Magnetic phases in the one-dimensional Kondo chain on a metallic surface

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We study the low-temperature properties of a one-dimensional spin-1/2 chain of magnetic impurities coupled to a (normal) metal environment by means of anisotropic Kondo exchange. In the case of easy-plane anisotropy, we obtain the phase diagram of this system at \( T = 0 \). We show that the in-plane Kondo coupling destabilizes the Tomonaga-Luttinger phase of the spin-chain, and leads to two different phases: i) At strong Kondo coupling, the spins in the chain form Kondo singlets and become screened by the metallic environment, and ii) At weak and intermediate Kondo coupling, we find a novel dissipative phase characterized by diffusive gapless spin excitations. The two phases are separated by a quantum critical point of the Wilson-Fisher universality class with dynamical exponent \( z \approx 2 \).

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I. INTRODUCTION

Magnetic structures of atomic size provide the smallest solid state systems in which it is possible to store (quantum) information. The possibility to build and manipulate such atomic-scale magnetic structures has been demonstrated in recent experiments using scanning tunneling microscopy (STM), a fact that paves the way for the realization of spin-devices of nanoscopic size.

Besides the interest in applications, magnetic systems at the nanoscale constitute an excellent playground to address fundamental questions in condensed matter physics. For instance, magnetic impurities inside a metallic host have been found in STM experiments to display the Kondo effect. This effect, consisting in the spin-compensation of a localized magnetic moment by conduction electrons in the metal, is one of the most paradigmatical phenomena in many-body physics. On the other hand, magnetic atoms inside a metal can interact non-locally via the electronic medium through the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange coupling, which is responsible for the magnetic properties of many heavy-fermion materials and for the giant-magneto-resistance effect in layered magnetic heterostructures. Direct evidence of RKKY interaction at the atomic scale (i.e., among pairs of magnetic Fe or Co atoms) has been reported recently in STM experiments. Due to the ability to control the distance between magnetic atoms using the STM tip, the RKKY interaction can be, in principle, tuned from ferromagnetic to antiferromagnetic, and this oscillating feature has been clearly revealed in recent experiments showing spin-polarized STM maps.

By depositing atoms one by one, STM also enables to build magnetic structures where the dimensionality is gradually changed from the zero-dimensional limit to the one-dimensional (1D) case. In particular, linear arrays of up to 10 magnetic Mn atoms have been recently built and analyzed with STM and inelastic electron tunnel spectroscopy (IETS). Theoretically, low-dimensional magnetic systems are of interest due to the prominent effect of quantum fluctuations, which inhibit magnetic order and, at low temperatures, lead to quantum phases with exotic properties.

Motivated by the experimental progress described above, in this work we study a one-dimensional (1D) chain of spin \( S = 1/2 \) magnetic atoms (i.e. Kondo impurities) embedded in (or, rather, deposited on) a host such like a metallic surface (cf. Fig 1). The magnetic atoms are coupled to each other and to the metallic host by means of an anisotropic exchange. The anisotropic coupling between the magnetic atoms may be regarded as a consequence of, e.g., a Dzyaloshinskii-Moriya interaction resulting from the spin-orbit coupling in the host. From a different perspective, this system also provides a realization of a 1D dissipative system. Indeed, the inter-
play between quantum fluctuations and dissipation can have important consequences for the phase diagram of a system. Examples of other physical realizations of 1D dissipative systems can be found in e.g. resistively shunted 1D Josephson junctions arrays, Tomonaga-Luttinger liquids coupled to dissipative baths, superconducting wires coupled to diffusive metals, and 1D ultra-cold atom gases embedded in a Bose-Einstein condensate.

Using a host of analytical methods, which include bosonization and renormalization group methods, we investigate the effects of the metallic environment on the spin chain. At $T = 0$, we predict that the Tomonaga-Luttinger liquid (TLL) phase of the impurity spin chain will be destabilized by the (in-plane) Kondo interaction, $J_{K}^\perp$, with the metallic host. Turning on $J_{K}^\perp$, yields a dissipative phase, whose ground state exhibits long-range order (LRO) of the in-plane magnetization. Upon increase of $J_{K}^\perp$, we predict a quantum phase transition towards a disordered Kondo-singlet phase, where the spins of 1D chain are locally screened by the host electrons, and the LRO along the chain is destroyed.

This work is organized as follows. In Section II we present the model for the anisotropic spin chain coupled to a normal metal, in Section III we show our main results, divided into weak-coupling (Sec. IIIA) and strong-coupling (IIIB) treatment of the Kondo Hamiltonian, in Section IV we present a summary and conclusions, and finally, Section V is an Appendix.

II. MODEL

The Hamiltonian of the spin-chain system embedded in a metallic host can be split into three terms,

$$\mathcal{H} = \mathcal{H}_C + \mathcal{H}_F + \mathcal{H}_K,$$

(1)

where $\mathcal{H}_C = \sum_{i,j,n} J_n^{\alpha\beta} (ij) S_i^\alpha S_j^\beta$, describes the (static) interactions between the magnetic atoms in the chain, $\mathcal{H}_K$ accounts for the coupling of the chain to the metallic host, and $\mathcal{H}_F$ describes the host electrons. We shall not attempt to fully specify the microscopic origin of the exchange couplings, $J_n^{\alpha\beta} (ij)$, since we want to address a generic situation in which different contributions (i.e., RKKY, direct exchange, dipolar, etc.) may exist. However, we shall assume that the dominant exchange couplings are short-ranged. Thus, we consider the model:

$$\mathcal{H}_C = \sum_{j} \frac{J_H^\perp}{2} \left( \tilde{S}_{j+1}^+ \tilde{S}_j^- + \tilde{S}_j^+ \tilde{S}_{j+1}^- \right) + \sum_{j} D \tilde{z} \cdot \left( \tilde{S}_j \times \tilde{S}_{j+1} \right)$$

(2)

For definiteness, we assume here that the index $j$ runs along the $\tilde{x}$–axis (cf. Fig. 1). The last term in Eq. (2) is a Dzyaloshinskii-Moriya (DM) interaction, which results from the spin-orbit coupling of the electrons at the surface of the metallic host. The symmetry conditions for the DM interaction to exist are rarely met in the bulk of typical metals. However, for an impurity chain that lies on a metallic surface where inversion symmetry is broken, a DM interaction term is in principle expected.

The above spin-chain model, Eq. (2), can be mapped onto a 1D Heisenberg-Ising (XXZ) $S = 1/2$ chain by the following transformation:

$$S_j^\pm = e^{i\eta_j \tilde{S}_j^\pm},$$

(3)

$$S_j^z = \tilde{S}_j^z,$$

(4)

where $\eta = \tan^{-1}(D/\tilde{J}_H)$ ($0 \leq \eta \leq \pi/2$). Thus, Eq. (2) becomes:

$$\mathcal{H}_{XXZ} = \sum_{j} \frac{J_H^\perp}{2} \left( S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+ \right) + \tilde{J}_H S_j^z S_{j+1}^z,$$

(5)

with $\tilde{J}_H = (\eta \tilde{J}_H)/\cos \eta$ and $\tilde{J}_H = \tilde{J}_H$. Although the DM interaction in metallic surfaces is small (i.e., $D/\tilde{J}_H \ll 1$), it can dramatically affect the properties of the spin chain. In particular, if the initial impurity-chain Hamiltonian (2) is isotropic (i.e., $\tilde{J}_H = \tilde{J}$), the above transformation (3) maps it onto an XXZ spin chain with easy-plane anisotropy: $|\tilde{J}_H/\tilde{J}_H| = (\cos \eta)^{-1} > 1$. Therefore, from here on, we shall focus on the case of the XXZ spin chain with in-plane anisotropy. Under these assumptions, it is well known that the low-energy sector of Hamiltonian Eq. (5) maps onto the XY—model, whose spectrum is described in terms of spinon modes and exhibits power-law magnetic correlations.

The coupling between the XXZ chain and the metal is described by the following anisotropic Kondo exchange interaction:

$$\mathcal{H}_K = \sum_j \frac{1}{2} J_K^\perp S_j^z \left[ c_j^\dagger (R_j) c_j (R_j) - c_j^\dagger (R_j) c_j^\dagger (R_j) \right]$$

$$+ \frac{J_K^\perp}{2} e^{i\eta_j} S_j^+ c_j^\dagger (R_j) c_j (R_j) + H.c.,$$

(6)

where Eqs. (6) and (4) have been used. In (6) every spin $S_j$ in the chain is coupled to the fermionic spin-density of the bath. The operator $c_j^\dagger (R)$ creates an electron with spin projection $\sigma$ at position $\mathbf{R} = (x, y, z)$ in the metal, and for a chain site $\mathbf{R}_j = (j a_0, 0, 0)$ with $a_0$ the lattice parameter of the impurity chain. We also assume an anisotropic Kondo interaction with in-plane anisotropy $|\tilde{J}_K/\tilde{J}_K^\perp| > 1$.

