Dissipative dynamics of an extended magnetic nanostructure: Spin necklace in a metallic environment

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We study theoretically the dynamics of an “xxz” spin necklace coupled to a conduction electron sea, a model system for a nanostructure in a dissipative environment. We extract the long-time behavior via a mapping to a multichannel Coulomb gas problem followed by a scaling analysis. The strong quantum fluctuations of the necklace cause a nontrivial dependence of couplings on system size which we extract via an analysis involving the “boundary condition changing operator”, and confirm via a detailed numerical evaluation of one case.

The dissipative dynamics of a magnetic nanostructure is important from both technological and fundamental points of view. For example, magnetic recording involves the polarization of small domains, whose stability over long times is crucial. Tunnelling of isolated magnetic particles has been extensively studied \cite{1} \cite{2}. We shall be interested here in the new physics brought by coupling to a conduction electron bath. There are two effects. Exchange of spin between the conduction electron system and the nanostructure changes the magnetic state of the nanostructure, leading effectively to a tunneling process. On the other hand, dissipation from the particle-hole excitations of the metal suppresses tunnelling \cite{3}. A finite cluster of spins coupled to a conduction electron bath is thus a model system for examining general issues of quantum coherence and dissipation in a system with many degrees of freedom. Also, recent experimental advances in atom manipulation \cite{4} \cite{5} mean that clusters of atoms (eg. quantum corrals) can now be placed in controllable arrays on suitably chosen solid surfaces, so it seems likely that in the near future controlled magnetic nano-arrays may be constructed and studied.

In the case of a single spin in a metal, the interplay between tunnelling and dissipation gives rise to the logarithmic renormalizations characteristic of the one-impurity Kondo effect \cite{6}. While the two \cite{7} \cite{8} and three \cite{9} impurity Kondo problems have been studied, there is less known about the behavior of systems containing larger numbers of spins. The subject has been recently studied in the context of the “Griffiths phase” scenario for the non-Fermi-liquid physics apparently observed in certain ‘heavy fermion’ metals \cite{10}. To study this physics, Castro-Neto and Jones \cite{8} considered a cluster of $N$ magnetic impurities, coupled strongly to each other and weakly to a conduction electron bath. They presented a series of qualitative arguments and approximate mappings from which they concluded that the system could undergo a more or less conventional Kondo screening (which they termed a “cluster Kondo effect”), at an $N$-dependent temperature which they estimated. The qualitative nature of the treatment suggests however that further analysis would be useful. One of us, with Morr and Schmalian \cite{11}, treated a similar problem of $N$ coupled moments from a functional integral point of view. In the Ising case, orthogonality effects were found to suppress tunnelling in all but the smallest nanostructures, while no definitive results were obtained in the continuous symmetry case.

In this paper we attack the problem from a different point of view. We identify a specific nanostructure, the finite-size spin necklace depicted in Fig.1. There are three motivations for this choice of cluster. First, it is (as can well be seen) amenable to a detailed analysis. Second, it exhibits large (but tractable) quantum fluctuations whereas in other works \cite{8} \cite{11} the quantum fluctuations within the cluster are not taken into account. Third, we can treat the continuous symmetry case as well.

![Fig.1 Sketch of ‘spin necklace’ in conduction electron bath for $N = 5$. Heavy dots represent local moments, which are coupled via an exchange coupling $K$. Shaded area represents conduction electron (c) sea, Kondo-coupled to local moments via exchange $J$.](image)

The Hamiltonian describing the physics of interest is

\begin{equation}
H = H_{\text{necklace}} + H_{\text{cond}} + H_{\text{coupling}}^z + H_{\text{coupling}}^\perp \tag{1}
\end{equation}

\begin{equation}
H_{\text{necklace}} = \sum_{j=0}^{N-1} (K_{\perp}(S_j^z S_{j+1}^z + S_j^y S_{j+1}^y) + K_z S_j^z S_{j+1}^z) \tag{2}
\end{equation}

\begin{equation}
H_{\text{cond}} = \sum_k \epsilon_k c_k^\dagger c_k \tag{3}
\end{equation}

