

# Superconducting quantum dot and the sub-gap states

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## ABSTRACT

Quantum dots are nanostructures made of semiconducting materials that are engineered to hold a small amount of electric charge (a few electrons) that is controlled by external gate and may hence be considered as tunable artificial atoms. A quantum dot may be contacted by conductive leads to become the active part of a single-electron transistor, a device that is highly conductive only at very specific gate voltages. In recent years a significant attention has been given to more complex hybrid devices, in particular superconductor-semiconductor heterostructures. Here I review the theoretical and experimental studies of small quantum-dot devices contacted by one or several superconducting leads. I focus on the research on the low-lying localized electronic excitations that exist inside the superconducting gap (Yu-Shiba-Rusinov states) and determine the transport properties of these devices. The sub-gap states can be accurately simulated using the numerical renormalization group technique, often providing full quantitative understanding of the observed phenomena.

**Keywords:** quantum dots, magnetic impurities, transport properties, Coulomb blockade, superconductivity, Yu-Shiba-Rusinov states, numerical renormalization group, Josephson current

## 1. INTRODUCTION

Soon after the discovery of superconductivity it was observed that magnetic impurity atoms are strongly antagonistic to the superconducting order: even a small concentration of magnetic dopants (below one percent) can suppress the critical temperature  $T_c$  down to zero temperature.<sup>1-3</sup> At the same time, superconductivity is remarkably robust to other kinds of impurities and persists in strongly disordered (even amorphous) samples.<sup>4</sup> The difference was shown to be related to the time-reversal invariance, a symmetry with respect to reversal of the direction of time flow, that is broken in magnets.<sup>4</sup> Controlled experiments revealed that the suppression of  $T_c$  can be correlated with the spin of the dopant atoms (rather than their magnetic moment), thus it must be associated with the exchange interaction between the impurity and the host.<sup>1</sup> In addition, the suppression was linear in the impurity concentration, indicating that this is not a collective phenomenon, but instead each impurity site acts independently.<sup>1</sup> Finally, it was observed that at high impurity concentrations the moments order magnetically,<sup>1</sup> implying that the impurities couple with the itinerant electrons of the superconductor. These three key insights show that the basic theoretical model for understanding the interplay between superconductivity and magnetic effects consists of a single magnetic impurity represented by a point-like quantum mechanical spin which is exchange coupled with the host electron gas.<sup>3</sup> After the Bardeen-Cooper-Schrieffer theory of superconductivity had been developed,<sup>5</sup> it was shown that a magnetic impurity modelled as a localized static magnetic moment induces a bound state inside the superconducting gap.<sup>6-9</sup> Such excitations are now known as Yu-Shiba-Rusinov states or Andreev bound states (the first name will here be used in the following; the two terms are equivalent when applied to quantum dots which behave as magnetic impurities). The theory was later extended to incorporate the fact that magnetic impurities actually have internal dynamics, i.e., that the impurity spin can flip when host electrons exchange-scatter on the impurity site.<sup>10-12</sup> This required a correct description of the impurity dynamics, a notoriously difficult theoretical problem known as the Kondo problem.<sup>13-22</sup>

The Kondo effect (anomalous behavior of normal-state metals at low temperatures due to magnetic dopants) was experimentally observed in 1930s, and theoretically understood much later in 1960s after noticing the