Finally, the dynamics of the electrons in the metallic host is described in terms of Landau quasi-particles:

$$\mathcal{H}_F = \sum_{\mathbf{k},\sigma} \epsilon_k c_{\mathbf{k}\sigma}^\dagger (\mathbf{k}) c_{\mathbf{k}\sigma} (\mathbf{k}) + \cdots,$$

(7)

where $\epsilon_k$ is the electron dispersion and $c_{\mathbf{k}\sigma} (\mathbf{k})$ annihilates one electron with quantum numbers $\mathbf{k}$ and spin projection $\sigma$. The dots in Eq. (7) stand for additional terms,
such as spin-orbit interactions, whose form needs not be specified.

The physics of model in Eq. (1) can be understood in part by noting that, whereas the Heisenberg interactions favor correlations along the spin chain, the Kondo coupling tends to screen the impurity-spins at every site, thus promoting a non-magnetic ground state. However, as we will show further below, this intuitive picture where the Heisenberg and Kondo interaction compete is not always correct. Indeed, the interplay between Heisenberg and Kondo interaction is subtle and leads to a counter-intuitive cooperation effect in a certain regime of parameters, resulting in a non-trivial phase diagram at $T = 0$ (cf. Fig. 3 below).

Note that our model significantly differs from previous approaches to the 1D Heisenberg-Kondo model or the 1D Kondo-lattice model. Those models assumed an entirely 1D situation in which the 1D spin-chain is coupled to a 1D electron gas which acts as a host. However, our model is closer to the experimental situations described in Sec. I, where the spin chain is embedded in or lies on a higher-dimensional metallic host.

In the following, we focus on the critical properties of model Eq. (1) at low-energies and for different regimes of parameters $J_{H}, J_{K}$ and $J_{K}$. Throughout we shall use units where $\hbar = 1$.

### III. RESULTS

#### A. Weak coupling scaling analysis

When the Heisenberg coupling $J_{H}$ is much larger than $J_{K}$ and $J_{K}^{2}$, it is a good starting point to treat the Kondo coupling, $\mathcal{H}_{K}$ (cf. Eq. (6)), as a small perturbation to the isolated spin-chain Hamiltonian, $\mathcal{H}_{XXZ}$ (cf. Eq. (5)). In this case, Hamiltonian (5) can be studied within the framework of Abelian bosonization, which allows to map it onto the continuous XY Hamiltonian

$$\mathcal{H}_{XXZ} = \frac{1}{2\pi} \int dx \left[ \frac{u}{K} (\nabla \Phi)^{2} + u K (\nabla \Theta)^{2} \right] + \ldots \quad (8)$$

Here $\Theta(x)$, $\Phi(x)$ are conjugate canonical fields obeying the usual commutation relations $[\Theta(x), \nabla \Phi(x')] = i\pi \delta(x - x')$. These fields are continuous in the scale of $a_{0}$, the original lattice spacing in the chain, and are related to the original spin operators by

$$S_{j}^{\pm} = a_{0} S_{j}^{\pm}(x_{j}) = \frac{e^{\mp i\Theta(x_{j})}}{\sqrt{2\pi}} \left[ e^{i x_{j} \pi / a_{0}} + \cos 2\Phi(x_{j}) \right],$$

$$S_{j}^{z} = a_{0} S_{j}^{z}(x_{j}) = -\frac{a_{0}}{\pi} \nabla \Phi(x_{j}) + \frac{e^{i x_{j} \pi / a_{0}}}{\sqrt{\pi}} \cos 2\Phi(x_{j}),$$

where $x_{j} = ja_{0}$ is the position of the $j$-th spin. The model describes 1D spinon excitations in the transverse direction propagating with velocity $u$, and is parametrized by the dimensionless Luttinger parameter $K \equiv \frac{\pi}{2} \arccos \left( -J_{H} / J_{K} \right)^{-1}$, which determines the decay of the correlation functions in the chain, e.g., $\langle S^{+}(x) S^{-}(0) \rangle \sim |x|^{-1/2K}$. The isotropic Heisenberg model is recovered for the particular value $K = 1/2$. As discussed above, in this work we focus on the regime of easy-plane anisotropy, which corresponds to the condition that $K > 1/2$. The ellipsis in (8) stands for additional perturbations, such as the sine-Gordon term $\sim \cos 4\Phi(x)$, which are irrelevant in the renormalization-group (RG) sense for $K > 3/2$ and will be neglected.

The continuum limit of the Kondo Hamiltonian, Eq. (6), reads:

$$\mathcal{H}_{K} = \int dx \frac{J_{K}}{k_{F}} S_{j}^{z} \left( x \right) S_{j}^{z} \left( x \right) + \int dx \frac{J_{K}}{2k_{F}} \left[ \cos q_{DM} \pi a_{0} S_{j}^{z} \left( x \right) + \text{H.c.} \right], \quad (11)$$

where we have defined $q_{DM} \equiv \eta / a_{0}$ and introduced the factors of the Fermi momentum $k_{F}$ in order for the Kondo couplings to have dimensions of energy. We have also defined the spin-density operator of the host electrons:

$$s_{a}^{z}(\mathbf{R}) \equiv \sum_{\sigma,\sigma'} c_{\sigma}(\mathbf{R}) \left[ \frac{1}{2} \sigma_{a}^{z} \right]_{\sigma,\sigma^{'}} c_{\sigma^{'}}(\mathbf{R}), \quad (12)$$

with $\sigma^{a}$ ($a = x, y, z$) the Pauli matrices. From Eqs. (10) and (11) we note that the operator $\nabla \Phi(x)$ couples to the uniform component of the spin-density in the electron-gas $s_{a}^{z}(x) \equiv s^{z}(x)$, and the operator $\cos 2\Phi(x)$ couples to the staggered component $s_{a}^{z}(x) = e^{i2\pi a_{0}} s^{z}(x)$. On the other hand, the operator $e^{-i\Theta(x)}$ couples to the staggered magnetization $s_{a}^{z}(x) = e^{i2\pi a_{0}} s^{z}(x)$. These contributions to Eq. (11) have different scaling dimensions, and we treat them independently in the following analysis.

Next, we assess the stability of the Tomonaga-Luttinger (TLL) phase, which is described by Hamiltonian in Eq. (5). To this end, we have considered the leading order corrections to the free energy per unit length of impurity spin-chain. The technical details of this calculation can be found in Appendix A. We shall not pursue the stability analysis beyond the leading order in this work, as our focus here is on the phase diagram in the $K > 1/2$ (i.e., $J_{H} > J_{K}$) regime, for which, as the following discussion demonstrates, there is only one relevant Kondo coupling, namely $J_{K}$. A more complete analysis will be reported elsewhere. To leading order in the Kondo couplings, for temperatures $T \ll J_{H}^{2}$, we find:

$$\frac{\Delta F}{L} = g_{z,a}^{2} \frac{KA_{z}^{2}}{2^{4}k_{F}a_{0}^{2}\pi} T^{3} + g_{x,a}^{2} \frac{A_{x}^{2}}{2^{4}k_{F}a_{0}^{2}\pi} \left( \frac{\pi a_{0}}{u} \right)^{2K} T^{1+2K}, \quad (13)$$

$$+ g_{z,a}^{2} \frac{A_{z}^{2}}{2^{4}k_{F}a_{0}^{2}\pi} \left( \frac{\pi a_{0}}{u} \right)^{1/2K} T^{1+1/2K}, \quad (14)$$

$$+ g_{y,a}^{2} \frac{A_{y}^{2}}{2^{4}k_{F}a_{0}^{2}\pi} \left( \frac{\pi a_{0}}{u} \right)^{1/2K} T^{1+1/2K}, \quad (15)$$
where $L \to +\infty$ is the impurity chain length and the dimensionless couplings $g_{z,u} = \frac{J_{K}^{z}}{v^2 k F}$, $g_{z,s} = \frac{J_{K}^{z}}{v k F}$ and $g_{\perp,s} = \frac{J_{K}^{\perp}}{v k F}$ have been introduced; $A_{z}^{u}$, $A_{z}^{s}$ and $A_{\perp}^{z}$ are non-universal numerical coefficients. The stability of the TLL phase with respect to the perturbation $\mathcal{H}_{K}$ can be now assessed by comparing the scaling with temperature of $\Delta F$ and the free energy of the spin-chain chain, $F_{0}$, when decoupled from the environment, which behaves as $\sim F_{0} \sim T^{2}$. Thus we look for divergences in the perturbative corrections to $\Delta F/F_{0}$ as the temperature is gradually decreased towards the ground state (i.e. $T = 0$). From (15), it can be seen that the term $\propto g_{\perp,s}^{2}$ yields a divergent contribution to $\Delta F/F_{0}$, which signals an instability of the TLL phase.

