Easy-axis ferromagnetic chain on a metallic surface

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Abstract

The phases and excitation spectrum of an easy-axis ferromagnetic chain of $S = 1/2$ magnetic impurities built on the top of a clean metallic surface are studied. As a function of the (Kondo) coupling to the metallic surface and at low temperatures, the spin chain exhibits a quantum phase transition from an Ising ferromagnetic phase with long-range order to a paramagnetic phase where quantum fluctuations destroy the magnetic order. In the paramagnetic phase, the system consists of a chain of Kondo singlets where the impurities are completely screened by the metallic host. In the ferromagnetic phase, the excitations above the Ising gap are damped magnons, with a finite lifetime arising due to the coupling to the substrate. We discuss the experimental consequences of our results to spin-polarized electron energy loss spectroscopy, and we finally analyze possible extensions to spin chains with $S > 1/2$.

1. Introduction

Recent progress in scanning tunneling microscopy (STM) and other surface-manipulation techniques at the atomic scale has made it possible to build low-dimensional magnetic structures with unprecedented control [1, 2]. Atomic-scale magnetic structures possess an enormous potential for applications in spintronics as well as in classical and quantum computation due to their ability to store and process (quantum) information in the atomic spins. However, in order to build reliable atomic-size memories or qubits out of such systems, it is crucial to understand how the coupling to the environment affects their properties. For instance, it is known that quantum nanomagnets coupled to electronic degrees of freedom are prone to the effects of decoherence induced by Ohmic quantum dissipation [3, 4].

In addition to their interest for information technologies, low-dimensional magnetic systems coupled to dissipative environments are also very important from the point of view of fundamental physics. This is because they allow one to study the crossover from quantum to classical behavior as the coupling to the environment is increased [5, 4]. Current theoretical models that describe local quantum degrees of freedom coupled to sources of dissipation predict rich and interesting physical phenomena at low temperatures, including quantum phase transitions and quantum criticality [6–9], as well as broken continuous symmetries and long-range order (LRO) in low-dimensional systems [10–15]. The interplay between quantum fluctuations, which are induced by quantum confinement and reduced dimensionality, and quantum dissipation, caused by the interaction with the environment, is at the core of this exotic behavior. From this perspective, magnetic nanostructures built on the top of clean metals offer a unique platform to test our understanding of dissipative quantum systems. For instance, the simplest zero-dimensional (0D) case of a single magnetic impurity coupled to a metallic environment (such as a Co or Mn adatom sitting on a Au(111) surface) is a practical realization of the celebrated Kondo effect, one of the most paradigmatic phenomena in the physics of strongly correlated electrons [16]. This phenomenon is the spin compensation by the conduction electrons of the magnetic moment $S_i$ of an...
impurity embedded in a metallic host at temperatures $T \ll T_K$, where $T_K$ is the so-called Kondo temperature. Eventually, at $T = 0$, the ground state of the system is a many-body singlet (termed a ‘Kondo singlet’), formed by a linear superposition of $S_i$ and the spin of a cloud of conduction electrons that is anti-ferromagnetically correlated with the impurity local moment. The original magnetic impurity $S_i$ is thus completely screened by the metallic environment. In the context of magnetic adatoms deposited on clean metallic surfaces, this is a well-established phenomenon, which reveals itself as a narrow Fano resonance at the Fermi energy in the STS spectra [17–19].

Unfortunately, the extension of the single Kondo impurity to the case of many interacting magnetic impurities embedded in a metallic host represents a formidable theoretical challenge. Due to the many-body nature of the problem, exact methods are only limited to simple cases (i.e., consisting of few magnetic impurities), and at the cost of expensive numerical calculations [20]. On the other hand, dynamical mean-field theory (DMFT) methods [21] provide reliable results in the case of bulk 3D compounds, but are much less successful when applied to low-dimensional systems.

One particular class of such low-dimensional systems, namely, one-dimensional (1D) chains of magnetic atoms or organic molecules with active magnetic atoms, are currently under intensive experimental investigation [22–26]. For instance, by depositing a $\approx 0.1$ monolayer (ML) of Co on Pt(997), which is a vicinal surface containing steps, chains of magnetic atoms have been created recently [22]. The magnetic Co atoms decorate the steps and form ferromagnetic chains, which, when probed by an external magnetic field, typically exhibit superparamagnetism. However, in the case of Co chains at temperatures $T \lesssim 8 \text{ K}$, the magneto-crystalline anisotropy results in relaxation times which are longer than the experimental typical timescale, and the response of the system becomes effectively ferromagnetic [22]. Another recently reported system, consisting of chains of Co atoms on Cu(775), has been shown to undergo a Peierls distortion leading to dimerization [27]. This dimerized phase has been explained by the strong correlations existing in the partially filled $d$ orbitals of the Co atoms, which are in the high-spin configuration. Maintaining the high spin in a geometry where the overlap between the $d$ orbitals is small and correlations are strong, favors a ferromagnetic ground state, which in turn makes the charge-density-wave instability possible.

In the above-mentioned systems, the coupling to the metallic substrate was assumed to be weak, and therefore was neglected in their analysis. However, as we show below, the metallic environment can have dramatic effects for the phase diagram at low temperatures, and it cannot be neglected when studying the magnetic excitations of the chain. For instance, in [15], it was shown that a $S = 1/2$ chain with easy-plane anisotropy (effectively described by a XY model in the gapless regime) and weakly coupled to a metal is able to develop long-range order (at $T = 0$) in the in-plane magnetization. Note that this is a very unusual situation in a strictly 1D system, where the presence of quantum fluctuations inhibits long-range ordered phases that break a continuous symmetry.