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diverging behavior of high-order perturbation-theory calculations with decreasing temperatures in a model for a single spin exchange-coupled to a normal-state metal (the  $s - d$  model), despite the fact that the exchange coupling  $J$  is in principle a small parameter.<sup>13</sup> Indeed, the problem was later shown to be non-perturbative in  $J$  and required the development of entirely new theoretical tools to reliably solve it.<sup>15–17,23–26</sup> In some very simplified cases a full analytical solution is possible for some properties of the model (e.g. for thermodynamics, but not for the full frequency dependence of spectral functions).<sup>17,24</sup> A more generally applicable numerical technique for tackling this problem was developed in 1970s by K. G. Wilson<sup>16,23,27,28</sup> and later refined and generalized.<sup>29–37</sup> This approach, now known as the Wilson’s numerical renormalization group (NRG), consists in reformulating the impurity problem as a one-dimensional continuum problem with a point-like defect. The continuum is then discretized and the discrete Hamiltonian is tridiagonalized to obtain a one-dimensional tight-binding chain representation of the host conduction-band. An appropriate choice of the discretization scheme leads to exponentially decreasing hopping constants along the chain.<sup>16</sup> The impurity is attached at the beginning of this half-infinite chain. The problem is then iteratively diagonalized: First an initial block consisting of the impurity and one or several chain sites is exactly solved by diagonalisation of the relevant Hamiltonian matrix. Then another chain site is taken into consideration, new Hamiltonian matrices in extended Hilbert space are constructed, and the resulting eigenproblem is solved again. Since the Hilbert space grows exponentially with the number of chain sites included, at some step the states need to be truncated to the low-energy subspace. This is actually a good approximation because the matrix elements relating the low-energy and high-energy sectors are quickly decaying with increasing energy difference (the property of energy-scale separation), thus discarding the high-energy states does not affect the physics on low energy scales.<sup>16</sup> The method allows to calculate the spectrum of many-body states, thermodynamic properties, expectation values of all local (neighborhood of the impurity) and some non-local operators, dynamic quantities, and even the response to quantum quenches (sudden changes of Hamiltonian parameters).<sup>36</sup> Importantly, the method is applicable to all those situations where the host Hamiltonian can be reliably approximated by a mean-field decoupling of the interaction terms. This is notably the case for the reduced Hamiltonian in the BCS theory of superconductivity.

In early 1990s, the NRG method was for the first time applied to the problem of magnetic impurities in a BCS superconducting host.<sup>38–41</sup> It confirmed the presence of Yu-Shiba-Rusinov (YSR) states and for the first time allowed to very accurately describe their properties. The interest in this class of problems was renewed in the early 2000s, when it was realized that a quantum dot embedded between two superconducting contacts has unusual behavior of the Josephson current (the current flowing in the absence of voltage difference between two superconductors with different superconducting phases) in the regime where it behaves as a magnetic impurity.<sup>42</sup> Furthermore, experimental techniques were developed to probe single magnetic atoms on superconductor surfaces using the tip of a scanning tunneling microscope, giving access to space resolved information.<sup>43</sup> A final impetus to this research field was the realization that hybrid semiconductor-superconductor devices may host robust (topologically protected) excitations known as Majorana zero-modes,<sup>44–46</sup> which are predicted to be non-Abelian anyons whose braiding corresponds to unitarily changing the state of the ground-state multiplet of the system that might lead to an implementation of quantum computers that are particularly resilient to environment-induced decoherence.

In section II, this contribution presents the basic physics of the YSR states in quantum dots coupled to superconducting leads. Section III reviews some experimentally relevant extensions of the model, such as the effects of additional normal-state tunneling probes and that of the external magnetic field, high-spin impurities and magnetic anisotropy effects. Section IV discusses more recent experiments involving multiple quantum dots and their theoretical interpretation.

## 2. YU-SHIBA-RUSINOV STATES

A quantum dot can be electrostatically defined using gate electrodes deposited on the surface of a semiconductor heterostructure that hosts a two-dimensional electron (2DEG) gas below its surface.<sup>47,48</sup> 2DEG electrons are repelled by the potential below the electrodes and using suitable patterning it is possible to obtain a small puddle of electrons coupled to neighboring 2DEG via tight constrictions: quantum point contacts. A further gate electrode controls the number of confined electrons. Alternatively, the electrons can be confined in sections of carbon nanotubes and semiconductor nanowires, again by suitable shaping the electrostatic potential using