To make contact with the renormalization group (RG), we shall define the effective couplings $g_{z,u}(\ell) \equiv g_{z,u} e^{-(1/2)\ell}$, $g_{z,s}(\ell) \equiv g_{z,s} e^{((1/2-K)\ell)}$ and $g_{\perp,s}(\ell) \equiv g_{\perp,s} e^{((1/2-1/4K)\ell)}$, where $\ell \equiv \ln(\Lambda_{0}/T)$ and $\Lambda_{0} \sim J_{K}^{z}$. This is a high-energy cutoff for the effective low-energy description of the spin-chain in terms of Eq. (8). Decreasing the temperature a bit towards the ground state (i.e. $T = 0$) can regarded as an infinitesimal change of $\ell \to \ell + \delta \ell$, and the corresponding change (“flow”) of the effective couplings can be described by the following set of differential equations:

$$
\frac{dg_{z,u}(\ell)}{d\ell} = -\frac{1}{2} g_{z,u}(\ell),
$$

$$
\frac{dg_{z,s}(\ell)}{d\ell} = \frac{1}{2} (1 - 2K) g_{z,s}(\ell),
$$

$$
\frac{dg_{\perp,s}(\ell)}{d\ell} = \frac{1}{2} \left( 1 - \frac{1}{2K} \right) g_{\perp,s}(\ell).
$$

Alternatively, we can regard these equations as describing the change in effective (dimensionless) couplings of an equivalent (coarse-grained) system with a reduced high-energy cutoff $\Lambda(\ell) = e^{-\ell} \Lambda_{0}$. This interpretation means that for in-plane anisotropy where $K > 1/2$, the couplings $g_{z,u}(\ell)$ and $g_{z,s}(\ell)$ decrease as the system is coarse-grained by integrating out the high-energy degrees of freedom and become irrelevant (in the RG sense). In other words, the terms in $\mathcal{H}_{K}$ proportional to those couplings yield subleading corrections and therefore can be neglected as $T \to 0$. On the other hand, $g_{\perp,s}(\ell)$ is a relevant (in the RG sense) perturbation, which, as $T \to 0$ yields an dominant correction and destabilizes the TLL phase of the spin-chain described by Eq. (8). Note that both $g_{z,s}(\ell)$ and $g_{\perp,s}(\ell)$ have the same scaling dimension at the Heisenberg point ($K = 1/2$), where they are marginally relevant, and a higher order perturbative analysis is required to fully assess the stability of the TLL phase.

Finally, as explained in the Appendix A, in the derivation of Eq. (15) we have assumed that the host is a normal metal. This means that it exhibits an ohmic spectrum of magnetic excitations over a broad range of momentum transfer along the spin-chain direction. Alternatively, this situation can be mimicked by an infinite set of fermionic baths, each bath being locally coupled to only one impurity spin (cf. Fig. 2), which yields a local (i.e. momentum independent) ohmic spin response: e.g. $\chi(x,\tau)^{z} \sim \delta(x)/\tau^{2}$. As it will be discussed in the next section, this model allows us to treat the relevant Kondo coupling $J_{K}^{z}$ in a non-perturbative way. In particular, it captures the important (non-perturbative) feature that the magnetic moment of the impurities will be fully screened by the metallic environment at large $J_{K}^{z} \gg J_{H}^{z}$. In the above analysis, the need for a non-perturbative treatment is evidenced by the fact that even an infinitesimal value of $J_{K}^{z}$ will destabilize the TLL phase for in-plane anisotropy ($K > 1/2$). However, different from the single-impurity Kondo problem, we will see below that the RG flow does not proceed from the TLL phase into a strong coupling Kondo-screened phase in a straightforward manner, but rather, another phase of dissipative nature intervenes between the TLL and the Kondo phase.

### B. Strong coupling analysis

1. Derivation of an effective 1D model

As mentioned before, when $J_{K}^{z}$ flows to strong coupling, the perturbative RG approach used in the previous Section IIIA is no longer valid, and we need to study the physical properties of the spin chain in a different way. The approach used in this section is motivated by the following arguments: i) the analysis made in the previous section indicates that the most relevant coupling of the spin-chain to the host stems from a local kind of coupling to the metallic host and, ii) even at strong-coupling, for a two- or three-dimensional host, the interference of two Kondo screening clouds belonging to spins located at a distance $d$ decays rapidly when $d$ is of the order of a few Fermi wavelengths ($\sim x$) i.e. $\sim k_{F}^{-1})$. Experimentally, this is confirmed by the behavior of the STS Fano line shapes in magnetic Co atoms deposited on Cu(100) and separated by distances $d > 10 \AA$, which are identical to the single-impurity STS line shapes.

These arguments suggest to perform an approximation on Hamiltonian $\mathcal{H}_{F}$, assuming a set of independent fermionic baths (i.e., semi-infinite 1D chains, cf. Fig. 2) coupled to each single spin in the chain $S_{i}$

$$
\mathcal{H}_{F} \simeq -t \sum_{ij} c_{i,j-1,\sigma}^{\dagger} c_{i,j,\sigma} + \text{H.c.}
$$

Here, the index $i$ runs along the $\hat{x}$-axis. Eq. (19) is a valid description in the limit $k_{F}a_{0} \gg 1$, consistent with the local limit of Sec. IIIA. Note that in this local-bath approximation, since the fermionic chains are not connected between them, the indirect RKKY exchange interaction mediated by conduction electrons is not dynamically generated at second order in the Kondo coupling and it is necessary to incorporate it explicitly in the
Heisenberg exchange parameters $J_H^\perp, J_H^\parallel$. In the following, we assume that both $J_H^\perp, J_H^\parallel$ already contain these corrections.

The advantage of the independent-bath approximation Eq. (19) is that it allows to use powerful analytical methods which have been applied successfully to describe the single Kondo-impurity problem. In the following, we implement the Abelian bosonization approach to the Kondo problem [15]. To avoid confusion with the previous Sec. [11], note that here bosonization is implemented to describe the fermionic 1D chains, and not the spin chain. At low energies the Hamiltonians $\mathcal{H}_F$ and $\mathcal{H}_K$ become in the bosonic representation[20]

$$\mathcal{H}_F = \sum_{i,\nu=\{c,s\}} \frac{v_F}{4\pi} \int_{-\infty}^{\infty} dy \left( \nabla \phi^R_{i,\nu}(y) \right)^2,$$

$$\mathcal{H}_K = \sum_{i} -\frac{2\delta_s}{\pi\rho_0} \nabla \phi_{i,0}(0) \sqrt{2\pi} + \frac{J_K b}{2} \left[ S_i^+ e^{-i\sqrt{2} \phi_{i,0}(0)} + S_i^- e^{i\sqrt{2} \phi_{i,0}(0)} \right],$$

where the chiral fields $\phi^R_{i,\nu}(y), \phi^I_{i,\nu}(y)$ obey the commutation relations $[\phi^R_{i,\nu}(y), \phi^I_{i,\nu}(y')] = i\pi\text{sign}(y-y') \delta_{i',i} \delta_{\nu',\nu}$, and are related to charge and spin density-fluctuations through the relations $\rho_i(y) = \sum_{\nu} \phi^R_{i,\nu}(y) R_{i,\nu}(y) = -\frac{1}{\pi} \nabla \phi^I_{i,\nu}(y)$ and $m_i(y) = \sum_{\nu} \phi^I_{i,\nu}(y) R_{i,\nu}(y) = -\frac{1}{\pi} \nabla \phi^R_{i,\nu}(y)$, respectively. In Eq. (20) $v_F$ is the Fermi velocity, and in Eq. (21) $\delta_s = \tan^{-1}(\pi\rho_0 J_K b_0/4)$ is the scattering phase-shift associated with the potential $J_K \delta_s^2/2$, $\rho_0 = (2\pi v_F)^{-1}$ the conduction electron density of states at the Fermi energy, and $b_0$ the lattice parameter in the fermionic chain. For simplicity we assume these parameters to be identical for all chains. We then introduce the (Emery-Kivelson) unitary transformation[16]

$$\mathcal{U} = \exp \left[ -i\gamma \sum_{i} S_i^\dagger \phi^R_{i,0}(0) \right],$$

under which the bosonic field $\nabla \phi^R_{i,0}(y)$ and the spin operator $S_i^\dagger$ transform as

$$\mathcal{U} \nabla \phi^R_{i,0}(y) \mathcal{U}^\dagger = \left[ \nabla \phi^R_{i,0}(y) + \delta(y) 2\pi \gamma S_i^z \right],$$

$$\mathcal{U} S_i^\dagger \mathcal{U}^\dagger = S_i^+ e^{i\gamma \phi^I_{i,0}(0)}.$$  

