi_{\mu'}, \tag{13}$$

where we assume now that S is a spin $1/2$ impurity. In this case, at the fixed point the scattering of conduction electrons can be described simply by phase shifts, which, however, *depends* on the relative spin of the incoming electron and the impurity $\delta_\mu(S_z) = \delta_0 2 S^z \mu$. Now suppose that we prepare the impurity in the eigenstate of S^x and we look at the scattering of a spin up electron. Applying the formalism above, we immediately find that the inelastic scattering rate is nonvanishing and is proportional to $\sigma_{inel} \sim 1 - \cos^2(2\delta_0)$. The physical reason for this is very simple: The impurity experiences the spin field of the conduction electron in course of the scaterring process through the exchange coupling. As a response to this field, the impurity spin is rotated around the z axis by an angle $2\delta_0$, and has only an overlap $\cos(2\delta_0)$ with the initial impurity spin state. This change in the "environment" is the ultimate reason for inelastic scattering. (Interestingly enough, while this process does not seem to destroy week localization corrections, it definitely destroys Aharonov-Bohm oscillations.)

This simple non-Fermi-liquid nature of the ferromagnetic anisotropic Kondo model may seem to be surprising at a first sight, since we know that by changing the anisotropy $J_\perp/J_z$ within the ferromagnetic Kondo model one gradually approaches the isotropic ferromagnetic Kondo fixed point of singular Fermi-liquid nature. But this is not very surprising and indeed in many ways this is analogous to the way one approaches the critical point of a ferromagnet from the ferromagnetic side: for $T < T_C$ the magnetization has a jump as a function of external magnetic field, corresponding to a first order transition, but this jump gradually vanishes as one approaches the the critical end point, $T = T_C$ where the thermodynamical quantities exhibits power law behavior, governed by the critical end point.

In the ferromagnetic Kondo problem at $T = 0$ a somewhat analogous quantum phase transition occurs as a function of $J_l \perp / J_z$: For $J_l \perp / J_z < 1$ the impurity magnetization exhibits a jump as a function of magnetic field, and the effective interaction strength J^*_z in Eq. (13) gradually vanishes as one approaches $J_l \perp / J_z = 1$. For $J_l \perp / J_z > 1$, on the other hand, the model has a Fermi-liquid ground state, and the impurity magnetization does not jump as a function of magnetic field. In this sense the singular Fermi-liquid point is just a critical endpoint. Note, however, that unlike the ferromagnetic phase transition mentioned above, in case of the Kondo model SU(2) symmetry usually *guarantees* that $J_\perp = J_z$, and therefore one is doomed to approach the singular Fermi-liquid state.

