Majorana Coupling and Kondo Screening of Localized Spins

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We perform a theoretical analysis of the fate of the local magnetic moment of a quantum dot coupled to a normal metallic lead and a topological superconducting wire hosting Majorana modes at the ends. By means of simple analytical tools and numerical renormalization group calculations, we show that the proximity of the Majorana mode reduces the magnetic moment from $\frac{1}{4}$, characteristic of a free spin $\frac{1}{2}$, to $\frac{1}{16}$. Coupling to the normal lead then causes the Kondo effect, such that the magnetic moment is fully screened below the Kondo temperature. The latter is vastly increased for strong coupling to Majorana mode.

1. Introduction

The quest for the realization of Majorana modes (MMs) in the solid state is mainly motivated by applications [1–3] and promising experimental results [4]. The hope for fault-tolerant quantum computing using MMs stems from their topological protection against local disturbances [5]. As a consequence, a rich field of research focused on realizing and manipulating MMs has emerged, as summarized in a number of reviews [6–9].

Recently, the field has been experiencing criticism as summarized in [10] concerning hasty publications with exaggerated conclusions. Furthermore, practical implementation for useful computation would require a large number of Majorana devices, which does not seem feasible soon. Here, we leave the mainstream application-oriented approach and address basic theoretical questions concerning the interplay of MMs with strongly interacting mesoscopic systems, hoping to gain some understanding. This relatively unexplored direction has been pioneered by [11] and remains relevant especially in the context of transport properties of quantum dots proximitized by topological superconducting wires [12–16]. We focus on the interplay between the Kondo effect [17] and the local MM-spin coupling by studying the minimal model — as elaborated further. We analyze this by looking at the fate of the magnetic moment localized on the quantum dot at low temperatures.

2. Model and methods

We consider a single quantum dot (QD) coupled to a one-dimensional topological superconducting nanowire, called further the Majorana wire (MW); see Fig. 1. MW is characterized by a superconducting gap and a pair of (Majorana) modes at Fermi energy, which are strongly localized at the ends of the wire. Therefore, especially at temperatures ($T$) much smaller than the superconducting gap, the only relevant coupling between QD and MW is electron hopping into and from these end-modes, and the in-gap Hamiltonian of QD and MW can be written in the form [11]

\begin{equation}
H_{\text{DM}} = \sum_{\sigma} \varepsilon n_{\sigma} + U n_\uparrow n_\downarrow + \lambda (\hat{d}_1^\dagger \hat{\gamma}_1 + \text{h.c.}) + i \varepsilon_M \hat{\gamma}_1 \hat{\gamma}_2,
\end{equation}

where $\varepsilon$ is the QD energy level, $U$ is the on-dot Coulomb repulsion, while $\lambda$ measures the QD–MW coupling strength. The operators $\hat{d}_\sigma^\dagger$ creates the spin-$\sigma$ electron at QD ($\hat{n}_{\sigma} = \hat{d}_\sigma^\dagger \hat{d}_\sigma$), and the Majorana operators $\hat{\gamma}_1$, $\hat{\gamma}_2$ are normalized such that $\{\hat{\gamma}_1, \hat{\gamma}_2\} = 1$. The last term in $H_{\text{DM}}$, proportional to $\varepsilon_M$, corresponds to the Majorana modes overlap, which is exponentially small for long wires and shall henceforth be neglected, i.e., $\varepsilon_M = 0$. Note that only $\sigma = \downarrow$ electrons are coupled to MW.

At first glance (1) may be seen as a fusion of the Anderson-like impurity with the Kitaev chain model [18], where bulk states are completely
removed and only in-gap states remain. One of them is then coupled via hopping with QD. In the experiment, MW is a complex hybrid nanostructure, typically comprising a semiconductor with strong spin-orbit coupling and a conventional superconductor, almost fully spin-polarized with the help of a magnetic field. While such a system is vastly more complicated than the Kitaev model, it eventually leads to a practically spin-polarized $p$-wave superconductor, with an energy gap and in-gap MMs. These are the generic features we model simply by (1), which serves very well at temperatures below the energy gap in the superconductor, as long as the MW is long enough for both the coupling to its other side and $\varepsilon_M$ to be neglected [19].