Upon this transformation, the model Hamiltonian, Eq. (1) transforms as $\mathcal{H} = \mathcal{U}^\dagger \mathcal{H} \mathcal{U} = \mathcal{H}_c + \mathcal{H}_K + \mathcal{H}_{XXZ}$, with

$$\mathcal{H}_c = \mathcal{H}_c, $$

$$\tilde{\mathcal{H}}_K = \sum_{i} -\frac{2\delta_s}{\pi\rho_0} \nabla \phi_{i,0}(0) \sqrt{2\pi} + \frac{J_K b}{2} \left[ S_i^+ e^{-i\sqrt{2} \gamma \phi^I_{i,0}(0)} + \text{H.c.} \right],$$

$$\tilde{\mathcal{H}}_{XXZ} = \sum_{i} J_{XXZ} S_i^z S_{i+1}^z + \frac{J_{XXZ}}{2} e^{i\gamma[\phi^I_{i,0}(0)-\phi^I_{i+1,0}(0)]} S_i^+ S_{i+1}^- + \text{H.c.},$$

where we have defined $\delta_s = \delta_s - \pi\gamma/2\sqrt{2}$. Note that in the transformed representation, the quantum dynamics of the bath [represented by the chiral field $\phi^I_{i,0}(0)$] appears explicitly in the Heisenberg term $\sim J_K \left( S_i^+ S_{i+1}^+ e^{i\gamma[\phi^I_{i,0}(0)-\phi^I_{i+1,0}(0)]} + \text{H.c.} \right)$. Physically, this means that the Heisenberg interaction is now ‘dressed’ by the spin-density fluctuations of the electron gas. Note that the independent-bath model (19) is crucial to implement bosonization along the chains, and to put these ideas on a clear mathematical framework.

Up to now the parameter $\gamma$ appearing in Eq. (22) remains completely arbitrary. We now set $\gamma = \sqrt{2}$ in Eqs. (26) and (27), and the transformed Hamiltonians simplify to

$$\tilde{\mathcal{H}}_K = \sum_{i} -\frac{2\delta_s}{\pi\rho_0} \nabla \phi_{i,0}(0) \sqrt{2\pi} + \frac{J_K}{2\pi} S_i^z,$$

$$\tilde{\mathcal{H}}_{XXZ} = \sum_{i} J_{XXZ} S_i^z S_{i+1}^z + \frac{J_{XXZ}}{2} e^{i\gamma[\phi^I_{i,0}(0)-\phi^I_{i+1,0}(0)]} S_i^+ S_{i+1}^- + \text{H.c.},$$

where now $\tilde{\mathcal{H}}_K$ is equivalent to the spin-boson model with Ohmic dissipation[21,22] with $\tilde{\delta}$ related to the dissipative parameter $\alpha$ in the context of macroscopic quantum coherence through $\alpha = (2\tilde{\delta}/\pi)^2$, and with the in-plane Kondo interaction playing the role of a magnetic field along the $x$−axis $h_x = -J_K^\perp/2\pi$. That model describes a quantum phase transition from a phase with a “frozen” spin state (either $S_i^z = +1/2$ or $S_i^z = -1/2$) for $\alpha > 1$, to a phase with an ‘untrapped’ spin state for $\alpha < 1$, where spin-flips induced by $S_i^z$ proliferate. The strong-coupling
regime of the single-impurity Kondo Hamiltonian therefore corresponds to this last case, where (not too close to the transition) the Kondo temperature is

$$T_K \propto J_K^1 \left( \frac{J_K h_0}{\sqrt{\beta}} \right)^{\alpha/(1-\alpha)}.$$  \hspace{1cm} (30)

The special case $\alpha = 0$ (i.e., $\delta_s = 0$) was analyzed in Ref. [27] and represents a particular limit where $\hat{\mathcal{H}}_K$ can be diagonalized in the eigenbasis $|\pm\rangle_i$ of the operator $S_i^z$. Note that the condition $\delta_s = 0$ implies that the original phase-shift is $\delta_s = \pi/2$, corresponding to the unitary limit $J_K b/\sqrt{\beta} \to \infty$. Unfortunately, the unitary limit is not consistent with the well-known local Fermi-liquid description of the strong-coupling Kondo fixed point. 

Intuitively, in the limit $\delta_s = 0$ the coupling to the bath vanishes and $\hat{\mathcal{H}}_K$ reduces to a Zeeman Hamiltonian, which is not equivalent to the Kondo problem. However, as shown by Kotliar and Si, a physically correct description of the strong-coupling limit is recovered by performing second-order perturbation expansion in $\delta_s$. Physically, this is equivalent to reintroducing the coupling to the bath.

In the case of plane-anisotropy, the Kondo couplings satisfy $J_K^2 > J_K^1$. This implies that in order to perform an expansion around the point $\delta_s = 0$, the microscopic parameters of the model should be in a regime such that strictly speaking the use of bosonization is not justified (i.e., the interactions are of the order or bigger than the Fermi energy). However, since this approach has been shown to successfully capture qualitatively the main features of the strong-coupling Kondo fixed point, we expect our approach to be correct only at a qualitative level.

An effective low-energy Hamiltonian valid near $\delta_s = 0$, and for the case where the Kondo interaction dominates over Heisenberg exchange, i.e., $J_K^1 \gg \{J_H^1, J_H^2\}$ can be obtained expanding Eq. (28) at order $\delta_s^2$ and projecting onto the lowest energy level on each site $|\pm\rangle_i$,

$$\hat{\mathcal{H}}'_K \equiv P_- \hat{\mathcal{H}}_K P_- = -\sum_i \delta_s^2 \frac{2\pi}{\beta_0} J_K^1 \left( \nabla \phi_{i,s}^R (0) \right)^2.$$  \hspace{1cm} (31)

where we have introduced the projector operator on the subspace spanned by $|\pm\rangle_i$, i.e., $P_- \equiv \prod_i \left( |\pm\rangle_i \langle \pm| \right)_i$, and where we have neglected a constant term $J_K^2/2\pi$. The effective magnetic field $h_x$ opens a gap of size $\Delta = 2h_x$ in the spin excitation spectrum and consequently the spin degrees of freedom are “frozen” in the lowest energy configuration $|\pm\rangle_i$. In contrast, spin-density fluctuations in the bath remain gapless and their dynamics becomes dominant at low energies. Projecting $\hat{\mathcal{H}}_{XXZ}$ onto this basis yields

$$\hat{\mathcal{H}}'_{XXZ} \equiv P_- \hat{\mathcal{H}}_{XXZ} P_- = \sum_i J_H^1 \frac{2}{4\pi} \cos \sqrt{2} \left[ \phi_{i,s}^R (0) - \phi_{i+1,s}^R (0) \right].$$  \hspace{1cm} (32)

In this representation, the Heisenberg term $J_H^1 (S_i^+ S_{i+1}^+ + \text{h.c.})$ induces an effective interaction between neighboring baths, encoded in the term $\cos \sqrt{2} \left[ \phi_{i,s}^R (0) - \phi_{i+1,s}^R (0) \right]$. This is an important result in our work, complementary to the situation analyzed in Sec. [32] where the opposite limit $J_H^1 \gg J_K^1$ was studied. In that case, the bath was integrated out, and we studied the stability of the Tomonaga-Luttinger liquid phase to leading order in perturbation theory. Here, we do just the opposite: we keep the degrees of freedom of the bath and eliminate the spin degrees of freedom.