The FL condition implies that electrons at the Fermi en-

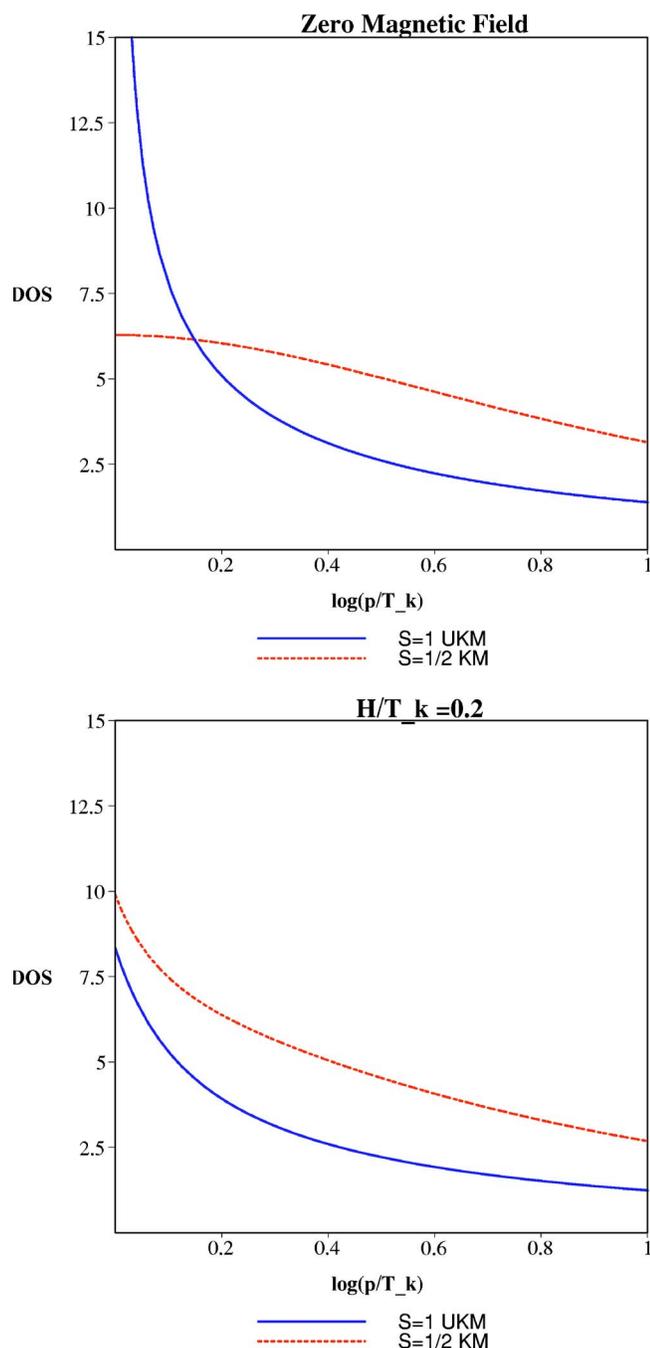**Zero Magnetic Field**

H/T_k =0.2

FIG. 2. (Color online) (a) The impurity induced (spinon) DOS of the $S=1/2$ Kondo model and the $S=1$ underscreened Kondo models as a function of the logarithm of the quasi-particle (spinon) energy. (b) The same quantities in a finite magnetic field H. For $S=1/2$, the impurity induced DOS is always finite. For the $S=1$ underscreened Kondo model, however, the DOS diverges in zero magnetic field as the energy of the excitation goes to zero. The presence of H cuts off the singularity of the DOS of the underscreened Kondo model.

ergy scatter completely *elastically* off the impurity, and that this scattering can be characterized in terms of simple phase shifts. In fact, most impurity models, such as screened or underscreened Kondo models, the Anderson impurity model, the resonant level model, or overscreened models in an external field, fall in the category of Fermi liquids, since in all these cases the single particle S matrix satisfies Eq. (12).

The structure of the energy dependence of the $s_\lambda(\omega)$'s, i.e., the renormalization group flow of the eigenvalues of the single particle S matrix, however, does depend on the specific Fermi-liquid model, and allow for further classification: We can define as singular Fermi liquids those models, where the convergence to the $\omega=0$ Fermi-liquid fixed point is singular in ω, while we shall call regular Fermi liquids those where the convergence is analytical. By these terms, the standard spin $1/2$ Kondo model is a regular Fermi liquid, while the underscreened Kondo models studied in this paper belong to the class of singular Fermi liquids. We shall see below that singular Fermi liquids have singularities in the low-energy thermodynamic properties while having only elastic (albeit singular) scattering on the Fermi surface.

III. BETHE ANSATZ CALCULATION OF THE DENSITY OF STATES FOR THE UNDERSCREENED KONDO MODEL

We proceed to show that the UKM is an example of a singular FL by studying its scattering properties. We show that in zero magnetic field the phase shift and resulting DOS is a singular function of electron energy. We also show that while $|s(\omega)| \to 1$ as $\omega \to 0$ the limit is approached in a singular manner. Finally, we study the effect of a magnetic field and show that the singularity in the DOS is cut off by a finite field.

The Hamiltonian for the UKM can be mapped to the following one-dimensional Hamiltonian:

$$H_{\text{UKM}} = -i\sum_a \int dx \, \psi_a^\dagger(x) \partial_x \psi_a(x) + J\psi_a^\dagger(0)\vec{\sigma}_{ab}\psi_b(0) \cdot \vec{S},$$

where $\psi_a^\dagger(x)$ is the creation operator of an electron with spin a and $\vec{S}$ is a localized spin at the origin coupled to the electron sea by an antiferromagnetic coupling J. In this equation the left-moving chiral Fermions $\psi_a^\dagger(x)$ in regions $x>0$ and $x<0$ simply represent the incoming and outgoing parts of the conduction electrons' s-wave function in the three-dimensional problem.