\begin{equation}
H_{\text{coupling}}^z = J_z \sum_{j=0}^{N-1} S_j^z (c_{R_{j,\uparrow}}^\dagger c_{R_{j,\downarrow}} - c_{R_{j,\downarrow}}^\dagger c_{R_{j,\uparrow}}) \tag{4}
\end{equation}

\begin{equation}
H_{\text{coupling}}^\perp = J_\perp \sum_{j=0}^{N-1} (S_j^x c_{R_{j,\downarrow}}^\dagger c_{R_{j,\uparrow}} + S_j^x c_{R_{j,\uparrow}}^\dagger c_{R_{j,\downarrow}}) \tag{5}
\end{equation}
with $\mathbf{R}_j$ the position of spin $j$. Here each spin value is $S_j = 1/2$ and $\mathbf{S}_N = \mathbf{S}_0$. We restrict to the case of $K_\perp > -|K_z|$, so the ground state of $H_{\text{necklace}}$ is not ferromagnetic. We further specialize to $N$ odd so the ground state is characterized by a spin quantum number $S^z = \pm 1/2$. For $K_\perp < 0$ the total momentum of each of the $S^z = \pm 1/2$ states is zero and the ground state is four-fold degenerate. For $K_\perp > 0$ the ground state also has non-zero total momentum $P = \kappa |\mathbf{P}|$, $\kappa = \pm 1$ implying four-fold degeneracy. In this paper we focus on the limit in which the Kondo coupling $J$, of the cluster to the conduction electrons is weak enough and the temperatures of interest low enough, that it is sufficient to consider only those spin flip processes that couple the degenerate ground states of the cluster. We expect that stronger couplings, implying mixing of higher energy states of the cluster, give rise to qualitatively similar physics. This case will be considered in a future paper [12].

If $H_{\text{coupling}} = 0$, then the $z-$component of the cluster spin is a good quantum number. The cluster remains in a definite spin state, the conduction electrons just feel a potential due to the longitudinal coupling $J_z$, and the Hamiltonian $H_0 = H_{\text{necklace}} + H_{\text{cond}} + H_{\text{coupling}}$ is easily diagonalized. For non-zero $J_\perp$ the problem is no longer trivially solvable. To study it, we use a perturbative expansion in $J_\perp$ to establish a mapping onto a Coulomb gas, following the approach introduced by Anderson and Yuval [6]. Let $|\Psi_\theta\rangle$ denote the ground state of $H_0$ when the cluster is in the $S^z = +1/2$ state, $|\theta\rangle$ and consider the ground-state-to-ground-state amplitude (alternatively the partition function in the imaginary time formulation) given in the interaction representation by

$$Z(t) = \left\langle \Psi_\theta | e^{iH_0t} T \exp[i \int_0^t H'(t')dt'] | \Psi_\theta \right\rangle$$

where $H'(t) = e^{-iH_0t} H_{\text{coupling}} e^{iH_0t}$ and $T$ is the “time ordering operator”. Restricting to the ground state of the cluster, and expanding to $O(J^2)$,

$$Z(t) = J^2 \int_{t_0}^{t_1} dt_1 \int_{t_2}^{t_1} dt_2 \sum_{\mathbf{R}_i} \sum_{\mathbf{R}_j} \langle \uparrow \uparrow | S_i^+ | \uparrow \uparrow \rangle \langle \uparrow \uparrow | S_j^+ | \uparrow \uparrow \rangle \times F_i(\mathbf{R}_{ij}, t_{12}) F_j(\mathbf{R}_{ij}, t_{12})$$

where $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j$, $t_{12} = t_1 - t_2$ and

$$F_i(\mathbf{R}_{ij}, t_{12}) = \left\langle \Psi_\theta | T c_i^{\dagger}(\mathbf{R}_i, t_{12}) c_i(\mathbf{R}_i, t_{12}) | \Psi_\theta \right\rangle$$

$$S(t_{12}) = T \exp[-i \int_{t_{12}}^{t_1} d\tau V(\tau)]$$

$$V(\tau) = -2J \sum_{\mathbf{R}_j} \langle \uparrow \uparrow | S_j^+ | \uparrow \uparrow \rangle c^{\dagger}_{\mathbf{R}_j}(\tau) c_{\mathbf{R}_j}(\tau).$$

The expressions above are similar to the ones introduced in the context of the X-ray [13] [14] and the Kondo problem [6], but with new features arising from the spatially extended nature of the magnetic object. The most important of these new features are the space dependence of $F$, arising from processes in which an electron is created at one site and destroyed at another, and a nontrivial dependence of matrix elements such as $\langle \uparrow | S_i^+ | \downarrow \rangle$ on necklace size and symmetry. We discuss these in turn.