Motivated by the above-mentioned systems, in this contribution we focus on the analysis of an easy-axis ferromagnetic (FM) 1D spin chain deposited on the top of a metallic surface. Interestingly, as a function of the coupling with the substrate, we predict a quantum phase transition from an Ising ferromagnetic phase with long-range order to a paramagnetic phase where quantum fluctuations proliferate and destroy the ordered phase. Although modifying the coupling to the substrate in the experimental systems created so far may be hard, in the future other systems can be created where the coupling to the substrate could be tuned, uncovering even more interesting phenomena. Compared to [15], where the authors studied a gapless XY spin chain coupled to a metallic environment, in the present work we focus on the Ising chain with gapped magnetic excitations, which constitute a complementary regime.

The paper is organized as follows: in section 2, we introduce a simple model to describe an easy-axis $S = 1/2$ ferromagnetic chain on a metallic substrate. This model is studied in the framework of mean-field theory in section 3, and the quantum phase diagram is thus obtained. The phase diagram is displayed in figure 4, and it is one of the most important results of this work. In section 4 we consider the excitation spectra of the ferromagnetic phase. We show that a weak coupling with the metallic substrate can have important consequences for the magnetic excitations of the ferromagnetic chain. These properties of the excitations, and in particular, the substrate-induced damping, can be accessible by experimental probes such as spin-polarized electron energy loss spectroscopy (SPEELS). In figure 5, we plot the spin response of the 1D spin chain due the substrate-modified magnon excitation spectrum, which is also an important result of this work. Finally, in section 6, we offer our conclusions and outlook for future research directions. In the appendix, we give more details about the technical aspects of our calculations.

2. Model

Let us consider a chain of magnetic atoms deposited on top of a metallic surface (see figure 1). We model the magnetic interactions between the atoms using the spin-$\frac{1}{2}$ XXZ Hamiltonian:

$$H_0 = -\sum_{i=1}^{N} J_{XX} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + J_{HF} S_i^z S_{i+1}^z.$$

![Figure 1. Graphical representation of a FM spin chain deposited on the top of a metallic surface. Kondo screening of the individual spins at low temperatures $T \ll T_K$ tends to destroy the FM long-range order and induce a quantum phase transition to a paramagnetic phase (see figure 4).](image-url)
In the above expression, we have assumed anisotropic exchange interactions, which originate from the reduced symmetry of the surface crystal environment, as well as from spin–orbit interactions of the electrons in the metallic substrate [2]. Assuming that the impurity spin is \( S = \frac{1}{2} \) implies that the single-ion anisotropy \( D \sum_{i} (S_i)^2 \) reduces to a constant term. Furthermore, for \( S = \frac{1}{2} \), exchange terms such as \( \sum_{i} (S_i \cdot S_{i+1})^2 \) can be expressed in terms of \( \sum_{i} (S_i \cdot S_{i+1}) \). However, for impurities with \( S > \frac{1}{2} \) such terms must be taken into account, but we shall not pursue their analysis here.

The nature of the ground state of equation (1) depends crucially on the ratio \( \Delta = J_{\parallel}/J_{\perp} \), where we assume \( J_{\perp} \geq 0 \). For \( \Delta > 1 \) (\( \Delta < -1 \)), equation (1) describes an easy-axis (i.e. Ising-like) ferromagnet (anti-ferromagnet). In this system, the spin waves (magnons) and their bound states are separated from the ground state by a gap [28, 29]. On the other hand, for \( |\Delta| < 1 \), the spin chain Hamiltonian (1) exhibits a XY phase with a gapless spin-wave spectrum [30, 31]. However, as anticipated in the introduction, in what follows we will focus only on the FM Ising limit \( \Delta > 1 \) of (1), and we refer the reader to [15] for a complementary study in the case of easy-plane anisotropy, where the spin chain exhibits an XY phase. Nevertheless, we note that the results reported in section 3 are also applicable to the anti-ferromagnetic (AFM) phase. Nevertheless, we note that the results reported in section 3 are also applicable to the anti-ferromagnetic (AFM) regime corresponding to \( \Delta < 1 \) (see section 6) [32]. Finally, for the sake of simplicity, we have neglected longer-range magnetic exchange interactions in equation (1), which may be present due to the Ruderman–Kittel–Kasuya–Yosida (RKKY) mechanism mediated by the metallic substrate [33]. We note that these interactions can be easily included, as long as they do not modify the nature of the Ising FM ground state. This means that, in addition, we are not considering the case of strong irregularities in the inter-impurity spacing, which would make the RKKY exchange site-dependent and would render spin-glass physics relevant.

The coupling between the spin chain and the metallic substrate is described by an anisotropic Kondo-exchange Hamiltonian [16]:

\[
H_K = \sum_{i=1}^{N} \left( J_K^{\parallel} S_i^x R_i^x + J_K^{\perp} S_i^y R_i^y \right) + J_K^{\perp} S_i^z R_i^z,
\]

where \( S^x \) (\( R_i \) \( (a = x, y, z) \)) is the spin density of conduction electrons at the position of the \( i \)-th spin impurity in the surface \( R_i = i \cdot a_0 \) (with \( a_0 \) the lattice parameter of the chain). Note that this model bears some similarity with the Kondo-lattice model, which is used to describe the properties of heavy-fermion systems [16, 34, 35]. In the case of impurities with \( S > \frac{1}{2} \), the Kondo exchange involves more channels (with channel-dependent couplings) and results in a dynamical screening of the impurity spins occurring in several stages, involving different Kondo temperatures [36]. We shall not pursue such an analysis here.