The spectrum of the UKM can be determined from the Bethe-ansatz solution.[15–17] The excitations consist of uncharged spin-$1/2$ excitations, spinons, and spinless charge excitations, holons. In the spinon-holon basis, the wave function for the electron can be written as a sum of products of a spin wave function and a charge wave function. Since the Kondo interaction affects only the spin sector, we will ignore the charge sector in the analysis that follows.

In the spin sector, an electron (not an eigenstate of the full hamiltonian) can be expressed as a *superposition* of spinons and antispinons. Formally, this is done through a form-factor expansion of the electron onto the spinon basis. At low energies, the coefficients of the the multispinon terms in the form factor expansion tend to zero. For this reason, at sufficiently low energies, it is a reasonable to approximate the

electron by a spinon.[18] Since we are interested in the low-energy properties of the UKM, we will employ this approximation. The validity of this approximation will be checked by comparing our results at the Fermi energy with those of the numerical renormalization group (NRG).

From the Bethe-ansatz solution, we can calculate the phase shift $\delta_s(k,H)$ of a spinon with momentum k when it is scattered off the impurity in the presence of a magnetic field H. The phase shift, in turn, is intimately related to the DOS of spinons at the impurity through the Friedel sum rule, which states that the spinon DOS $N_s(\omega)$ is proportional to the derivative of the phase shift with respect to the energy:[19]

$$N_s(\omega,H) = \frac{1}{\pi}\frac{d\delta_s(\omega,H)}{d\omega}. \qquad (14)$$

Note that as the energy of the spinon is linear in its momentum we shall use the symbols for momentum k and energy ω interchageably (we have chosen units where $v_F=1$, so $\omega=k$).

To calculate the phase shift, we place our physical system in a finite ring of length L. The momentum k of a free spinon will satisfy $k=(2\pi/L)n$, but in the presence of a impurity, by definition, the momentum will be shifted from its free value by twice the phase shift

$$k = \frac{2\pi}{L}n + 2\delta_s(k=\omega,H)\frac{1}{L}. \qquad (15)$$

Since one can, using the Bethe-ansatz solution, determine spinon momenta to accuracy $O(1/L)$, the phase shift can be exactly determined directly from the Bethe-ansatz spectrum.[20–23]

To solve for the spectrum of the UKM and to determine the phase shifts, it is necessary to solve a set of coupled integral equations called the Bethe-ansatz equations (BAEs).[24] The BAEs are written in terms of the spin rapidities Λ and a spinon magnetic field Λ_B (related to H, see later). Each set of $\{\Lambda\}$'s and Λ_B which solve the BAE give rise to a set of physical momenta $\{k\}$ and physical magnetic field H.

In the thermodynamic limit, instead of examining specific solutions of the BAE, it is sufficient to study the density of solutions. Let $\sigma(\Lambda)$ denote the density of solutions of the BAE in an interval $d\Lambda$ (not to be confused with the scattering cross section). A spinon excitation corresponds to removing a $\Lambda=\Lambda^h$ from the ground state, i.e., to adding a density of "holes" $\sigma^h(\Lambda)=\delta(\Lambda-\Lambda^h)$.[25] The "hole" position Λ^h determines the spinon momentum $k(\Lambda^h)$ and its phase shift $\delta_s[k(\Lambda^h),H]$. It should be noted that the hole density is "dressed" by the back flow of the Fermi sea, which corresponds to a small change in the ground state density $\Delta\sigma(\Lambda)$. It is essential to take this back flow into account when calculating the excitation energy $E=\Sigma_{j=1}^{N^e}(2\pi/L)n_j +D\int d\Lambda\sigma(\Lambda)[\Theta(2\Lambda-2)-\pi]$, where $D=N_e/L$ denotes the energy cutoff and $\Theta(x)=-2\tan^{-1}(x/c)$.