Following Ref. [13] we express $F$ as the product of open line part $g = F/|S|$ and a closed loop part $S$ $\equiv e^C$ which may be computed by an expansion in $J_z$. The crucial object in this expansion is the Green’s functions $G(\mathbf{r}, t)$ of $H_{\text{cond}}$. We require the long time limit $(t \gg R/v_F$ with $R$ the radius of the necklace) in which $G(\mathbf{r}, t) \rightarrow \rho_F G(\mathbf{r})/it :$ for a spherical Fermi surface $G(\mathbf{r}) = 2 \sin(k_F)/v_F$. In order to obtain a closed form for $g$ we exploit the specific geometry of the necklace. We parametrize the positions of the spins by the azimuthal angle $\phi_j = 2\pi j/N$, $j \in [0, N - 1]$. Using $R_{kl} = 2R \sin(\phi_{kl}/2)$, where $\phi_{kl} \equiv \phi_k - \phi_l$, $G(R_{kl}) \rightarrow G(\phi_{kl})$. We finally define the one-dimensional Fourier transform

$$G_m = \sum_{k=\pm 0}^{N-1} G(\phi_{kl}) e^{im\phi_{kl}}$$

$$G(\phi_{kl}) = \frac{1}{N} \sum_{m} G_m e^{-im\phi_{kl}}$$

where we choose $m = -\frac{N-1}{2}, ... 0, ... \frac{N-1}{2}$ to make the symmetry of the problem most apparent: $G_{-m} = G_m$. Using the $m-$basis and defining $V = -2J_z \tilde{V} |\uparrow \rangle |S^+_i | \uparrow \rangle$,

$$g(\phi_{ij}, t_{12}) \equiv \sum_{m} \frac{\rho_{F} G_m}{iN(t_{12})} e^{-i\alpha_{ij}} \left\langle \tau_{12} \right\rangle \sum_{m} G_m^2$$

$$e^{C(t_{12})} = \left\langle \tau_{12} \right\rangle \sum_{m} \sum_{m} G_m^2$$

where $\tau_c$ is the short-time cut-off separating two spin-flips and we have neglected terms of $O(J^4)$ in the exponent.

We now consider the matrix elements. We first note that if $K_\perp > 0$ then the necklace ground states $|\uparrow \rangle$, $|\uparrow \rangle$ have a nonvanishing momentum $\pm P_{\phi}$, and the matrix element depends on the momentum transfer: $\langle \uparrow | S_i^+ | \uparrow \rangle = \langle \uparrow | S_i^+ | \uparrow \rangle \exp[iQj]$ where $Q = (P_0 - P_\phi)$. When $K_\perp > 0$, the absolute value of the matrix element decays faster with $N$ when $P_\phi = P_0$. For $K_\perp > 0$ when $P_\phi = -P_0$ and for $K_\perp < 0$ we find, defining $\alpha \leq 1$,

$$|\langle \uparrow | S_i^+ | \uparrow \rangle| \sim 1$$

$$|\langle \uparrow | S_i^+ | \uparrow \rangle| \sim 1$$

For $|K_\perp| \leq |K_z|$, in terms of the Jordan-Wigner fermion representation [17], the states $|\uparrow \rangle$ and $|\downarrow \rangle$ have different boundary conditions, one periodic and the other antiperiodic. Considering the low energy form of the Hamiltonian given by the Luttinger (massless) model
and adopting the “boundary-condition changing operator” formalism [15] [16] we find
\[ \alpha = \frac{1}{2} \left( 1 - \frac{1}{3} \cos^{-1} \frac{K}{|K_z|} \right) \quad \text{for } |K_z| \leq |K_\perp| \] (17)
which we verify by a detailed numerical analysis (see Fig.2) of the exact lattice solution for the \( K_z = 0 \) case (\( xx \)-model [17]) for which \( \alpha = 1/4 \).