Despite its simplicity, the model introduced above still represents a formidable theoretical challenge, and in order to make analytical progress we shall introduce some simplifying assumptions. We approximate the metallic substrate by a collection of one-dimensional metals (see figure 2) described by the Hamiltonian

\[
H_F = \sum_{i=1}^{N} \sum_{\alpha, \beta} (\epsilon_k - \mu) c_{\alpha i}^\dagger(k) c_{\alpha i}(k),
\]

where \( c_{\alpha i}^\dagger(k) \) creates an electron with linear momentum \( k \) and spin projection \( \alpha \). The index \( i \) indicates that the electron reservoir described by the operators \( c_{\alpha i}^\dagger(k), c_{\alpha i}(k) \) is only coupled to the impurity located at \( R_i \) and not to others with \( j \neq i \). For this reason, we dubbed this approximation the ‘local bath approximation’ (LBA) [15]. Within the LBA, the spin-density operator reads:

\[
s^\alpha (R) = \sum_{a, \alpha', k, k'} c_{\alpha a i}^\dagger(k) \left( \frac{\sigma^\alpha}{2} \right)_{\alpha' \beta} c_{\beta i}'(k'),
\]

where \( \sigma^\alpha \) are the Pauli matrices.

The dimensionality of the substrate is crucial for the justification of the LBA. When the magnetic impurities embedded in a high-dimensional (2D or 3D) metallic substrate are separated by a distance of the order of a few \( k_F^{-1} \), with \( k_F \) the Fermi wavevector of conduction electrons, the interference of Kondo screening clouds that dynamically quench the magnetic moments becomes negligible [37–39]. Consequently, at distances \( a_0 \gg k_F^{-1} \) the impurities can be considered as independently screened [15]. This is an important difference with respect to the case of a strictly 1D metallic substrate, as in the case of the 1D Kondo-lattice model [40]. In that case, the single Kondo-impurity limit is reached only at distances \( a_0 \gg \xi_K \sim v_F/T_K \). Since the Kondo temperature \( T_K \) is an exponentially small scale, in the purely 1D geometry the single-impurity regime is only reached at extremely dilute impurity-spin concentrations [37–39].

In actual experiments, although the magnetic nanostructures are built on the top of a metallic surface, \( k_F \) is determined by the 3D bulk electron density due to a non-vanishing overlap between the bulk and surface conduction states [19]. For instance, the Fermi wavenumber for Au bulk free conduction electrons is \( \pi/k_{F, b} = 2.6 \) Å, while for Au(111) surface states it is \( \pi/k_{F, s} = 16.6 \) Å [41]. This fact dramatically increases
the range of applicability of the LBA. The physical picture provided by the LBA is also supported by the behavior of the STS Fano line shapes in experiments on magnetic Co atoms deposited on Cu(100) and separated by distances $a_0 > 8 \, \text{Å}$, which are identical to the single-impurity STS line shapes [42].

Note that the same LBA has been implemented before in the case of few Kondo or Anderson impurities [43–45] and in the case of many impurities forming an infinite chain with easy-plane anisotropy (i.e., $XY$ spin chain in the gapless regime) [15], where the interplay of local screening and inter-impurity Heisenberg or Ising coupling results in a non-trivial low-temperature phase diagram of these systems.

Finally, although in the actual experimental realizations the limit $a_0 \gg k_F^{-1}$ might not be strictly realized, the model resulting from applying the LBA to equations (1), (2) can be considered as the simplest ‘toy model’ that captures the competition between the Kondo physics, which is a local quantum critical phenomenon, and the magnetic interactions along the chain [15]. Concerning the latter, it is worth noting that the LBA cannot reproduce the non-local RKKY exchange coupling mediated by the metal and arising at order $O(J_0^2)$. As mentioned before, this is not a crucial drawback, since one can always redefine the couplings $J_{H,i}, J_{H}^{\perp}$ in equation (1) to take the RKKY contribution explicitly into account. Moreover, one could introduce all the complexities inherent to the long-range RKKY interaction (as long as the spectrum of the chain remain gapped) by first integrating out the high-energy degrees of freedom of the electronic bath, as described in [46] by Castro Neto and Jones. The local bath approximation is used subsequently, in order to account for the Kondo physics. More importantly, what eventually justifies the separate treatment of RKKY and Kondo interactions is that, although both originate in the same Hamiltonian (2), the RKKY interaction results from electronic states deep inside the Fermi sea and is a static coupling, while the Kondo effect is a purely dynamical effect originated predominantly in the Fermi surface [35, 46].

3. Mean-field analysis of the $T \to 0$ phase diagram

In order to gain insight into the low-temperature phase diagram of the system, we now focus on the limit $\Delta > 1$ of equation (1), describing an isolated FM Ising spin chain. In that case, the ground state of the isolated chain is separated from the single-magnon excitation spectrum by a gap $E_g = E_{g0}^H(1 - \Delta^{-1})$ and by a gap $E_{g}^{\perp} = J_{H}^{\perp}(1 - \Delta^{-2}) > E_g$ from the two-magnon bound states [28, 29]. This means that the long-range FM order in the isolated chain is stable at low temperatures and, to a first approximation, it is safe to take $J_{H}^{\perp} = 0$ in equation (1).

We now introduce the coupling to the substrate equation (2), which has important consequences for the low-temperature behavior of the spin chain. For instance, the nature of the ferromagnetic to paramagnetic phase transition is modified. As we show in the appendix, in the case $J_{H}^{\perp} = 0$ the model for the Ising chain coupled to the substrate can be mapped onto the 1D dissipative quantum Ising model, which is in the universality class of the classical 3D (instead of 1D) Ising model. In the following, we exploit this fact to introduce a mean-field (MF) approach, which therefore provides a good description of the phases of the spin chain in the (easy-axis) Ising limit.