QD is further attached to metallic electrode, modeled as non-interacting, with energy dispersion $\varepsilon_k$. This means the lead part of the Hamiltonian is $H_L = \sum_{k,\sigma} \varepsilon_k \hat{n}_{k,\sigma}$, with $\hat{n}_{k,\sigma} = \hat{c}_{k,\sigma} \hat{c}_{k,\sigma}^\dagger$ and $\hat{c}_{k,\sigma}^\dagger$ creating the corresponding electron. Finally, the hybridization term takes the form $H_h = \sum_{k,\sigma} v(d^*_{k,\sigma} \hat{c}_{k,\sigma} + \text{h.c.})$, where $v$ is the tunneling matrix element and h.c. stands for a Hermitian-conjugate term. The total Hamiltonian of the system is $H = H_{DM} + H_h + H_L$. In the calculations we take the wide-band limit, i.e., we assume the (normalized) density of leads states $\rho(\omega)$ is a constant within the cut-off window, $\omega \in [-D, D]$, and vanishes outside (we use $D = 2U$). The broadening of the dot level denoted by $\Gamma = \pi \rho(0) \sigma^2$ measures the coupling strength to normal lead.

In general, the magnetic susceptibility $\chi$ is defined as a linear coefficient of the spin polarization response induced by the application of a small external magnetic field $B$. In impurity or QD systems, the relevant quantity is the impurity contribution to $\chi(T)$ [17], which can be defined as

$$\chi(T) = -\frac{\partial}{\partial B} \langle \hat{S}_z \rangle_T \bigg|_{B=0}, \quad (2)$$

where $\hat{S}_z$ is the $z$-th component of the QD spin, $B$ is the magnetic field acting locally at QD, and $\langle \ldots \rangle_T$ denotes a thermal expectation value. The magnetic moment is simply $\mu(T) = T \chi(T)$. To calculate these quantities numerically at given $T$, we add a small field $B \ll T$ into $H (H \rightarrow H + g\mu_B BS_z)$, with gyromagnetic ratio $g$, Bohr magneton $\mu_B$; units of $B$ adjusted such that $g\mu_B = 1$, and $\hat{S}_z = (\hat{n}_\uparrow - \hat{n}_\downarrow)/2$.

Then, $\chi(T) = -\langle \hat{S}_z \rangle_T/B$ follows from (2). To reliably solve the model in the Kondo regime, we use the numerical renormalization group (NRG) technique [20]. Our implementation is based on open-access code [21], exploiting the symmetries of charge parity and total spin-$\gamma$ electron number conservation. We use the discretization parameter $\Lambda = 3$ and keep around the $N = 1000$ states during NRG iteration. We also provide a number of exact analytical results where possible.

3. Results

For a free spin $S$ at low $T$, the magnetic susceptibility can be calculated directly as defined in (2) as

$$\chi_S(T) = \frac{S(S+1)}{3T},$$

which implies $\mu(T) = 1/4$ for $S = 1/2$. This high fragility to the magnetic field leads to the vulnerability of localized spins, often suppressed at low $T$ due to one of the following circumstances:

(i) Ordering tendencies. In practice, spins are often coupled by the exchange interaction $J$, which in the case of just 2 local moments leave them in a singlet (for antiferromagnetic (AFM) $J > 0$) or triplet (for ferromagnetic (FM) $J < 0$) ground state at $T = 0$, with $\langle \hat{S} \rangle_z$ independent of $B$ unless it exceeds the binding energy $\sim |J|$. The same mechanism leads to magnetic instabilities in lattices possessing local moments, which tend to form a magnetic order (FM or AFM, depending on the sign of effective exchange coupling between the localized spins).

(ii) The Kondo effect. Coupling to the continuous bath drives the Kondo effect. Then, a portion of free conduction electrons bind into a singlet with a localized QD spin at $T$ below the so-called Kondo temperature, $T_K$. Then, the divergence of $\chi$ is suppressed below $T_K$, such that for $T \ll T_K$ we have $\chi \sim 1/T_K$ and $\mu = 0$ [17] (see in particular Appendix K there).