![Fig.2 Plot of absolute value of \( M = \langle \uparrow | S_0^x | \downarrow \rangle \) evaluated numerically for the \( K_z = 0 \) case as a function of \( N \). \( \Delta_{\mu} \) is the matrix element when the Jordan-Wigner fermion is added (when spin is flipped) in the unoccupied momentum \( k_\mu \), each of which contributes to \( M \). The inset plots its real, imaginary parts and the absolute value as a function of \( k_\mu \) for \( N = 283 \). The maximum contribution is near the Fermi point. We find that \( |M| \) is equal to \( |\Delta_{\mu}| \) (obtained when \( k_\mu \) is closest (\( \mu = 0 \)) to the Fermi point) and when plotted against \( N \), the two plots overlap.

For the Ising case (\( K_z = \infty \)) for \( K_z > 0 \), the energy is minimized by having alternating up and down spins, but \( N \) being odd there is one frustrated bond with \( N \) possible locations for each of \( S^z = -\frac{1}{2} \) and \( \frac{1}{2} \). A perturbative analysis around this \( 2N \) fold degenerate point yields
\[ \alpha = 1 \quad \text{for } K_z \gg |K_\perp|. \] (18)
We expect \( \alpha = 1 \) for all \( K_z > |K_\perp| \) (Ising regime).

The results for \( \alpha \) indicate that it is much easier than one might guess, to flip a large cluster between its two ground states. Quantum fluctuations, which for example in the Ising regime delocalize the frustrated bond, bring about dramatic enhancement in the tunneling caused by one spin flip by a conduction electron. By distributing \( S^z = \pm 1/2 \) over \( N \) sites, they also decrease the expectation value of \( S_\perp^z \), thereby reducing the potential felt by the conduction electrons at each spin site.

We are now in a position to present our result for the ground-state-to-ground-state amplitude for the spin necklace embedded in a conduction bath,
\[ Z(t) = \sum_m u^*_m \int_0^t dt_1 \int_0^{t_1} dt_2 \frac{d\tau_c}{\tau_c} \] (19)
\[ \times \exp \left\{ -2 \alpha \right\} \ln \left( \frac{\tau_c}{t_2 - t} \right) \] (20)
where using \( 2\pi \bar{Q}/N = Q = (P_y - P_y) \),
\[ \varepsilon_m = \bar{J}_z [G_m + G_{m+Q}] - \bar{J}_z^2 \sum_{m'} G^{2}_{m'} \] (21)
\[ u_m = \bar{J}_L G_m G_{m+Q} \] (22)
with \( \bar{J}_\perp = J_{\perp} \rho_F \langle \langle S_0^x | \downarrow \rangle \rangle \sim J_{\perp} \rho_F / N^\alpha \) and \( \bar{J}_z = 2 \rho_F J_z \langle \langle S_0^z | \downarrow \rangle \rangle \sim J_z \rho_F / N \). Note that since \( \sum_m G^2_m \sim N \), the two terms in \( \varepsilon_m \) are of the same order in \( N \) and its leading behavior is given by the term linear in \( J_z \rho_F \) (assumed \( \ll 1 \)). In the corresponding expression obtained in Ref. [11] it was assumed that only one channel was important and in the expression for \( \varepsilon_m \), the term linear in \( J_z \) was overlooked. The above expression for \( Z \), Eq.(19), is the second-order term in the expansion of a multicomponent Coulomb gas model in which each spin flip event (Coulomb gas charge) is labelled by the channel \( (m - \text{value}) \) of the electron-hole pair created. Higher order terms in the expansion in \( J_z \) may be treated similarly, but compact expressions cannot be obtained because (as noted in a related context [18]) in the multi-channel case, the higher order terms do not combine into the Cauchy determinant form [6]. However we may define a scaling procedure as usual [19] by eliminating close-pair spin flips of the same channel. To the leading order the different channels are not coupled, and standard arguments show that near the weak coupling fixed point, the partition function retains the form Eq.(19) but with parameters \( \varepsilon_m(\tau_c) \) and \( u_m(\tau_c) \) which evolve according to
\[ d\varepsilon_m / d(\ln \tau_c) = 2u^2_m \] (23)
\[ du_m / d(\ln \tau_c) = u_m \varepsilon_m / 2 \] (24)
with initial conditions given by Eq.(21) and (22). The flow implied by Eq.(23) and (24) is shown in Fig.3.