We introduce the MF approximation to the Ising term in equation (1) by making the replacement $i S_i^z \rightarrow S_i^{\perp} \left[ S_i^{\perp} \right]_{i+1} + \left[ S_i^{\perp} \right]_{i+1} - \left[ S_i^{\perp} \right]_{i+1}$, which leads to the MF Hamiltonian of the spin chain:

$$H_0^{\text{MF}} = \frac{N h_{\text{eff}}^2}{4 J_{H}} - \sum_{i=1}^{N} h_{\text{eff}} S_i^z,$$

where

$$h_{\text{eff}} = 2 J_{H} \langle S_i^z \rangle$$

is the local Weiss field. The MF Hamiltonian of the system is therefore written as

$$H_{\text{MF}} = \sum_{i=1}^{N} H_i^{\text{MF}} + \sum_{i=1}^{N} \left[ \frac{N h_{\text{eff}}^2}{4 J_{H}} \right],$$

$$H_i^{\text{MF}} = J_{K}^H \left[ S_i^z \hat{c}^\dagger (R_i) + S_i^z \hat{c} (R_i) \right] + J_{K}^\perp \left[ S_i^\perp \hat{c}^\dagger (R_i) \right] - h_{\text{eff}} S_i^z + H_{Fi},$$

with $H_{Fi} = \sum_{i,k} c_{\alpha}(k)c_{\alpha}^\dagger(k) \delta_{\alpha,\beta}$ describing the $i$th conduction electron bath. In the following we drop the lattice sub-index $i$ in $H_i^{\text{MF}}$ and $H_{Fi}$ in order to lighten the notation.

We note that the MF approximation together with the LBA leads to a set of independent Kondo-impurity problems in an effective magnetic field $h_{\text{eff}}$, which is a quantity that must be obtained self-consistently. The MF thermodynamical properties of the spin chain can therefore be obtained from the free energy $f(T, h_{\text{eff}}) = - T \ln \text{Tr} [e^{-H_{\text{MF}}(h_{\text{eff}})/T}]$ for a single Kondo impurity in a magnetic field $h_{\text{eff}}$. Note that the Weiss field $h_{\text{eff}}$ does not act upon the conduction electrons, it only acts on the impurity. The mean-field self-consistency condition is obtained from the relation between the impurity magnetization,

$$m_{\text{imp}}(T, h_{\text{eff}}) = \langle S_i^z \rangle = -\frac{\partial f(T, h_{\text{eff}})}{\partial h_{\text{eff}}}$$

and the definition of the Weiss field equation (6):

$$m_{\text{imp}}(T, h_{\text{eff}}) = \frac{h_{\text{eff}}}{2 J_{H}}.$$

To make further progress we now need to know the function $m_{\text{imp}}(T, h_{\text{eff}})$ for a single Kondo impurity. Introducing the Abelian bosonization method [31] to describe the metallic 1D chains in figure 2, and the unitary Emery–Kivelson transformation [47] (see equation (A.3)), the anisotropic Kondo model can be mapped onto the resonant-level model [48–50]. The resonant-level model is exactly solvable when the parameter $J_{K}^H$ is chosen at the so-called ‘Toulouse line’ [51], defined by $\tan^{-1}(\pi \rho_0 h_0 J_{K}^H / 4) = \frac{\pi}{4}(1 - \frac{1}{\sqrt{2}})$, where $\rho_0$ and $h_0$ are the density of states and lattice parameter of the bosonized 1D chains, respectively (see appendix). In combination with the renormalization
where $T$ is the Pauli paramagnetic response obtained from (10) in the limit $\hbar \chi_{\text{imp}} \propto T$. The above result can be also obtained using the scaling equations, and it is modified by anisotropy at the Toulouse point. Thus, a non-vanishing solution for $h_{\text{eff}}$ is found from equation (10) in the limit $h_{\text{eff}} \rightarrow 0$

$$\frac{1}{2T_{\text{H}}} < \chi_{\text{imp}}(0) \left[ 1 - \frac{\pi^2}{3} \left( \frac{T}{T_{K}} \right)^2 \right].$$

(15)

From the above considerations, the phase boundary is therefore given by the critical line

$$\frac{T_{c}}{T_{K}} = \sqrt{\frac{2}{\pi}} \sqrt{1 - \frac{\pi T_{K}}{2T_{H}}},$$

(16)

and from here we can obtain the MF phase diagram of the spin chain (see figure 4).

It is interesting to note that, in the FM phase, as $J_{\text{H}}/T_{K}$ increases from the phase boundary, the value of the Weiss field $h_{\text{eff}}$ crosses over from a regime $h_{\text{eff}} \ll T_{K}$ where the Kondo singlet is still robust, to the regime of large $h_{\text{eff}} \gg T_{K}$ where

$$m_{\text{imp}}(T, h_{\text{eff}}) \sim \frac{1}{\pi} \arctan \left[ \frac{h_{\text{eff}}}{2\pi T + T_{K}} \right].$$

(14)

Figure 3. Graphical solution of the mean-field equation, equation (10), for $T = 0$. For $J_{\text{H}}$ larger than the critical value there are two kinds of mean-field solutions: those for which $h_{\text{eff}} < T_{K}$ and those for which $h_{\text{eff}} > T_{K}$. In the first case, the coupling between the impurities does not suffice to destroy the Kondo singlet. However, in the latter case, the coupling is strong enough to break the Kondo singlets.

Figure 4. Mean-field phase diagram of the Ising chain coupled to the metallic substrate. At low enough temperatures, and in the regime $J_{\text{H}} \ll T_{K}$, quantum fluctuations induced by the (Kondo) coupling to the substrate completely destroy the long-range magnetic order.
the Kondo singlet is destroyed (see figure 3). Therefore, the above mean-field theory yields a regime where the Kondo effect and a FM LRO coexist. In section 4, we shall return to this point again.