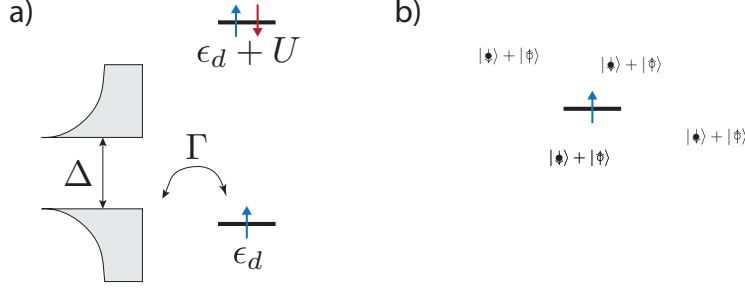


Figure 1. (a) Level diagram of the system under discussion: an impurity level  $\epsilon_d$  with electron-electron repulsion  $U$  is hybridized with a continuum of excitations in a superconductor with a gap  $\Delta$  through hybridization with strength  $\Gamma$ . (b) Schematic representation of a Yu-Shiba-Rusinov state as the bound state of the impurity spin up (blue arrow) and spin-down Bogoliubov quasiparticles (superpositions of spin-down electrons and spin-up holes) from the superconducting conduction lead.

metallic electrodes. The transport properties of such devices can then be probed by measuring the current as a function of source-drain bias and gate voltage.<sup>49</sup> One or both of the source/drain electrodes can be made of a material which becomes superconducting below the critical temperature  $T_C$ , giving rise to hybrid superconductor-semiconductor devices and superconducting quantum dots.<sup>50</sup>

The simplified description of such a device is obtained by retaining solely the electron level that is closest to the chemical potential. (As discussed in the following, this is in fact an excellent approximation on low energy and temperature scales.<sup>51</sup>) The corresponding Hamiltonian then takes the form of the Anderson impurity model<sup>14</sup> with superconducting leads:<sup>52</sup>

$$H = H_{\text{QD}} + \sum_{\alpha} H_{\text{lead},\alpha} + \sum_{\alpha} H_{c,\alpha}. \quad (1)$$

Here

$$H_{\text{QD}} = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} \quad (2)$$

describes the QD energy level  $\epsilon_d$  with electron-electron repulsion  $U$ , the charge operator is  $n_d = n_{d\uparrow} + n_{d\downarrow}$  with  $n_{d\sigma} = d_{\sigma}^{\dagger} d_{\sigma}$ , where  $d_{\sigma}$  is the electron annihilation operator. Further,

$$H_{\text{lead},\alpha} = \sum_{k\sigma} \epsilon_k c_{k\sigma,\alpha}^{\dagger} c_{k\sigma,\alpha} + \sum_k \left( \Delta_{\alpha} c_{k\uparrow,\alpha}^{\dagger} c_{-k\downarrow,\alpha}^{\dagger} + \text{H.c.} \right), \quad (3)$$

is the BCS Hamiltonian for lead  $\alpha = 1, 2, \dots$ , where the operator  $c_{k\sigma,\alpha}$  corresponds to an electron with momentum  $k$ , spin  $\sigma$  and energy  $\epsilon_k$  in lead  $\alpha$ , while  $\Delta_{\alpha} = |\Delta_{\alpha}| \exp(i\phi_{\alpha})$  is the BCS order parameter of lead  $\alpha$ . Finally,

$$H_{c,\alpha} = \sum_{k\sigma} \left( V_{\alpha} c_{k\sigma,\alpha}^{\dagger} d_{\sigma} + \text{H.c.} \right) \quad (4)$$

is the coupling between the lead  $\alpha$  and the impurity;  $V_{\alpha}$  is the tunnel coupling. The strength of the hybridisation between the dot and the leads can be conveniently quantified by scalar quantities  $\Gamma_{\alpha} = \pi \rho_{\alpha} |V_{\alpha}|^2$ , where  $\rho_{\alpha}$  is the density of states at the Fermi level in the normal-state of lead  $\alpha$ . The parameters can be widely tuned in the experiments, giving access to very different regimes.<sup>53</sup> A schematic representation of the problem is shown in Fig. 1(a).