![Fig.3 Plot showing the flow for each channel, near the weak coupling fixed point. The heavy solid line is the separatrix \( \varepsilon_m = -u_m/2 \). The shaded oval region shows the generic initial conditions for the \( xx \) symmetry. The dotted circle shows the generic initial conditions for the Ising limit. The striped region near \( u_m = 0 \) is the range of initial conditions for ‘imperfect’ necklaces.

For each channel the flow is to the no-flip fixed line (\( u_m = 0 \)) if \( \varepsilon_m < -u_m/2 \) and towards the strongly
coupled (rapidly flipping) regime (with $\varepsilon_m = u_m/2$) if
$\varepsilon_m > -u_m/2$. Scaling amplifies the differences between
channels. For example, in the $K_1 < 0$ case of the
$xx$–model, the initial condition is $u_0^0 = J^2 \rho_F G_m/N^{1/4}$
and $\varepsilon_0^0 = 2Jz \rho_F G_m/N$. For large $N$, $\varepsilon_0^0$ is thus
parametrically smaller than $u_0^0 m$; all initial conditions are near
the vertical axis and the dominant channels are those with the largest
$G_m$. Representative results are shown in Fig.4. Note that for the ideal
ring studied here, $G_{-m} = G_m$. We see that all channels with $m < Nk_F/2\pi$
roughly equal strength, but generically there is one largest pair, so after a
transient many channel regime, the asymptotic behavior is of the two-channel
Kondo problem. Extensions can occur, and in particular for $k_F \lesssim 2\pi/N$, the $m = 0$ channel dominates. The
same generic behavior occurs in other cases we have studied, but we note that in the Ising regime the $J_z$ and $J_\perp$
couplings are both $\sim 1/N$, so the initial conditions are shifted as indicated in Fig.3.

To summarize: we have shown that the generic long-
time dynamics of a spin necklace coupled to a conduction
electron bath is of the two-channel Kondo class. We
emphasize that generic deviations from perfect translation invariance break the
two-channel symmetry. A key feature of the model is the large quantum fluctuations
characteristic of the isolated necklace: these ensure that the
dominant spin flip amplitude between the ground states
of the spin necklace decays only as a power of the system size ($N^{-\alpha}$ with $0 < \alpha \leq 1$) and that the static
field exerted by the necklace on the conduction bath is
small, of order $1/N$, so “orthogonality” effects do not
dominate. To explore the changes occurring as quantum
fluctuations are reduced, we consider a necklace in the
extreme Ising limit ($K_z \gg |K_\perp|$) and with one weak link
($K_{z_0} \rightarrow K_z(1-\delta)$) which acts to localize the frustrated
bond. A detailed discussion and extension to other cases
will be published elsewhere [12]. Here we note that although the residual reflection symmetry allows two chan-

nel behavior, the spin flip amplitude changes from $\sim 1/N$
to $\sim \exp[-N \ln(K_\perp/\delta K_z)]$ (moving the initial condition
much closer to the $u_m = 0$ axis of Fig.3). More
importantly, because the frustrated bond is localized, the
quadratic, “orthogonality” term in $\varepsilon_m$ (Eq.(21)) becomes
$\sim J_{\perp}^2 N$, moving the initial condition substantially to the
left (independent of the sign of $J_z$); and, for large enough
$N$, into the stable (no asymptotic flip) region.

Extensions of the present work include a treatment of
systems with open boundary conditions, and of other
nanostructures. We expect generically that internal quantum fluctuations of a nanoscale object (neglected in
many treatments, Ref. [8] and [11] for example) will have
a dramatic effect on the long time dynamics.

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Fig.4 Plot showing $G_m$ in the $K_1 < 0$ case of the $xx$–model
for two values of $k_F$. For $k_F = \pi$, the pair $m = -10$ and 10 and
for $k_F = \pi/2$, the pair $m = -4$ and 4 is the highest, constituting
the dominant pair which governs the low energy behavior.

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