In terms of these densities, the BAE can be written as

$$\sigma(\Lambda) + \sigma_h(\Lambda) = f(\Lambda) - \int_{\Lambda_B}^{\infty} K(\Lambda - \Lambda')\sigma(\Lambda')d\Lambda'$$

with

$$f(x) = \frac{N^e}{\pi}\frac{c/2}{(c/2)^2 + (x-1)^2} + \frac{N^i}{\pi}\frac{(cs)}{(cS)^2 + x^2},$$

$$K(x) = \frac{1}{\pi}\frac{c}{c^2 + x^2},$$

where S is the spin of the impurity, N^e is the number of electrons, N^i is the number of "dilute" impurities, and c is the coupling constant.[16] The coupling c is related to the original coupling J, however, the precise relation between these two couplings depends on the specific scheme used to regularize the local interactions.[27] Using the chain rule, we can write the spinon DOS as

$$N_s(\omega) = \frac{1}{\pi}\frac{d\delta_s}{d\omega} = \frac{1}{\pi}\left(\frac{d\omega}{d\Lambda^h}\right)^{-1}\frac{d\delta_s}{d\Lambda^h}, \qquad (16)$$

where ω is calculated from the expression for the energy. To proceed, we note that the density of solutions in the presence of a spinon excitation $\sigma(\Lambda,\Lambda^h)$ can be written as

$$\sigma(\Lambda,\Lambda^h) = \sigma_o(\Lambda) + \Delta\sigma(\Lambda,\Lambda^h), \qquad (17)$$

where σ_o is the density in the ground state (with no holes present) and $\Delta\sigma$ is the change in the density due to the excitation (presence of the hole Λ^h). We can further divide σ_0 into two terms σ_{el}, the electron contribution to the ground state and σ_{im}, the impurity contribution to the ground state. It is known that the derivative of the phase shift as a function Λ^h, $d\delta_s/d\Lambda^h$, is precisely the impurity contribution of to ground-state density of solutions evaluated at Λ^h, $\sigma_{im}(\Lambda^h)$ (see Ref. 21). Note that $\sigma_{im}(\Lambda)$ depends only on the ground state and does not know about the presence of the spinon. The information about the spinon in the DOS comes only through the spinon excitation energy ω. Finally, it should be noted that since we are interested in the behavior around $H=0$, the results we present here are valid only for magnetic fields much smaller than the Kondo temperature temperature $H/T_k\ll 1$.

The details of the explicit solution of the BAE and the and computation of the DOS $N_s(\omega)$ are given in cond-mat/0404122. The final results read

$$N_s(\omega) = \frac{1}{2\pi}\left[\frac{1}{\omega + H'}\beta\left(S + i\frac{1}{\pi}\ln[(\omega+H')/T_k]\right)\right.$$
$$\left. + \frac{H}{2\pi(\omega+H')^2}\beta\left(S + i\frac{1}{\pi}\ln(H'/T_k)\right)\right] \qquad (18)$$

with $H'=(e/2\pi)^{1/2}H$ and $\beta(x)$ defined to be

$$\beta(x) = \frac{1}{2}\text{Re}\left\{\psi\left(\frac{x+1}{2}\right) - \psi\left(\frac{x}{2}\right)\right\}, \qquad (19)$$

with $\psi(x)$ the digamma function.

In Fig. 2, the DOS versus energy is plotted for the UKM. Notice that for the UKM, the DOS is singular in the absence of a magnetic field. As a result, characteristics of quasiparticles are not analytic near the Fermi surface leading to singular thermodynamical behavior.

Note that the singular behavior is cut off by a finite field magnetic field. To compare with numerical RG, we must explicitly calculate the phase shift. To do so, we integrate the above expression with respect to ω to get

$$\delta(\omega,H) = \frac{\pi}{2} + \frac{1}{2i} \ln\left(\frac{\Gamma\left[S + \frac{1}{2} + \frac{i}{\pi} \ln\left(\frac{\omega + H'}{T_k}\right)\right] \Gamma\left[S - \frac{i}{\pi} \ln\left(\frac{\omega + H'}{T_K}\right)\right]}{\Gamma\left[S + \frac{1}{2} - \frac{i}{\pi} \ln\left(\frac{\omega + H'}{T_k}\right)\right] \Gamma\left[S + \frac{i}{\pi} \ln\left(\frac{\omega + H'}{T_K}\right)\right]} \right) - \frac{H'}{\sqrt{2\pi e}(\omega + H')} \operatorname{Re}\left[\beta\left(S + i\frac{1}{\pi} \ln(H'/T_k)\right)\right].$$