Although a general derivation of an effective low-energy model (i.e., for an arbitrary value of $\gamma$), is beyond the scope of the present work, it is worth noting that the effective coupling between fermionic baths that appears in (32) is a physical feature that goes beyond our particular derivation for $\gamma = \sqrt{2}$. This can be understood using, for example, similar arguments as those leading to the Nozières’ local Fermi-liquid. Indeed, when $J_K^1 \gg J_H^1$, a natural approach is to start from the Kondo singlets at neighboring sites $i$ and $i + 1$, i.e., $|G_i\rangle$ and $|G_{i+1}\rangle$ respectively, where $|G_i\rangle = \langle |0\rangle_i |c_{0,i}^+ \rangle - |\psi_i\rangle |c_{1,i}^+ \rangle \big) / \sqrt{2}$. The perturbation $H' = -t \sum_{i\ell=i,i+1} \langle c_{\ell,i}^+ c_{0,i} \rangle + \text{h.c.}$ acting on these neighboring singlets produces virtual excitations to the $\nu_0 = 1$ triplet subspace, at order $(t/J_K^1)^2$ on each one of them. Eventually, the Heisenberg interaction $J_H^1 (S_i^+ S_{i+1}^+ + \text{h.c.})$ restores the initial singlet ground states $|G_i\rangle$ and $|G_{i+1}\rangle$ and, as a net result, virtual processes generate an effective spin interaction $\sim (\gamma/J_K^1)^2 \left[ c_{1,i}^+ c_{i+1}^+ \right]$ between the second sites in the chains $i$ and $i + 1$. Bosonizing this induced effective interaction yields a term of the form $\sim \cos \sqrt{2} \left[ \phi_{i,s}^R (0) - \phi_{i+1,s}^R (0) \right]$, analogous to Eq. (32).

Next we can proceed to derive an effective 1D model, which first proceeds by the integrating out of the modes $\phi_{i,s}^R (y)$ for $y \neq 0$. This can be done exactly using the functional integral representation of the partition function, and generates a term of the form $\sim \cos \gamma \nabla \phi_i$ in the effective action, which stems from the (ohmic) dissipation induced by the coupling to local bath (cf. Refs. [16,11] for details). The resulting Euclidean action of the system reads:

$$S' = S_0' + S_H',$$  \hspace{1cm} (33)

$$S_0' = \sum_i \left[ \int_0^\beta d\tau \frac{|\omega_m|}{4\pi \gamma} \left| \varphi_1 (i \omega_m) \right|^2 + \int_0^\beta d\tau \left( \frac{\partial_\tau \varphi_1 (\tau)}{2\pi E_0} \right)^2 \right]$$  \hspace{1cm} (34)

$$S_H' = \int_0^\beta d\tau \frac{J_H^1}{4\pi} \cos \left[ \varphi_1 (\tau) - \varphi_i (\tau) \right],$$  \hspace{1cm} (35)

where we have defined the more compact notation for local field $\varphi_i \equiv \sqrt{2} \phi_{i,s}^R (y = 0)$, and where we have used the equation of motion of chiral fields, i.e., $\partial_\tau \varphi_i - iv_F \nabla \varphi_i = 0$ to express $\nabla \varphi_i$ in terms of $\partial_\tau \varphi_i$. In addition, in (33) we...
have defined the parameter

$$E_0 \equiv \frac{J_K^1}{2\delta_s^2},$$  \hfill (36)$$

where the singularity at $\delta_s = 0$ is a consequence of the unphysical unitary limit mentioned above.

Note that the effective model Eq. (33) is formally equivalent to the action of a 1D Josephson-junction array with local Ohmic dissipation, with $\varphi_i$ the phase of the superconducting parameter order at site $i$, $J_{ij}$ the Josephson coupling and $E_0$ the charging energy with respect to the ground state. It can also be brought to a form equivalent to a 1D O(2) dissipative quantum rotor model if we write it in terms of $N_i$, $H_0$ and to a form equivalent to a 1D O(2) dissipative quantum rotor model if we write it in terms of $N_i$, $H_0$, $J_{ij}$ and $E_0$.

To appreciate the physical consequences of the effective model in Eq. (33), we concentrate on the transverse spin correlation function $C^{++}(n, \tau) \equiv \langle T_{\tau} S_{i+n}^{\perp} S_i^{\perp} (0) \rangle$. In the transformed representation, this correlation is evaluated as (cf. Appendix B) $C^{++}(n, \tau) = \langle T_{\tau} e^{i\varphi_{i+n}(\tau)} e^{-i\varphi_i(0)} \rangle$. Near the strong-coupling singlet-impurity Kondo limit $J_K^1 \gg \{ J_H^1, J_H^2 \}$, we obtain the result (cf. Eq. [B14]) $C^{++}(0, \tau) \sim \tau^{-2}$, as expected for the local Fermi-liquid description of the Kondo problem. \[73\]

This slow decay is a consequence of the ohmic dissipation term $\sim |\omega_m|$ in Eq. (34), inherited from the dynamics of the semi-infinite fermionic chain. This behavior is consistent with the strong-coupling Kondo picture where, at long times, the spin degrees of freedom are merged with those of the fermion bath. On the other hand, the exponentially decaying non-local correlation [cf. Eq. (B15)]

$$C_{++}(n, 0) = \frac{e^{-n/\xi_c}}{2n+1},$$  \hfill (37)$$

with $\xi_c \equiv 1/\ln \left( \frac{E_0}{\tau_0^2} \right)$, the correlation length, indicates that the spins are not spatially correlated beyond a distance $\xi_c$, supporting the idea that in this limit the spin chain realizes a disordered phase of nearly independent Kondo singlets.

2. Hubbard-Stratonovich decoupling and RG analysis of the effective $\psi^3$-theory

The properties and phases of action (33) can be investigated introducing an auxiliary bosonic field $\psi_i(\tau)$ to decouple the Heisenberg term $J_H^1$ (cf. e.g. Refs. [58–60])

$$\frac{J_H^1}{16} \sum_i \int_0^\beta d\tau \cos[\varphi_i(\tau) - \varphi_{i+1}(\tau)] \to \int_0^\beta d\tau \sum_{i,j} \psi_i^* (\tau) \left[ J^{-1} \right]_{ij} \psi_j (\tau) - \frac{1}{2} \int_0^\beta d\tau \sum_i \left[ \psi_i^* (\tau) e^{i\varphi_i(\tau)} + \psi_i (\tau) e^{-i\varphi_i(\tau)} \right],$$  \hfill (38)$$

where we have defined the matrix $\left[ J \right]_{ij} \equiv \frac{1}{32} J_H^1 (\delta_{i,j+1} + \delta_{i+1,j})$. Then, the partition function reads $Z = Z_0 \int D[\psi] e^{-S[\psi]}$, where

$$S[\psi] = \sum_{i,j} \int_0^{1/T} d\tau \psi_i^* (\tau) \left[ J^{-1} \right]_{ij} \psi_j (\tau) - \ln \left( \frac{1}{2} \int_0^{1/T} d\tau \psi_i^* (\tau) e^{i\varphi_i(\tau)} + \text{h.c.} \right),$$  \hfill (39)$$

is the effective action for the auxiliary field $\psi_i(\tau)$. Here, the notation $\langle \ldots \rangle_0$ means average with respect to the local action (34). A cumulant expansion of the last term in Eq. (39) to order $\psi_i^3$ yields

$$S[\psi] = \frac{T}{2N_i} \sum_q G^{-1}_0(q) |\psi_q|^2 + \frac{2}{4!} \sum_i \int_0^{1/T} d\tau |\psi_i(\tau)|^4,$$  \hfill (40)$$

where the compact notation $q = (k, \omega_m)$, with $\omega_m = 2\pi n T$ the bosonic Matsubara frequencies has been used, and where $N_i$ is the number of spins. Here we have defined the Gaussian propagator

$$G^{-1}_0(q) \equiv r + \frac{16}{J_H^1} k^2 + \frac{\pi e^{-2\gamma}}{E_0} |\omega_m|,$$  \hfill (41)$$

where

$$r = \frac{\pi e^{-\gamma E}}{2E_0},$$  \hfill (42)$$

$$u = \frac{\gamma_E}{E_0},$$  \hfill (43)$$

with $\gamma_E = 0.577 \ldots$ the Euler gamma constant and $c = 21.8 \ldots$ At the mean-field level (i.e., the saddle-point approximation to Eq. (40)), this model describes a QPT when
Disordered Kondo Phase
\langle S^x \rangle = 0

Dissipative Phase
\langle S^x \rangle \neq 0

Luttinger liquid

\[ J_K \]

Figure 3: Schematic $T = 0$ phase diagram of the dissipative 1D Kondo-Heisenberg spin chain. The blue line corresponds to the Tomonaga-Luttinger liquid phase, which is unstable against a small perturbation $J_K^\perp$. The dashed line is the critical line separating a phase of disordered Kondo-singlets (upper white area), from a dissipative phase (shaded bottom area), characterized by gapless diffusive spin excitations. In this phase, at $T = 0$, the dissipative dynamics induced by the metallic environment stabilizes long-range order in the transverse magnetization.