It is also worth mentioning that the result in equation (16) clearly contrasts with the case of the isolated Ising chain, for which the analytical form of $T_c$ equation (16) is very different from the expression for $T_c$ encountered in the study of the classical Ising model, where $T_c \propto J_{hi}^{-1}$ [54]. Physically, in the present case, the spin-flip processes induced by the Kondo coupling to the metal equation (2) can be considered as quantum fluctuations that tend to destroy the LRO in the Ising chain as $T \rightarrow 0$ for $J_{hi}/T_K \lesssim 1.6$ (see figure 4).

In section 4 we characterize the excitations of the ordered FM phase.

4. Magnetic excitations in the FM phase

We next focus on the FM phase, in the regime $J_{hi}/T_K \gtrsim 1$ (right-bottom region in figure 4), where the spectrum of the system is gapped and the effective Weiss field $h_{eff}$ is large enough so as to inhibit the Kondo screening of the impurities. We shall focus in particular on single-magnon excitations that can be created by probes (such as spin-polarized electron energy loss spectroscopy, SPEELS, see section 5) that couple weakly to the ferromagnetic system. Such probes are assumed to produce single spin-flips, and thus the calculation of the system response can be carried out within linear response theory. This approximation allows us to neglect the effect of magnon bound states in the spectrum of the FM XXZ chain. Thus, the low-lying excitations involving a single spin-flip can be described using the Holstein–Primakoff (HP) representation of the spin operators [55]:

$$S_i^+ = b_i^\dagger \sqrt{2S - b_i^\dagger b_i} = \sqrt{2S} \left[ b_i^\dagger + O\left(\frac{1}{S}\right)\right],$$

$$S_i^- = \sqrt{2S - b_i^\dagger b_i} = \sqrt{2S} \left[ b_i + O\left(\frac{1}{S}\right)\right],$$

$$S_i^z = (b_i^\dagger b_i - S),$$

where $b_i, b_i^\dagger$ are bosonic annihilation and destruction operators, obeying $[b_i, b_j^\dagger] = \delta_{ij}$, which physically represent a single spin-flip. For the XXZ chain introduced in section 2, we should take $S = \frac{1}{2}$ in the above expressions. However, below we shall work assuming that $S$ is large, which is known to provide an accurate description of the lowest energy excitations [55]. Assuming $S$ large means that our results also apply to spin chains with $S \gtrsim \frac{1}{2}$, provided the Hamiltonian is of the XXZ form and we assume that the Kondo-exchange coupling with the substrate describes the strongest channel of substrate electrons that couple to each impurity along the chain. Thus, working to leading order in $S$ (i.e. in the large-$S$ approximation), we find:

$$H_{0}^{\text{HP}} \simeq \sum_{i=1}^{N} \left[-J_{hi}^2 S_i^z - J_{hi} S_i^z \left( b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \right) + J_{hi}^2 S_i^z \left( b_i^\dagger b_i + b_{i+1}^\dagger b_{i+1} \right)\right].$$

$$H_{0}^{\text{HP}} = \sum_{q} E_{q} b_{q}^\dagger b_{q} - N J_{hi}^2 S^2 + O(1),$$

which can be easily diagonalized in a running-wave basis

$$b_i = \frac{1}{\sqrt{N}} \sum_{q} e^{i q R_{i}} b_{q},$$

and leads to

$$H_{0}^{\text{HP}} \simeq 2 S J_{hi}^2 - 2 S J_{hi}^2 \cos(q a_0),$$

$$\simeq 2 S (J_{hi}^2 - J_{hi}^2) + 2 S \frac{q^2 a_0^2}{2} + O(q^4)$$

is the dispersion relation for magnons, and $a_0$ is the lattice parameter. In addition, in equation (22) we have neglected terms of $O(1)$, which involve interactions between the magnons. From equation (23), we see that for $J_{hi}^2 > J_{hi}^2 > 0$ (i.e. $\Delta > 1$) the excitation spectrum of the spin chain is gapped, and the spin waves exhibit a quadratic dispersion for momentum $q \rightarrow 0$.

Let us next consider on the Kondo-exchange coupling to the metal, equation (2). We shall treat this coupling using the HP representation in the large-$S$ limit:

$$H_{K}^{\text{HP}} \simeq \sum_{i=1}^{N} [J_{K}^{\text{HP}} \sqrt{2/2(b_i^\dagger s^- (R_i) + s^+(R_i)b_i)} + J_{K}^{\text{HP}} (b_i^\dagger b_i - S)s^z (R_i)].$$

$$H_{K}^{\text{HP}} \simeq \sum_{i=1}^{N} \left[J_{K}^{\text{HP}} \sqrt{2/2(b_i^\dagger s^- (R_i) + s^+(R_i)b_i)} + J_{K}^{\text{HP}} (b_i^\dagger b_i - S)s^z (R_i)\right].$$

As we will see, although this Hamiltonian no longer describes the Kondo effect (we recall that we are working in the limit of...
large $h_{\text{eff}}$), the coupling to the gapless degrees of freedom in the metal still can have important consequences to the spin chain. To make further progress, we now need to integrate out the electronic degrees of freedom in the conduction band. To this end, we shall rely upon the coherent-state functional integral representation of the partition function [56]:

$$Z = \int \prod_{i=1}^{N} D[\hat{b}_i, \hat{b}_i^\dagger] e^{-S_{\text{eff}}^{\text{HP}}[\hat{b}, \hat{b}^\dagger]},$$  

(25)

where $S_{\text{eff}}^{\text{HP}}[\hat{b}_i, \hat{b}_i^\dagger]$ is the effective Euclidean action of the spin chain (with convention $\hbar = 1$)

$$S_{\text{eff}}^{\text{HP}}[\hat{b}, \hat{b}^\dagger] = S_0^{\text{HP}}[\hat{b}, \hat{b}^\dagger] + S_{\text{diss}}^{\text{HP}}[\hat{b}, \hat{b}^\dagger],$$  