The integration constant could be fixed by noting that the expression for the DOS is valid for any spin S allowing us to compare it to a spin-1/2 calculation carried out in Ref. 17. As a further check, note that for $S=1/2$ and zero magnetic field, the above expression can be simplified using various gamma function identities and yields

$$\delta_{S=1/2}(\omega) = \pi/2 - \tan^{-1}\left(\frac{\omega}{T_k}\right) \qquad (20)$$

in agreement with earlier calculations.[21]

For small energies and magnetic field, the above expression can be simplified using Stirlings approximation and yields

$$\frac{\delta_s(\omega,H=0)}{\pi} = 0.5 + \left(S - \frac{1}{2}\right)\frac{1}{2 \ln \frac{T_k}{\omega}} + \cdots,$$

$$\frac{\delta_s(\omega=0,H)}{\pi} = 0.5 + \left(S - \frac{1}{2}\right)\frac{1}{2 \ln \frac{T_k}{H}} + \cdots. \qquad (21)$$

Thus, when $H=0$, the quasiparticle (spinon) phase shift approaches a unitary value, a hallmark of FL. However, as promised earlier, it does it in a singular manner. Furthemore, note that this singular behavior disappears for the ordinary Kondo model when $S=1/2$. For these reasons, we classify the UKM as a singular Fermi-liquid (SFL) state. This singularity has interesting consequences for the phenomenological strong coupling picture developed by Nozières for the $S=1/2$ Kondo model.

IV. NUMERICAL RENORMALIZATION GROUP

In this section we shall use Wilson's numerical renormalization group (NRG) method to compute the magnetic field dependence of the phase shift of the quasiparticles and compare these numerical results with those of the Bethe ansatz.[28] An early NRG study of the underscreened Kondo model has been carried out by Cragg and Lloyd.[7] However, Cragg and Lloyd have not discussed the case of a finite magnetic field,

which we analyze here. As we argued earlier, although this is not true in general, at the Fermi energy the phase shifts of the spinons obtained from the Bethe ansatz should coincide with that of electrons.

In Wilson's NRG technique one maps the original Hamiltonian of the impurity problem to a semi-infinite chain with the magnetic impurity at the end of the chain. The hopping amplitude decreases exponentially along the chain, $t_{n,n+1} \sim \Lambda^{-n/2}$, where $\Lambda \sim 3$ is a discretization parameter and n labels the lattice sites along the chain. As a next step, one considers the Hamiltonians H_N of chains of length N, and diagonalizes them iteratively to obtain the approximate ground state and the excitation spectrum of the infinite chain

$$\cdots \to H_{N-1} \to H_N \to H_{N+1} \to \cdots.$$

The Hamiltonian H_N in this series simply describes the spectrum of H_L, the original Hamiltonian, in a finite one-dimensional box of size $L \sim \Lambda^{N/2}$. The spectrum of H_N is rather complicated in general, however, in the vicinity of a low-energy fixed point the finite size spectrum H_L becomes *universal*, implying that the spectrum of the fixed point Hamiltonian

$$H^* \equiv \Lambda^{N/2} H_N \sim \frac{L}{2\pi} H_L \qquad (22)$$

does not depend on the iteration number N apart from an even-odd oscillation, due to the change of boundary conditions with N.