$J_H^\perp$ reaches the critical value $J_H^\perp, c = 64E_0/\pi e^{-\gamma E} \propto J_K^\perp$. In Fig. 3 we show schematically this critical line as a dashed black line, separating the disordered phase with $\langle \psi_i \rangle = 0$, corresponding to the disordered Kondo phase described in Section IIIB [cf. Eq. (37)], from the ordered phase with $\langle \psi_i \rangle \neq 0$, corresponding to the dissipative phase of Section IIIA. Physically, when $J_H^\perp > J_H^\perp, c$ the Heisenberg interaction is large enough to induce long-range coherence in the transverse magnetization $\langle S^x \rangle \propto \langle e^{i\varphi} \rangle \propto \langle \psi_i \rangle$ along the spin-chain. On the other hand, when $J_H^\perp < J_H^\perp, c$ the “charging” term $E_0$ induces large quantum fluctuations of the field $\varphi_i$ (i.e., local spin-flips induced by the term $J_K^\perp$) and therefore tends to destroy the ordered state. In this representation, the competition between the couplings $J_K^\perp$ and $J_H^\perp$ is transparent.

Beyond the mean-field level, the quantum critical properties of this model, generalized to describe a $N$-component field $\{ \psi_i(x) \} = \{ \psi_1(x), \psi_2(x), \ldots, \psi_N(x) \}$ in $d$ dimensions, are well-known and have been studied in the context of antiferromagnetic instabilities of Fermi-liquids. Using the framework of the Hertz-Moriya-Millis theory, this theory describe quantum fluctuations of the order parameter $\psi_0(x)$, with critical dynamical exponent $z = 2$, around the Gaussian fixed-point [i.e., $u = 0$ in Eq. (40)]. A standard momentum-shell RG procedure, performing a two-loop expansion in $u$, and in the small parameter $\epsilon = 4 - D$, where $D = d + z$, allows to obtain the RG-flow equations for the parameters model

\[
\frac{dr (\ell)}{d\ell} = 2r (\ell) + u (\ell) \frac{N + 2}{6} A_D \frac{1}{1 + r (\ell)},
\]

\[
\frac{du (\ell)}{d\ell} = cu (\ell) - u^2 (\ell) \frac{N + 8}{6} A_D \frac{1}{(1 + r (\ell))^2},
\]

where $A_D = 2\pi^{(D/2)}/\Gamma (d/2)$ is the surface area of the $D$-dimensional sphere, and where the units are such that the high-energy cutoff of the theory (40) is $\Lambda = 1$. For $\epsilon$ small and positive ($d < 2$), this RG-flow is controlled by a Wilson-Fisher fixed-point located at $r^* = -\epsilon (N + 2)/2 (N + 8)$, $u^* = 6\epsilon/A_D (N + 8)$.

The stability of the Wilson-Fisher fixed point can be studied upon expansion of Eqs. (45) and (46) in the small deviations $\delta r = r - r^*$, $\delta u = u - u^*$, and allows to obtain the eigen-coupling equation $\delta w_i / d\ell = \lambda_i w_i$, $(i = 1, 2)$, with eigenvalues $\lambda_1 = 2 - \epsilon (N + 2)/(N + 8) + \mathcal{O} (\epsilon^2)$ and $\lambda_2 = -\epsilon + \mathcal{O} (\epsilon^2)$, determining the critical exponents of the transition. Although for $d = 1$ the parameter $\epsilon = 4 - (d + z) = 1$, which is not small, recent quantum Monte Carlo simulations have shown evidence of a QPT in $XY$-spin chains subject to local Ohmic dissipation, with critical exponents in good agreement with those predicted using the the $\epsilon$-expansion.

In the ordered phase $\langle \psi_i \rangle \neq 0$ occurring for $J_H^\perp > J_H^\perp, c$, since the U(1) symmetry of Eq. (39) is spontaneously broken, a Goldstone-mode arises from smooth fluctuations of the phase of the order parameter $\psi_i \sim |\psi_i| e^{i\varphi_i}$, and it becomes necessary to check the stability of the ordered-phase. To that end, we return to Eq. (40) and perform an expansion in small fluctuations of the phase $\delta \varphi_i = \varphi_i - \varphi_0$, around an arbitrary value $\varphi_0$. At Gaussian order in $\delta \varphi_i$ we obtain the effective action

\[
S_{\text{eff}} [\varphi] = \frac{1}{2} \frac{1}{\beta N} \sum_{\mathbf{q}} G^{-1}_{\text{eff}} (\mathbf{q}) |\varphi (\mathbf{q})|^2,
\]

\[
G^{-1}_{\text{eff}} (\mathbf{q}) = \frac{\pi e^{-2} \psi_0^2}{E_0^2} |\omega_m| + \frac{16\psi_0^2}{J_H^\perp} \beta N,
\]

where $G^{-1}_{\text{eff}} (\mathbf{q})$ is the propagator of the Goldstone mode, and where $\psi_0$ is the saddle-point solution of (40). This propagator describes a gapless phase characterized by diffusive ($z = 2$) excitations of the field $\varphi (\mathbf{q})$, and by correlation functions $C^+ (x, \tau) \equiv \langle T_x S^+ (x, \tau) S^- (0) \rangle$ decaying as $C^+ (x, \tau) \sim |x|^{-1}$ at long distances, and $C^+ (\tau) \sim |\tau|^{-1/2}$ at long times (cf. Appendix B). Using Eq. (47) to evaluate the average of the order parameter $\langle \psi_i \rangle = \psi_0 \langle e^{i\varphi_i} \rangle = \psi_0 e^{-\frac{1}{2} |\varphi_0^2|}$, we obtain the result

\[
\langle \psi_i \rangle = \psi_0 \exp \left[ - \frac{\epsilon^2}{2\pi} \frac{E_0}{\psi_0^2} \frac{1}{J_H^\perp} \right] \quad (\text{for } T = 0).
\]

Interestingly, due to the presence of the dissipative term $\sim |\omega_m|$, the (Gaussian) fluctuations of the spin-chain
are strongly suppressed relative to the isolated (XY) chain. Indeed, contrary to the case of isolated 1D systems, quantum fluctuations do not destroy the LRO because the effective dimensionality of the quantum system is \(D = d + z = 3\), larger than the critical dimension \(D_c = 2\) determined by the Gaussian theory for the Goldstone mode Eq. (17). Note that this is not in contradiction with the Mermin-Wagner theorem, which predicts the destruction of LRO at \(T = 0\) in 1D systems with short range interactions. In our case, due to the presence of a higher dimensional fermionic bath which induces long-ranged (imaginary) time correlations, the system cannot be considered strictly one dimensional. Therefore, the Mermin-Wagner theorem is not applicable to our system.

At this point, it is interesting to note the connection with the weak-coupling TLL description of Sec. IIIA, which becomes apparent using, for instance, the self-consistent harmonic approximation (SCHA) method. This method consists in finding the optimal propagator \(G^{-1}_{\text{trial}}(q)\) of a trial Gaussian action, such that the variational free-energy of the system is minimized. For reader to Refs. [25,27], where this method was applied to show the derivation of the SCHA equations, and refer the consistent harmonic approximation (SCHA) method.

The similar forms (in the limit \(d \to 0\)) of \(G^{-1}_{\text{trial}}(q)\) and \(G^{-1}_{\text{eff}}(q)\) in Eq. (48) suggests that the dissipative gapless phase with \(z = 2\), obtained in the strong-coupling regime, is also stable in the weak-coupling regime (see lower part of Fig. 3). The thick solid line at the bottom (i.e., \(J_K \to 0\)) corresponds to the gapless TLL phase described by the Hamiltonian (9). As shown by the RG-flow Eq. (18), this line is unstable against a vanishingly small perturbation \(J_K\).

IV. SUMMARY AND CONCLUSIONS

We have studied the quantum critical properties of a \(S = 1/2\) spin chain described by the anisotropic XXZ Hamiltonian \(\mathcal{H}_{XXZ}\), coupled to a metallic environment via the anisotropic Kondo model \(\mathcal{H}_K\). We study this system in different regimes of parameters using various analytical approaches (i.e., Abelian bosonization, renormalization-group method, analysis of the Ginzburg-Landau functional, etc.), and obtain the quantum phases at \(T = 0\). We focus on the case of plane-anisotropy in \(\mathcal{H}_{XXZ}\) and \(\mathcal{H}_K\), that favors the couplings in the transverse direction. In real systems, this kind of anisotropy is expected in a system with lack of inversion symmetry (see Fig. 1).