These two mechanisms typically compete with each other [22], driving many strongly-correlated phases of matter [23, 24].

In the model introduced in Sect. 2, free spin behavior is present in the absence of QD–leads couplings, $\Gamma = \lambda = 0$. A direct calculation following from (2) then gives

$$\mu_{QD} = \frac{1}{4} \left[ 1 + \exp \left( -\frac{U}{2T} \right) \cosh \left( \frac{\delta}{T} \right) \right]^{-1}, \quad (4)$$

Fig. 1. Scheme of a structure comprising a single quantum dot hybridized with a normal-metal contact with overall coupling strength $T$ and coupled to a long topological superconductor nanowire hosting Majorana modes $\gamma_1$ and $\gamma_2$. K.P. Wójcik et al.
The significance of this result can be better understood by contrasting it with the result obtained for QD proximitized by a conventional superconductor. Indeed, taking the BCS Hamiltonian with states outside the gap integrated out [25], \( H_{\text{DM}} = \sum_{n} \epsilon \hat{n}_n + U \hat{n}_n \hat{n}_n + \Gamma_5 \hat{d}_n \hat{d}_n + \text{h.c.} \) instead of \( H_{\text{DM}} \) of (1), we get

\[
\mu_{\text{DM}} = \frac{1}{4} \left[ 1 + \cosh \left( \frac{\sqrt{T^2 + \delta^2}}{T} \right) \exp \left( \frac{-U}{2T} \right) \right].
\]  

(7)

This differs from (4) only by replacement \( \delta \to \sqrt{T^2 + \Gamma_5^2} \), which for small \( \Gamma_5 \) simply slows the approach to the asymptotic free-spin behavior at \( T = 0 \) in singly-occupied regime \((|\delta| \ll U)\). However, at \( \Gamma_5 = \sqrt{U^2 - \delta^2} \) there is a quantum phase transition from a spin doublet for small \( \Gamma_5 \) to a spin singlet at large \( \Gamma_5 \) [26], and \( \mu_{\text{DM}}(0) \) discontinuously switches from 1/4 to 0. This is in stark contrast to continuous and always incomplete suppression of \( \mu_{\text{DM}} \), see (5).

In the presence of a normal lead, the situation changes dramatically. Already for \( \lambda = 0 \) (i.e., with MW completely detached) \( H \) takes the form of the Anderson model, where the Kondo effect leads to a screening of \( \mu(T) \) below \( T \to T_K \) [17]. However, \( T_K \) decreases rapidly for small \( \Gamma \), such that in reality at the lowest experimentally relevant temperature \( T \) (modeled here by \( T = 10^{-7} U \)) a crossover is observed between the weak coupling regime for small \( \Gamma \), with \( \mu(T) \approx 1/4 \), and the strong coupling regime for large \( \Gamma \), characterized by the Kondo-screened moment \( \mu(T) = 0 \). The weak coupling case is realized e.g. for \( \Gamma = 10^{-3} U \), as presented in Fig. 2 with a solid black line lying on top of the dashed free-spin (\( \lambda = 0 \)) one.

While without MW, \( \Gamma = 10^{-3} U \) is too small to affect the fate of the magnetic moment at the relevant temperatures (corresponding \( T_K \sim 10^{-12} U \) [27]). The presence of MW changes this situation dramatically. This is clearly visible as the difference between the dashed and solid lines in Fig. 2 for \( \lambda > 0 \). In all these cases, \( \mu(T) \) is partially suppressed — as for \( \Gamma = 0 \) at the intermediate \( T \), but drops to 0 for \( T \to 0 \) — similarly to the Kondo regime. This is even more evident in Fig. 3, where \( \mu \) is plotted as a function of \( \lambda \) for a few values of \( \Gamma \) at \( T = 10^{-7} U \), mimicking a cryogenic experiment. Even for \( \Gamma = 10^{-5} U \), a large \( \lambda \) leads to complete suppression of \( \mu \), which requires screening by conduction band electrons. This shows that the presence of MW vastly increases the Kondo temperature, by hastening the renormalization group flow away from the local moment fixed point at high energies before the Kondo coupling becomes relevant there. Apparently, the Kondo coupling is even more relevant around the \( \Gamma = 0 \) fixed point for \( \lambda > 0 \). Not only does it scale to strong coupling [11, 15], but it also does so at much higher \( T \). This result agrees