A typical finite size spectrum in zero magnetic field is shown in Fig. 3. Only the spectra of even iterations corresponding to periodic boundary conditions in the non-interacting problem are shown. For $N>5$ the excitation spectra approach very slowly ($\sim 1/N$) a universal spectrum.[7] This universal spectrum is identical to that of a free residual spin $S^*=1/2$ and the spectrum of the following Hamiltonian:
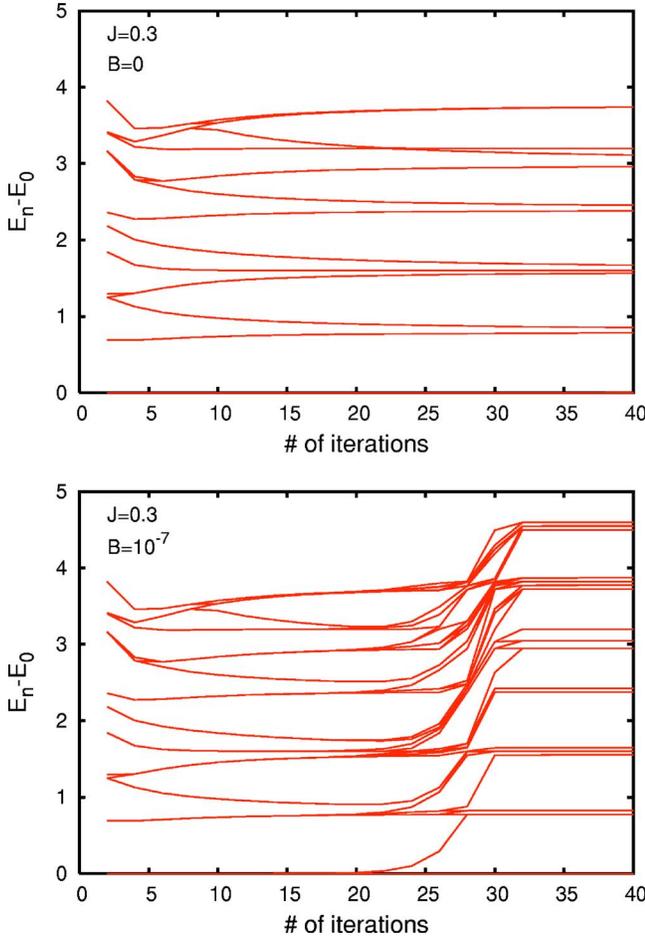
FIG. 3. (Color online) Finite size spectrum of the $S=1$ under-screened Kondo problem in the even sector in the absence (a) and presence (b) of a magnetic field. In the absence of a magnetic field the fixed point spectrum is that of a free Fermion field twisted by a phase shift $\pi/2$, and a residual spin $S^*=1/2$. In a magnetic field a second scale appears below which the fluctuations of the residual spin $S^*=1/2$ are frozen, and the spectrum can be characterized by a single, field-dependent phase shift $\delta(H)$.

$$H^* = \frac{L}{2\pi}\sum_{\sigma=\pm}\int_{-L/2}^{L/2}dx\,\widetilde{\psi}_\sigma^\dagger(x)[-i\partial\widetilde{\psi}_\sigma(x)], \qquad (23)$$

where, in contrast to the original fields, the free fermionic fields $\widetilde{\psi}_\sigma(x)$ obey now *antiperiodic* boundary conditions

$$\widetilde{\psi}_\sigma(-L/2) = -\widetilde{\psi}_\sigma(L/2). \qquad (24)$$

Thus in the absence of a magnetic field fermions at the Fermi energy simply acquire a phase shift $\pi/2$. As a consequence, the spectrum of Eq. (23) is gapped for a finite system size, and the ground state of the system is only twofold degenerate due to the presence of the residual spin S^*. As shown in Fig. 3(b), in the presence of a small magnetic field H a new scale $\sim H$ emerges, below which the fluctuations of the residual spin are frozen out, and the ground-state degeneracy is lifted. Below this scale the spectrum can be described simply by Eq. (23) with the modified boundary conditions
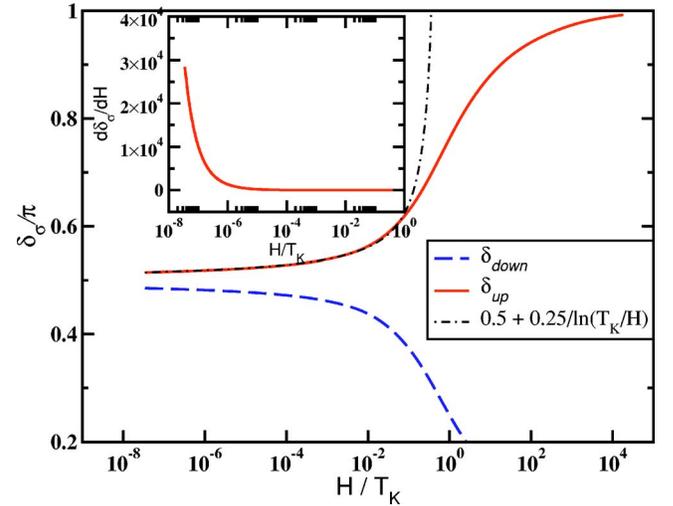