(26)

where the first term is the Euclidean action corresponding to (22)

$$S_0^{\text{HP}}[\hat{b}, \hat{b}^\dagger] = \sum_{q} \int_{0}^{\beta} d\tau \bar{b}_q(\tau) \left[ \partial_\tau + E_q \right] b_q(\tau),$$  

(27)

$$\overset{\text{=}}{=} \frac{1}{\beta} \sum_{q, \omega_0} \left[ -i\omega_0 + E_q \right] \bar{b}_q(\omega_0) b_q(\omega_0),$$  

(28)

and $S_{\text{diss}}^{\text{HP}}[\hat{b}, \hat{b}^\dagger] = -\ln(\exp[-\int_0^\beta d\tau H_{\text{HP}}^\text{eff}(\tau)])$ is the contribution arising from Hamiltonian (24), where we integrate over the fermions $(\bar{c}_{\alpha i}, \hat{c}_{\alpha i})$. Note that this can be done exactly, as $H_{\text{F}}$ is quadratic (we assume that Fermi liquid theory applies) and it can be interpreted as Landau damping [57–59]. Interestingly, this damping does not vanish in the limit $q \to 0$. At first sight, this may seem surprising, since in the $q \to 0$ limit, magnon excitations correspond to a uniform magnetization along the $z$ direction. Thus, the total projection $S_{\text{T}}^z = \sum_{\alpha i} s_{\alpha i}^z$ is a conserved quantity in the absence of coupling to the substrate. In other words, the number of magnons $\sum_{\alpha i} b_{\alpha i}^\dagger b_{\alpha i}$ is a conserved quantity of the Hamiltonian in (20). However, in the presence of $H_{\text{K}}^{\text{HP}}$ (equation (24)), $S_{\text{T}}^z$ is no longer conserved (i.e. the magnons $b_{\alpha i}$ can 'leak out' from the chain), and therefore total magnetization fluctuations also become damped out by the coupling to the substrate.

The above treatment is valid provided the coupling to the substrate is weak and can be treated perturbatively. At stronger coupling, we have to worry about the possibility that the magnetic moments of the impurities are Kondo screened by the substrate electrons. To deal with this situation, we shall rely on the non-perturbative treatment discussed in the appendix. As shown there, in the strong coupling limit where $K_{\text{HP}}$ is quadratic, and replacing it into (26) leads to the effective action

$$S_{\text{eff}}^{\text{HP}}[\hat{b}, \hat{b}^\dagger] = -\frac{1}{\beta} \sum_{q, \omega_0} \left[ \bar{b}_q(\omega_0) b_q(\omega_0) \right] - i\omega_0.$$  

Thus, the pole of the propagator becomes $\omega_0 = E_q(1 + i\alpha)^{-1}$, which implies that the coupling to the metal equation (24) induces a finite lifetime $\Gamma = (\alpha E_q)^{-1}$ and damping on the magnon excitations. Physically, this happens due to the presence of gapless particle–hole excitations in the exciton spectrum of the metallic substrate, and it can be interpreted as Landau damping [57–59]. Interestingly, this damping does not vanish in the limit $q \to 0$. At first sight, this may seem surprising, since in the $q \to 0$ limit, magnon excitations correspond to a uniform magnetization along the $z$ direction. Thus, the total projection $S_{\text{T}}^z = \sum_{\alpha i} s_{\alpha i}^z$ is a conserved quantity in the absence of coupling to the substrate. In other words, the number of magnons $\sum_{\alpha i} b_{\alpha i}^\dagger b_{\alpha i}$ is a conserved quantity of the Hamiltonian in (20). However, in the presence of $H_{\text{K}}^{\text{HP}}$ (equation (24)), $S_{\text{T}}^z$ is no longer conserved (i.e. the magnons $b_{\alpha i}$ can 'leak out' from the chain), and therefore total magnetization fluctuations also become damped out by the coupling to the substrate.
partition function is \( Z = \int [d\phi] e^{-S[\phi]} \), where the action \( S[\phi] \) is given by the expression [11]:

\[
S[\phi] = \frac{1}{4} \sum_{q,\omega_n} \left[ |\omega_n| + Dq^2 + r \right] |\phi(q, \omega_n)|^2 + \frac{g}{4} \int dx \, dr \, \phi^4(x, \tau),
\]

where \( \phi(x, \tau) = (\beta)^{-1/2} \sum_q e^{i(qx-\omega_n \tau)} \phi(q, \omega_n) \) \((\beta = 1/T)\) is the coarse-grained magnetization along the easy axis, i.e. \( \phi(x = x_0) = R^{-1} \sum_{n=1}^{R/2} S^z_{n+1} \), where \( 1 \ll R \ll N \). This result suggests that the quantum critical point (QPC) separating the paramagnetic and ferromagnetic ground states (see figure 4) can be described by this field theory, and therefore the critical exponents around the QCP will correspond to those of the Wilson–Fisher fixed point of the renormalization group (see e.g. [60], for a review). However, in deriving the map to the dissipative quantum Ising model, we have neglected the Heisenberg term \( \sim \frac{\delta}{2} \sum_i \sum_j S^z_i S^z_{i+1} \) from equation (1). If this term is included, we cannot rule out that the actual values of the critical exponents near the QCP turn out to be different from those of the Wilson–Fisher fixed point of the universality class. Addressing this question in detail requires a numerical investigation of the full model, which is beyond the scope of the present work.