First, we investigated the weak-coupling regime \(J_K \ll J_H\) (see Sec. IIIA), where \(\mathcal{H}_K\) can be considered a perturbation to the isolated spin-chain. In that case, we derive a set of RG-flow equations [cf. Eqs. (16)-18] at first order in in the parameters \(J_K\) and \(J_H\). This RG-flow is determined by the value of the Luttinger parameter \(K\) of the chain, and is drastically different the RG-flow expected for the single-impurity Kondo problem. Far away from the isotropic SU(2) point \(K = 1/2\), while \(J_K\) becomes an irrelevant coupling (in the RG sense), \(J_H\) becomes relevant and destabilizes the Tomonaga-Luttinger liquid fixed-point (cf. thick bottom line in Fig. 3). This situation is analogous to other Luttinger-liquid systems coupled to a dissipative environment.

In the opposite limit \(J_K \gg J_H\), we consider the problem starting from the limit of decoupled Kondo-screened impurities. We show that the effective model for coupled Kondo impurities [cf. Eq. (23)] is formally equivalent to that of a 1D Josephson-junction array with on-site Ohmic dissipation, which is known to undergo a quantum phase transition as a function of the dissipation parameter. To extract the properties of the spin chain in this limit, we derive an effective Ginzburg-Landau theory [cf. Eq. (40)] in terms of a U(1) bosonic Hubbard-Stratonovich field \(\psi_i\), and study the critical properties around the Gaussian fixed-point. Physically, the order parameter \(\psi_i\) describes coherence in the transverse magnetization \(\langle S^z_i \rangle \propto \langle \psi_i \rangle\) along the direction of the spin chain. In the limit \(J_K \gg J_H\), the system is characterized by a vanishing order parameter \(\langle \psi_i \rangle = 0\), which we interpret as a manifestation that the system realizes a disordered Kondo-singlet phase, where the spins are screened by their local fermionic bath. Upon the increase of \(J_H\), the system experiences a QPT (dashed line in Fig. 3) towards a phase with LRO, characterized by a non-vanishing order-parameter \(\langle \psi_i \rangle \neq 0\) at \(T = 0\). Interestingly, the dynamics of the emerging Goldstone mode [cf. Eq. (17)] is not able to destroy the mean-field solution, which would be the usual situation for 1D systems. This anomaly is because of the dissipative character of the dynamics of this mode.

Our results, summarized in the \(T = 0\) phase-diagram in Fig. 3, crucially depend on the assumption of in-plane anisotropy in the problem. As shown in Refs. [30,31], this assumption is physically reasonable due to the presence of Dzyaloshinskii-Moriya interactions (induced by spin-orbit coupling at the surface of metals) which break the SU(2) invariance, and enhance the transverse Heisenberg coupling \(J_H\) [cf. Eq. (3)]. Other physical mechanisms producing other types of anisotropy, such as magnetocrystalline effects in the metallic host are beyond the scope of the present work.

An important approximation we used is the assumption of locality in the spin-response of the metal. The conditions when this approximation is justified are discussed in detail in Sec. IIIA.

It would be very interesting to verify our predictions on experimental level. Experimentally, the phase diagram could be studied with STM techniques either by varying the strength of the Kondo exchange coupling (i.e., by
growing the 1D spin chain on the top of a decoupling layer\cite{3}, or by changing the distance between spins, which has the effect of changing the magnitude and sign of the exchange interaction.

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Appendix A: Leading corrections to the spin-chain free energy

We begin by considering the partition function

\[ Z = \text{Tr} \, e^{-(\mathcal{H}_0 + \mathcal{H}_K)/T} = Z_0 \left\langle T_r e^{-J_0 / T} d\tau \mathcal{H}_K(\tau) \right\rangle_0, \]

where \( Z_0 = \text{Tr} \, e^{-\mathcal{H}_0/T} \) is the partition function of the uncoupled host-chain system, and \( \mathcal{H}_0 = \mathcal{H}_{XXZ} + \mathcal{H}_F \) (cf. Eqs. [8] and [7], and \( \tau \) is the Matsubara imaginary time\cite{60}. The average \( \left\langle A \right\rangle_0 = \text{Tr} \, e^{-\mathcal{H}_0/ T} A/\text{Tr} \, e^{-\mathcal{H}_0/T} \) stands for the thermodynamic average of an operator \( A \) over the Gibbsian ensemble defined by \( \mathcal{H}_0 \).

The free-energy of the system (removing the bath contribution) is given by

\[ F - F_0 = -T \ln(Z/Z_0) = -T \ln \left\langle T_r e^{-J_0 / T} d\tau \mathcal{H}_K(\tau) \right\rangle_0. \]

Upon expanding the exponential to the lowest order non-trivial, we obtain the leading free energy correction:

\[ \Delta F = -T \ln \left[ 1 + \frac{1}{2} \int_0^{1/T} d\tau_1 d\tau_2 \left\langle T_r \mathcal{H}_K(\tau_1) \mathcal{H}_K(\tau_2) \right\rangle_0 + \cdots \right] = -\frac{T}{2} \int dr_1 dr_2 \left[ \left( \frac{J_K}{2k_F} \right)^2 \left\langle T_r \mathcal{S}^z(r_1) \mathcal{S}^z(r_2) \right\rangle_0 \mathcal{S}^{zz}(r_12) \right] + \cdots, \]

where \( \mathcal{S}^{zz}(r_12) \) lacks of the in-plane spin-rotation \([U(1)]\) symmetry of the spin-chain due to e.g. spin-orbit interactions (i.e. \( \chi^{xy}(r, \tau) \neq 0 \), et cetera), the leading corrections to the free energy are insensitive to it. However, one factor that complicates the weak-coupling analysis is the fact that the spin correlation functions of the host electrons have very different behavior as compared to the spin correlators of the uncoupled spin chain. In particular, the conformal invariance (e.g., homogeneous scaling upon space and time rescaling) present in the XY model, Eq. (8), implies the spin correlators of the uncoupled chain read\cite{60}
\[ \langle T_r S^z (r) S^z (0) \rangle_0 = -\frac{K}{4\pi^2} \left[ \frac{T^2}{\sinh^2 \left( \frac{\pi T}{u} \right)} + \text{h.c.} \right] + \frac{\cos \left( \frac{\pi x}{a_0} \right)}{a_0^2 \pi} \frac{\pi T_{a_0}}{\sinh \left( \frac{\pi T}{u} \right)} \frac{2K}{\sinh \left( \frac{\pi T}{u} \right)} \], \quad (A3)

\[ \langle T_r S^+ (r) S^- (0) \rangle_0 = \frac{\cos \left( \frac{\pi x}{a_0} \right)}{2\pi a_0 \sinh \left( \frac{\pi T}{u} \right) \sinh \left( \frac{\pi T}{u} \right)^{1/2K}} \left( \frac{\pi T_{a_0}}{u} \right)^{1/2K}, \quad (A4) \]

where we have kept the leading terms at large distances and times. The uniform component of \( S^+ \) \([\sim e^{-i\Theta(x)} \cos 2\Phi (x)]\) is less relevant than the staggered part \([\sim e^{i\pi/a_0} e^{-i\Theta(x)}]\) and will be neglected in what follows.

Estimating the temperature of the various contributions to Eq. (A2) is possible by realizing that the functions that multiply the staggered (\( \propto \cos (\pi x/a_0) \)) part of the spin-chain correlation functions vary very in space slowly compared to the oscillatory factors \( e^{i(q_{DM} \pm \pi/a_0)x} \). For instance, this allows us to approximate the integral:

\[ \int dx_1 dx_2 e^{i(q_{DM} \pm \pi/a_0)(x_1-x_2)} F_K(x_1-x_2, \tau_1) \chi^{+-}(x_1-x_2, \tau_1-\tau_2) \approx L F_K(0, \tau_1-\tau_2) \chi^{+-}(q_{DM} \pm \pi/a_0, \tau_1-\tau_2) \quad (A5) \]

where we have defined the dimensionless couplings \( g_{z,u} \equiv J^z_K/v_F k_F \), \( g_{z,s} \equiv J^z_K/v_F k_F \) and \( g_{J,s} \equiv J^J_K/v_F k_F \), and where \( A^z_u \), \( A^z_s \) and \( A^z_{s} \) are non-universal numerical coefficients.