FIG. 4. (Color online) Magnetic field dependence of the phase shifts extracted from the NRG finite size spectrum. The phase shifts scale to $\pi/2$ as $\sim 1/\ln(T_K/|H|)$. Inset: The derivative of the phase shift diverges as $1/|H|$ for $|H| \ll T_K$.

$$\widetilde{\psi}_\sigma(-L/2) = -e^{-i2\delta_\sigma(H)}\widetilde{\psi}_\sigma(L/2), \qquad (25)$$

where $\delta_\sigma(H)$ denote field-dependent phase shifts. Note that these phase shifts are the phase shifts of charged excitations, i.e., from the NRG spectrum we determine directly the phase shifts of the electrons at the Fermi energy.

We can thus determine the magnetic field dependence of the phase shifts directly from the NRG spectrum. As shown in shown in Fig. 4, the phase shifts $\delta_\sigma(H)$ approach $\pi/2$ as $0.25/\ln(T_K/H)$ in good agreement with the Bethe-ansatz result for $S=1$ Eq. (21). In the inset of Fig. 4 we plotted the derivative of the phase shift too, that we computed by numerically differentiating the NRG results. This derivative is proportional to the quasiparticle density of states at the Fermi level, and indeed diverges approximately as $\sim 1/H$ for $H\rightarrow 0$.

V. THE BREAKDOWN OF NOZIÈRES' FERMI-LIQUID PICTURE FOR THE UKM

In his seminal papers,[1] Nozières argued that one could perform a "Fermi-liquid expansion of phase shifts" at strong coupling. He argued that since the impurity is frozen into a singlet at strong coupling, the only remaining degrees of freedom in the problem were those of the Fermi liquid. He showed that all the physics could be captured by examining the phase shifts of quasiparticles as they pass the impurity. We shall now argue that this picture is valid for RFL but fails in the case of SFL.

Nozières' prescription to describe a Fermi liquid is to *assume* that the phase shift for a quasiparticle of energy ω and spin σ has the general form

$$\delta_\sigma(\omega) = \delta_\sigma[\omega,\{n_{\sigma'}(\omega')\}], \qquad (26)$$

where $\{n_{\sigma'}(\omega')\}$ denotes the occupation number of all other quasiparticle states. It is not clear from Nozières original

paper how exactly the phase shift can be defined for a particle of finite energy, which scatters generically inelastically off the impurity. Implicitly, Nozières' prescription assumes, that sufficiently close to the Fermi surface the inelastic scattering of a quasiparticle of energy ω is suppressed as $\sim \omega^2$, and thus quasiparticles are indeed well defined. With this assumption, and assuming further that in the strong coupling fixed point everything is *analytic* near the Fermi surface one can proceed and expand the phase shift in powers of ω and the change of quasiparticle occupation number δn as

$$\delta_\sigma(\omega) = \delta_0(\omega) + \sum_{\omega',\sigma'} \phi_{\sigma,\sigma'}(\omega,\omega')\delta n_{\sigma'}(\omega'),$$

$$\delta_0(\omega) = \delta_0 + \alpha\omega + \beta\omega^2, \tag{27}$$

where for the sake of simplicity we assumed $H=0$. These equations are the main constituents of Nozières' Fermi-liquid theory. The assumption that $\delta_0(\omega)$ is analytical in ω implies that the impurity-induced DOS remains finite at the Fermi energy with $\alpha \sim 1/T_K$.

Our Bethe ansatz solution, however, shows that in the absence of a magnetic field the spinon phase shifts take the form

$$\delta_s(\omega) = \frac{\pi}{2} + \gamma \frac{\text{sgn}(\omega)}{\ln\left(\frac{T_K}{\omega}\right)} + \cdots, \tag{28}$$

leading to the singular density of states for the spinon excitations shown in Fig. 2,

$$N_s(\omega) = \frac{1}{\pi}\frac{\partial \delta_s}{\partial \omega} = \frac{\gamma}{\pi|\omega|\left[\ln\left(\frac{T_K}{\omega}\right)\right]^2}. \tag{29}$$

As a results the conventional Fermi-liquid expansion of the phase shift can not be carried out.