Nevertheless, the field theory of equation (39), is capable of describing the phases of the system. Focusing on the ferromagnetic phase where \( \langle \phi(x, \tau) \rangle \neq 0 \), which corresponds to \( r < 0 \), it can be seen that the magnon excitations are indeed described by the propagator:

\[
\langle \phi^*(q, \omega_n) \phi(q, \omega_n) \rangle = \frac{1}{|\omega_n| + \frac{\omega_n^2}{E_g} + Dq^2 + r}.
\]

where \( E_g = 2|q| - J_{HF}^z - J_{HF}^\perp \) is the energy gap. This magnon propagator indicates that the magnetic excitations of the chain in the strong coupling regime are overdamped by their coupling to the metallic substrate. Physically, this makes sense, as the impurity spins are screened by the metal electrons and their magnetic moments undergo strong damping by the collective nature of their screening clouds. This regime must be contrasted with the weak coupling regime, where we found the damping to be weak. Thus, a physical picture emerges that allows us to distinguish the two mean-field solutions that we briefly described at the end of section 3 (see figure 3): in the weak coupling regime, the strong Weiss field (i.e. \( h_{\text{eff}} \gg T_K \)) due to the FM coupling of the impurities along the chain does not allow the Kondo screening of the local moments of the atoms in the chain. As a consequence, the magnetic excitations of the chain are only weakly affected by their coupling to the substrate, and thus acquire a small line width. On the other hand, in the strong coupling regime, the Weiss field is much weaker (i.e. \( h_{\text{eff}} \ll T_K \)) and the magnetic moments are effectively screened by the metal electrons, leading to overdamped magnetic excitations. In section 5, we shall study some experimental consequences of our findings.

5. Relation to SPEELS experiments

In this section, we focus on the effects of the dissipative environment on observable quantities. The magnetic properties of low-dimensional spin systems deposited on metals have been studied with a variety of experimental techniques, such as x-ray magnetic circular dichroism (XMCD), used to measure directly the magnetization of FM 1D spin chains [22], or local probes, such as spin-polarized STM, which can provide information on the magnon dispersion relation [61]. Here we focus on the spin-polarized electron energy loss spectroscopy (SPEELS) experiment [62–64], which provides direct information of the magnon dispersion relation.

The SPEELS cross section \( d^2P/d\Omega d\omega_o \) corresponds to the fractional number of electrons which emerge into the solid angle \( d\Omega \) after being scattered by a magnetic excitations \( \omega(q) \) in the energy range \( d\omega_o \). According to the theory of the SPEELS experiment [62], \( d^2P/d\Omega d\omega_o \) is related to the spin response function by

\[
\frac{d^2P}{d\Omega d\omega_o} \propto -\text{Im} \chi^\pm(\omega),
\]

where \( \chi^\pm(\omega) \) is the retarded spin correlation function obtained by analytic continuation from \( \chi^\pm(\omega) = \int d^4R e^{i\mathbf{q} \cdot \mathbf{R}} \langle \mathbf{S}^-(\mathbf{R}, \tau) S^+(0, 0) \rangle \). Using the HP representation equations (17)–(19), we can express

\[
\chi^\pm(\omega_o) \approx 2S \left[ \tilde{b}_q (\omega_o) \tilde{b}^*_q (\omega_o) \right],
\]

\[
= \frac{2S}{\omega_o - \alpha |\omega_o| - E_q}.
\]

where we have used equations (36) and (37), and the fact that in the 1D geometry \( \mathbf{q} \rightarrow q \). Introducing this result into equation (41) and performing the analytic continuation to real frequencies, we obtain:

\[
\text{Im} \chi^\pm(\omega) = -\frac{\alpha \omega}{(\omega - E_q)^2 + \alpha^2 \omega^2}.
\]

In figure 5 we show the spin response function \( -\text{Im} \chi^\pm(\omega) \) as a function of \( q \) and \( \omega \). The curves \( -\text{Im} \chi^\pm(\omega) \) show resonances centered at the magnon frequencies \( \omega = E_q \) (red line in the bottom \( q-\omega \) plane), which are broadened by the effect of \( \alpha \), the dimensionless coupling to the metal.

6. Conclusions and outlook

We have studied the phase diagram and the excitation spectrum of a magnetic chain of atoms or molecules with easy-axis ferromagnetic interactions. We focused on a simple model of \( S = \frac{1}{4} \) magnetic impurities displaying a Kondo-exchange interaction with the substrate. In the Ising
limit, which provides a good approximation to the ground state of an easy-axis ferromagnet, we obtained the phase diagram using a mean-field theory approach. We find that this system exhibits two possible phases at zero temperature: a paramagnetic phase where the impurity spins are screened by the substrate, and a gapped ferromagnetic phase whose excitations are damped by the magnetic (Kondo) exchange with the metallic substrate. Using a bosonic representation for the spins as well as various types of mathematical mappings between models, we have also investigated the excitation spectrum in the ferromagnetic phase, which may be accessible through probes such as spin-polarized electron energy loss (SPEELS). Although we have focused mainly on an easy-axis ferromagnetic (FM) chain, it is worth describing how our results can be modified in the case of the anti-ferromagnetic (AFM) chain corresponding to the parameter regime \( 1 < J_{\text{H}} \). The results can be modified in the case of the anti-ferromagnetic phase (especially for large \( J_{\text{H}} \)), due to the existence of a gap that separates the ferromagnetic ground state from the excitations and therefore protects the ground state from perturbations.