### Appendix B: Spin-spin correlation functions

Starting from the original spin representation (i.e., before the rotation \( \mathcal{U} \)), the transverse spin-correlator is defined as

\[ C_n^{+-} (\tau) \equiv \langle T_r S^z_{i+n} (\tau) S^z_i (0) \rangle_{\mathcal{U}}, \quad (B1) \]

\[ = \frac{\int \mathcal{D}[S] e^{-S} e^{i\tau \sigma^+_{i+n} \sigma^-_i} e^{-\tau \sigma^-_{i+n} \sigma^+_i}}{\int \mathcal{D}[S] e^{-S}}, \quad (B2) \]

where the average is taken with respect to the total Hamiltonian of the system Eq. (1). The correlation function is a physical quantity that does not depend on our particular choice of representation. Using the transformation \( \mathcal{U} \), the Hamiltonian is transformed as in Eqs. 25 and 26 while the spin operators become \( \mathcal{U}^\dagger S^z_i \mathcal{U} = S^z_i e^{i\phi^z_{i,0}} \) (see Eq. 24). Thus,

\[ C_n^{+-} (\tau) = \langle T_r (U e^{i\tau \mathcal{U}}) (U^\dagger S^z_{i+n} \mathcal{U}) \times (U e^{-i\tau \mathcal{U}}) (U^\dagger S^z_i \mathcal{U}) \rangle \]

\[ \quad = \langle T_r S^z_{i+n} (\tau) e^{i\phi_{i+n}^z} e^{-i\phi_{i}^z} \rangle \mathcal{U}, \quad (B3) \]

\[ = \langle T_r S^z_{i+n} (\tau) e^{i\phi_{i+n}^z} S^z_i (0) e^{-i\phi_{i}^z} \rangle \mathcal{U}. \quad (B4) \]

\[ = \langle T_r S^z_{i+n} (\tau) e^{i\phi_{i+n}^z} S^z_i (0) e^{-i\phi_{i}^z} \rangle \mathcal{U}. \quad (B5) \]
Imposing $\gamma = \sqrt{2}$, and near the strong-coupling Kondo fixed-point, the Hamiltonian $\mathcal{H}$ maps onto Eqs. [31] and [32] (the conduction electron term $\mathcal{H}_c$ is not changed since it doesn’t depend on spin operators). We therefore eliminate the spin-degrees of freedom in the correlation function and obtain

$$C_n^{\pm}(\tau) = \langle T_n e^{i\varphi_{i+n}(\tau)} e^{-i\varphi_i(0)} \rangle_{\mathcal{H}'} = \frac{\int \mathcal{D}[\varphi] e^{-S'_{\varphi}[\varphi]} e^{i\varphi_{i+n}(\tau)} e^{-i\varphi_i(0)}}{\int \mathcal{D}[\varphi] e^{-S'_{\varphi}[\varphi]}},$$

(B7)

where we have truncated the perturbative expansion at leading order. This is to be expected, since the Heisenberg term only couples nearest-neighbors, and therefore spins at a distance of $n$ sites only become correlated at order $(J_H^n)_{\mathcal{H}}$ in the perturbative expansion. The product

$$\langle T_n e^{i\varphi_{i+n}(\tau)} e^{-i\varphi_{i+n}(\tau)} \cdots e^{-i\varphi_{i+n}(\tau)_{\beta}} e^{i\varphi_i(\tau)_0} \rangle_{\mathcal{H}'}$$

can be calculated using Wick’s theorem. For compactness in notation, we define the local two-point correlation function

$$F(\tau) \equiv \langle T_n e^{i\varphi_{i+n}(\tau)} e^{-i\varphi_i(\tau)} \rangle_{0},$$

(B11)

where $a$ is a numerical factor $a = 4e^{-2\gamma_e} \approx 1.261\ldots$, and its Fourier transform

$$F(\omega_m) = \int_0^{\beta} d\tau e^{i\omega_m \tau} F(\tau),$$

$$= \frac{\pi e^{-\gamma_e}}{E_0} \exp \left[- \frac{\omega_m^2 2e^{-\gamma_e}}{E_0} \right].$$

(B13)

Then, the expression for $C_n^{\pm}(\tau)$ compactly writes

$$C_n^{\pm}(\tau) = \left\{ \begin{array}{ll}
\left( \frac{\beta}{\omega_m} \right)^n \frac{1}{\beta} \sum_{\omega_m} e^{i\omega_m \tau} [F(\omega_m)]^{n+1}, & n > 0 \\
F(\tau), & n = 0
\end{array} \right. \quad \text{for } n \geq 0$$

(B14)

One particularly interesting case is the local dynamical correlation $C_0^{\pm}(\tau) \propto \tau^{-2}$ cf. Eq. [B12], which encodes the properties of a local Fermi liquid. Another one is the static, non-local correlation

$$C_n^{\pm}(0) = \frac{1}{2} \frac{e^{-n/\xi_c}}{n + 1},$$

(B15)

where we have defined the correlation length $\xi_c \equiv \left[ \ln \left( \frac{E_0}{J_H^{32} \pi e^{-\gamma_e}} \right) \right]^{-1}.$

1. Spin-correlators in the disordered Kondo-singlet phase

In the disordered “Kondo” phase $J_K \gg \{J_H, J_H'\}$, the Heisenberg coupling $J_H$ in $\mathcal{H}$ Eq. [35] is a suitable expansion parameter to compute the correlation function. Explicitly

$$C_n^{\pm}(\tau) = \frac{\int \mathcal{D}[\varphi] e^{-S_0[\varphi] - S_H'[\varphi] e^{i\varphi_{i+n}(\tau)} e^{-i\varphi_i(0)}}}{\int \mathcal{D}[\varphi] e^{-S_0[\varphi] - S_H'[\varphi]}}$$

(B8)

where

$$\langle T_n e^{i\varphi_{i+n}(\tau)} e^{-i\varphi_{i+n}(\tau)} \cdots e^{-i\varphi_{i+n}(\tau)_{\beta}} e^{i\varphi_i(\tau)_0} \rangle_{\mathcal{H}'} = \frac{1}{m!} \int_0^{\beta} d\tau_1 \cdots d\tau_m \left( \langle T_n e^{i\varphi_{i+n}(\tau)} e^{-i\varphi_{i+n}(\tau)} \cdots e^{-i\varphi_{i+n}(\tau)_{\beta}} \rangle_{\mathcal{H}'} \right)_{\tau_0} = 0$$

(B9)

as $\langle \varphi \rangle = 0$, and $\langle \varphi \rangle^2 = 1$. In the ordered phase, the dynamics of the spin-chain is effectively given by the action of the Goldstone mode Eqs. [47]. With this Gaussian action, and using the saddle-point equations in Eq. (39) to express $e^{i\varphi_i(\tau)} = \psi_i^0(\tau)$, we can calculate the spin-correlation in Eq. (B6) as

$$C_n^{\pm}(\tau) = \langle T_n e^{i\varphi_{i+n}(\tau)} e^{-i\varphi_i(0)} \rangle = \psi_i^0 \langle T_n e^{-i\varphi_i(\tau)} e^{i\varphi_i(0)} \rangle$$

(B16)

where

$$\langle T_n e^{i\varphi_i(\tau)} e^{i\varphi_i(0)} \rangle = \frac{1}{\beta L} \sum_{\omega_m} \frac{1 - e^{i\omega_m (n-i\varphi_n)}}{\omega_m^2 |\omega_m| + \frac{16\omega_m^2}{\beta L} k^2}$$

(B17)

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We study this correlation function in two different limits: the local limit $n = 0$, and $\tau = 0$. In the first case we have

$$
\langle T_\tau [\vartheta_i (\tau) - \vartheta_i (0)]^2 \rangle = \frac{1}{\beta L} \sum_{k, \omega_m} \frac{1}{E_0} \left( 1 - e^{-\omega_m \tau} \right) \left| \omega_m \right| + \frac{16 \pi^2}{J_H^2} k^2 \left( \frac{1}{2\pi} \right)^2 \int d\omega \left( 1 - e^{-\omega \tau} \right) \int dk \frac{1}{16 E_0^2} |\omega| + k^2
$$

(B20)

where we have introduced the short-time cutoff $\tau_0$. With similar tools it can be shown that the static correlation decays as

$$
\langle T_\tau [\vartheta_{i+n} (0) - \vartheta_i (0)]^2 \rangle \sim |n|^{-1}.
$$

(B21)

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