Another essential feature of the Nozières Fermi-liquid approach, is the assumption of adiabaticity—that the excitations of the interacting system can be mapped onto the excitations of a corresponding noninteracting impurity problem. Since the interacting and noninteracting systems contain the same quasiparticles, the difference between the two situations can only be due to scattering by a one-particle potential.

We are thus lead to ask whether there is adiabaticity in the UKM. In light of the above observation, we can phrase the question in an alternative manner—is there any noninteracting scattering potential that can give rise to the observed energy-dependent spinon phase shift? In a conventional impurity scattering problem, the scattering potential and the phase shift are related by the relation

$$\delta(\omega) = \tan^{-1}[-\pi V(\omega)\rho], \tag{30}$$

where $V(\omega)$ is the bare scattering potential at energy ω,[29] so that

$$V(\omega) = -\frac{1}{\pi\rho}\tan\delta(\omega). \tag{31}$$

In the Nozières expansion, we have

$$\delta = \frac{\pi}{2} + \alpha\omega \tag{32}$$

so that the corresponding potential is given by

$$V(\omega) = \frac{1}{\pi\rho\alpha}\frac{1}{\omega}. \tag{33}$$

A $1/\omega$ phase shift indicates the formation of single bound-state inside the Kondo resonance. In fact, the scattering potential (33) is the same as that of a simple resonant level model with a resonance of width $\Gamma \sim \alpha^{-1} \sim T_K$ positioned right at the Fermi energy, $\epsilon_d=0$, implying that we can indeed map the excitations of the fluid onto a noninteracting Anderson impurity model.

If we now carry out the same procedure on the phase shift of the UKM, we find that

$$V^*(\omega) = \frac{1}{\pi\rho\gamma}\left[\ln\left(\frac{T_K}{\omega}\right)\right]\text{sgn}(\omega). \tag{34}$$

This singular elastic scattering potential can not be replaced by a simple scattering pole, but would require a singular distribution of noninteracting scattering resonances for its correct description. Thus the singular Fermi liquid of the underscreened model can not be obtained from the adiabatic evolution of a simple, noninteracting impurity model.

VI. CONCLUSION

The underlying mechanism for the singular behavior in the singular Fermi-liquid models is the slowness of approach of the coupling to the fixed point. In this respect also the ferromagnetic Kondo model is a SFL with a particularly simple fixed point.[30] Another example to study in detail would be fixed points of screened multichannel Kondo models.

Finally, in the spirit of the Nozières picture, Affleck and Ludwig have analyzed the low energy behavior of Kondo impurity models in the framework of boundary conformal field theory (BCFT).[31] In this method, the various fixed points correspond to different conformally invariant boundary conditions. Although the overscreened and exactly screened Kondo models were analyzed in great detail, the UKM were never properly examined, and it is still an open question how to incorporate the SFL behavior of the UKM we have found in terms of BCFT.

Let us finally make a remark on our distinction between non-Fermi-liquid and Fermi-liquid models. In this paper we defined an impurity model to be of non-Fermi-liquid type whenever at $T=0$ temperature a conduction electron at the Fermi energy can scatter in an inelastic way, i.e., by changing its environment in course of the scattering process. Depending on the way one tries to measure this inelastic scattering, one may, however, get rather different answers. The

Aharonov-Bohm (AB) interference mentioned before is, e.g., always destroyed by the inelastic scattering defined in this paper, and it provides therefore a reliable way to distinguish between singular Fermi liquids and non-Fermi-liquids: In a non-Fermi-liquid the AB interference is destroyed even at $T=0$ temperature, while in a singular Fermi liquid it is not.

However, we may sometimes get different results if we try to use weak localization to detect inelastic scattering. In the rather special case of the Hamiltonian, (13), e.g., the AB oscillations are trivially destroyed even at $T=0$ temperature, however, the weak localization corrections are not. This simple but important example should alert us that various ways to measure inelastic scattering processes may be inequivalent.

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