Fig. 2. The temperature dependence of the magnetic moment \( \mu(T) \) for \( \epsilon = -U/2 \) and \( \Gamma = 0.001U \) (solid lines, NRG results), as well as for \( \Gamma = 0 \) (dashed lines, exact (5)), and different values of \( \lambda \) as indicated in the figure.

Fig. 3. The magnetic moment \( \mu \) for \( T = 10^{-7} \) as a function of the QD-MW coupling \( \lambda \) for the indicated values of \( \Gamma \).

where \( \delta = \epsilon + U/2 \). In the limit \( T/U \to 0 \) this result asymptotically reaches \((4T)^{-1} \) expected from (3) for \( S = 1/2 \), as long as \( |\delta| \) does not exceed \( U/2 \) (QD is singly occupied then). This is shown (for \( \delta = 0 \)) in Fig. 2 as a dashed black curve.

In fact, (2) can be exactly solved in a relatively simple form also for the case \( \lambda \neq 0, \delta = 0 \), while \( H_{\text{DM}} \) can be diagonalized exactly [14]. The result is

\[
\mu_{\text{DM}} = \frac{1}{4} \left[ \frac{w+16u^2 T/U}{2w^{3/2}} \tanh \left( \frac{\sqrt{w}}{4T/U} \right) + \frac{1+4u^2}{2w} \right],
\]

where we set \( u = \lambda/U \) and \( w = 1 + 8u^2 \). This is presented for several values of \( \lambda \) as dashed lines in Fig. 2. As expected, for \( \lambda = 0 \) we have \( u = 0, w = 1 \), and at low \( T \) (when the argument of \( \tanh \) function becomes very large) \( \mu_{\text{DM}} \to 1/4 \). However, for \( \lambda > 0 \), the \( T = 0 \) magnetic moment becomes

\[
\mu_{\text{DM}}^{T \to 0} = \frac{1}{4} \left[ \frac{1 + \sqrt{1 + 8u^2} + 4u^2}{2(1 + 8u^2)} \right],
\]

which is plotted in Fig. 3 with a thick black line. Strikingly, \( 1/4 \geq \mu_{\text{DM}}^{T \to 0} > 1/16 \), so the magnetic moment is partially suppressed in the vicinity of MW. This reflects the fractional nature of MMs. Note that the suppressed fraction is not universal and even the minimal value \( \min(\mu_{\text{DM}}^{T \to 0}) = 1/16 \) does not correspond to any intuitive effective free spin \( S \) in (3). Inverting it with \( \chi_S = (16T)^{-1} \) gives \( S = (\sqrt{7} - 2)/4 \approx 0.161 \).
with the general tendencies of $\lambda$ increasing $T_K$, reported in [13, 14], but due to the large $\lambda$ considered here, the effect is much more spectacular. This intriguing effect calls for a better understanding.

4. Conclusions

Our analytical results for a quantum dot coupled to large-gap topological superconductor wire in the absence of a normal leads show a universal partial suppression of the QD’s local magnetic moment for strong QD–MW coupling $\lambda$. This is in contrast to the conventional superconductor behavior, where the low-temperature magnetic moment does not change. In the presence of the normal lead, even smaller magnitude of $\lambda = 0.01U$ causes a tremendous increase in the Kondo temperature. In particular, $\lambda = 0.01U$ is sufficient to enhance it for $\Gamma = 0.001U$ from hundreds of orders of magnitude below $U$ to around $10^{-7}U$. Together with the recent reinterpretation [28] of existing experimental data concerning candidate Majorana observation [29] in terms of conventional Kondo effect, this shows that proper understanding of the Kondo physics in the Majorana systems might be crucial for correct interpretation of the measurements.

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