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**Appendix. Bosonization of the fermionic chains and mapping to the dissipative quantum Ising model**

In this Appendix, we implement the Abelian bosonization approach to the semi-infinite fermionic 1D chains along the \( y \) direction in figure 2 [31, 66]. This procedure is standard and has been successfully applied to describe the low-energy properties of the single Kondo impurity. We refer the reader to the standard bibliography [31, 66, 48, 47, 67, 68]. In the present case, the LBA greatly simplifies the complexity of the problem and enables a straightforward generalization to the case of many impurities, each one coupled to an independent fermionic bath. At low temperature, in the bosonic representation [68] the Hamiltonians (3) and (2) become

\[
H_F = \sum_{i,v=\{\nu,\sigma\}} \frac{v y}{4\pi} \int_{-\infty}^{\infty} dy \left( \nabla \phi^F_{i,v}(y) \right)^2, \tag{A.1}
\]

\[
H_K = \sum_i \frac{2\delta_{i,\nu}}{\pi \rho_0} S_i^z \nabla \phi^K_{i,\nu}(0) \sqrt{2\pi} + \frac{J_{\text{K}} b_0}{2} \left[ S_i^+ e^{-i \sqrt{2} \phi^K_{i,\nu}(0)} - \frac{2\pi \rho_0}{\delta^2_{i,j} \delta_{\nu,\eta}} \right], \tag{A.2}
\]

where \( \phi^F_{i,\nu}(y), \phi^K_{i,\nu}(y) \) are bosonic chiral fields which obey the commutation relations \([\phi^F_{i,\nu}(y), \phi^F_{i',\nu'}(y')] = i \pi \text{sign} (y - y') \delta_{i,i'} \delta_{\nu,\nu'}\), and which are related to charge and spin density...
fluctuations in the 1D fermionic chains through the relations \( \rho_i(y) = -\frac{1}{2}\nabla \phi^R_{1i}(y) \) and \( s_i(y) = -\frac{1}{2}\nabla \phi^L_{1i}(y) \), respectively [31, 68]. In equation (A.1) \( \nu \) is the Fermi velocity, and in equation (A.2) \( \delta_i = \tan^{-1}(\pi \rho_0 K b_0/4) \) is the scattering phase shift associated with the potential \( J_F S_i^z/2, \rho_0 = (2\pi \nu)^{-1} \) 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 in the fermionic chain. For simplicity we assume these states at the Fermi energy, and

In this case, the Hamiltonian reads

\[
H = \sum_i J_F S_i^z S_{i+1}^z + \frac{J_K}{2} b_0 \sum_i \left[ S_i^z e^{-i(\sqrt{2}-\gamma)\phi^R_{1i}(0)} + \text{h.c.} \right]
\]

\[
\bar{H}_K = \sum \left[ \frac{2\hat{\delta}_i}{\pi \rho_0} \sqrt{\frac{\gamma}{2\pi}} \nabla \phi^R_{1i}(0) S_i^z - \frac{J_K}{2} b_0 \sum_i \left[ S_i^z e^{-i(\sqrt{2}-\gamma)\phi^R_{1i}(0)} + \text{h.c.} \right] \right],
\]

\[
\bar{H}_F = H_F,
\]

where we have defined \( \hat{\delta}_i \equiv \delta_i - \gamma / 2\sqrt{2} \). Note that the local bath approximation equation (3) is crucial to implement bosonization along the chains, and to put these ideas on a clear mathematical framework. It is also interesting to note that in the transformed representation, the quantum dynamics of the bath (represented by the chiral field \( \phi^R_{1i}(0) \)) appears explicitly in the Heisenberg term \( -J_H^+ (S_i^+ S_{i+1}^- e^{-i[\phi^R_{1i}(0) - \phi^L_{i+1}(0)]} + \text{h.c.}) \). Physically, this means that the Heisenberg interaction is now ‘dressed’ by the spin-density fluctuations of the electron gas. In the case of an easy-axis spin chain in Ising limit \( J_H^+ \gg J_F \), the effect of this term is negligible and can be ignored in a first approximation.

We now exploit the freedom to choose \( \gamma \) and set \( \gamma = \sqrt{2} \). In this case, the Hamiltonian reads

\[
\hat{H} = \hat{H}_0 + \bar{H}_K + \bar{H}_F
\]

\[
\simeq \sum_i \left[ J_F S_i^z S_{i+1}^z + \frac{2\hat{\delta}_i}{\pi \rho_0} \sqrt{\frac{2\pi}{\gamma}} \nabla \phi^R_{1i}(0) S_i^z + \frac{J_K}{2\pi} S_i^z \right] + \bar{H}_F.
\]

This Hamiltonian corresponds to the 1D dissipative quantum Ising model (DQIM), where now the Kondo Hamiltonian \( \bar{H}_K \) is equivalent to the spin-boson model with Ohmic dissipation [67, 5, 4, 14], with \( \hat{\delta}_i \) related to the dissipative parameter \( \alpha \) in the context of macroscopic quantum coherence through \( \alpha = (2\hat{\delta}_i/\gamma)^2 \), and with the in-plane Kondo interaction playing the role of a magnetic field along the z-axis \( h_z = -J_K^+ /2\pi \). At \( T = 0 \), the 1D DQIM is known to display a paramagnetic to ferromagnetic quantum phase transition which is in the universality class of quantum dissipative systems and whose dynamical critical exponent is \( \gamma = 2 \). Note that this is very different from the case of the 1D quantum Ising chain, which is in the universality class of the 2D classical Ising model and where \( \gamma = 1 \). The critical properties of this model near the quantum phase transition have been studied in the context of anti-ferromagnetic instabilities of Fermi liquids [60, 11] using the framework of the Hertz–Moriya–Millis theory [69–71]. This theory describes critical quantum fluctuations of the order parameter around the Gaussian fixed point of the theory. The predicted value of the critical dynamical exponent \( \gamma = 2 \) and has been confirmed numerically with Monte Carlo simulations [12, 13]. Physically speaking, such a dynamical exponent implies that the effective dimensionality of the 1D spin chain coupled to the metallic bath is \( d_{eff} = 1 + \gamma = 3 \), and therefore fluctuations of the order parameter are expected to be much less important than the case of the non-dissipative classical or quantum Ising model. This fact supports our MF approximation, which allows one to extend these results to \( T > 0 \).

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