We first consider the simplest case of a single conduction lead with  $\alpha = 1$ . The BCS gap  $\Delta_1 \equiv \Delta$  can be assumed to be real with no loss of generality in this case, and we write  $\Gamma_1 \equiv \Gamma$ . In the absence of the impurity, this model would have a spin-singlet ground state (the BCS superconducting wave-function), separated by  $\Delta$  from the onset of the continuum of spin-doublet excitations (Bogoliubov quasiparticles). For large  $U \gtrsim \pi\Gamma$ , the impurity is magnetic<sup>54</sup> and the Anderson impurity model in this regime maps<sup>55</sup> onto the Kondo impurity model with Kondo exchange coupling  $\rho J \approx 8\Gamma/\pi U$ . It turns out that the ground state of the system then depends on the ratio of two quantities,  $T_K/\Delta$ .<sup>3,10,11,56</sup>  $T_K$  is known as the Kondo temperature and it is given approximately by

$T_K \sim U\sqrt{\rho J} \exp(-1/\rho J)$ .<sup>18</sup> This defines the characteristic temperature and energy scale in the Kondo problem with normal-state lead: for  $T \lesssim T_K$  the effects of the exchange coupling between the impurity spin and the conduction-band electrons lead to large effects. In particular, in a normal-state lead the impurity spin becomes effectively screened for  $T \ll T_K$ , meaning that a spatially-extended many-body Kondo state is formed between the localized spin and the itinerant electrons. This state is a spin-singlet. In the superconducting case, however, the fermions required to form the Kondo state are not available to form the Kondo singlet if  $\Delta \gg T_K$ . The ground state of the system is then well approximated by a tensor product of an unperturbed BCS state (a spin-singlet) and a free impurity spin (a spin-doublet), producing a many-body ground state that is an over-all spin-doublet. On the contrary, if  $T_K \gg \Delta$ , the gap is so small that it hardly perturbs the Kondo screening and the ground state is essentially the Kondo singlet state. These considerations imply that with varying ratio  $T_K/\Delta$  an abrupt change of the ground state is expected. It is indeed directly observed in the NRG calculations: a level crossing occurs at  $T_K/\Delta \approx 0.3$  between a spin-singlet and a spin-doublet many-particle states. This first-order quantum phase transition (QPT) between singlet and doublet ground states has a number of observable consequences, in particular in the spectral function.<sup>3,50,57</sup> The singlet and doublet states are namely connected by the matrix elements that contribute to the single-particle excitation spectrum, thus the transition between them is visible in tunneling spectroscopy (see also below and the subsection 3.1). At the QPT, the singlet and doublet state switch their roles as the ground state and excited state, respectively, thus spectroscopically this is visible as a crossing of excitation lines.

The original works by Yu, Shiba, and Rusinov addressed a simplified version of this problem by freezing the impurity spin and neglecting all spin-flip events.<sup>6-8</sup> This is also known as the “semi-classical approximation” that is formally achieved by taking the  $S \rightarrow \infty$  and  $J \rightarrow 0$  limit, so that  $JS = \text{const}$ . These authors have shown that a static magnetic impurity acts as an attractive potential for Bogoliubov quasiparticles for one spin orientation (that opposite to the polarisation of the impurity) and repulsive for the other spin species. Since an impurity is effectively a 1D problem, this implies that a bound state must exist for attracted Bogoliubov quasiparticles. The binding energy is given as [see Fig. 2(a)]:

$$E_{\text{YSR}} = \Delta \frac{1 - \alpha^2}{1 + \alpha^2}, \quad (5)$$

where  $\alpha$  is the dimensionless coupling constant,  $\alpha = \pi\rho JS/2$ . For low Kondo coupling  $J$ , the YSR state is located just below the continuum of Bogoliubov states, but it descends deep down in the gap region and eventually crosses zero (at  $\alpha = 1$ , i.e.,  $J = 2/\pi\rho S$ ). At this point, a Bogoliubov quasiparticle becomes trapped at the impurity site,<sup>9</sup> thereby “screening” the impurity spin, see Fig. 1(b). This is actually highly reminiscent of the behavior in the full quantum problem: apart from the quantitative details (dependence of the excitation energy on  $J$ ) and the degeneracy (a doublet of both spin orientations in quantum case, a single spin polarization in the classical case), the qualitative behavior is essentially the same. For this reason, the sub-gap states in the quantum case are also commonly referred to as YSR states. In general, several such sub-gap can exist at the same time, see Fig. 2(b) for illustration.

There are several approaches for characterizing superconducting QD devices.<sup>50,58-60</sup> One involves measuring the Josephson current, which is a ground-state property of the system.<sup>61-64</sup> In particular, it can be shown that the singlet state is associated with the so-called 0-junction behavior, where  $j \approx j_c \sin \phi$ , with  $j_c > 0$  being the critical current and  $\phi = \phi_2 - \phi_1$  is the phase difference between the SC order parameters  $\Delta_1$  and  $\Delta_2$  of the two superconducting leads contacting the device. The doublet state is, however, associated with the so-called  $\pi$ -junction behavior, where  $j \approx j_c \sin(\phi + \pi) \approx -j_c \sin(\phi)$ . Such reversals of the Josephson current at QPTs are indeed experimentally detectable.<sup>42,50,65</sup> Another commonly used technique is tunneling spectroscopy, whereby a further (ideally weakly coupled) electrode at finite voltage is used as a tunneling probe to measure the density of states (spectral function) at the impurity site.<sup>52,66-68</sup> In addition, non-equilibrium Andreev transport can also be used.<sup>69,70</sup>

Experiments have shown that the simple QD devices are often surprisingly well described by the simplest version of the Anderson impurity model as introduced in this section. The tunneling spectra match the calculated spectral functions both on the energy scale within the gap, as well as somewhat beyond the gap edges in the continuum.<sup>51</sup> The agreement between the measured tunneling spectra and the computed equilibrium spectral

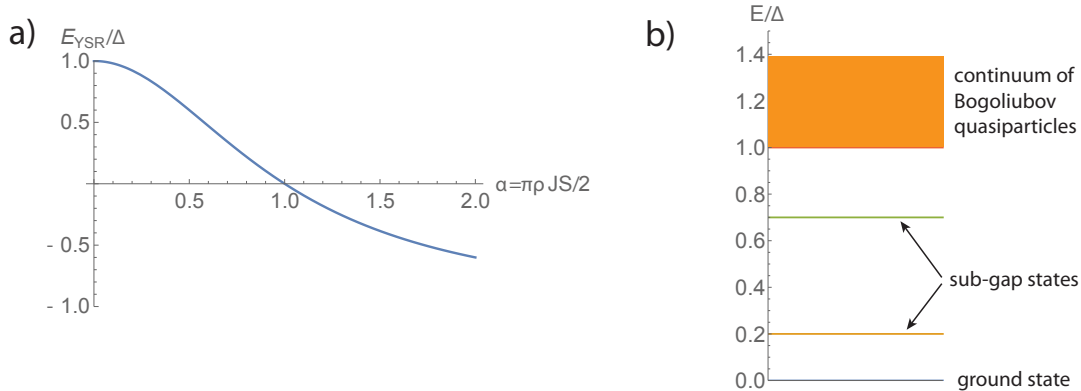


Figure 2. (a) The binding energy of the Yu-Shiba-Rusinov single-particle state in the semi-classical approximation. (b) The level diagram for many-particle states in the full quantum impurity problem.

functions is in fact rather surprising, since the dominant transport mechanism at the lowest temperatures is expected to be that associated with Andreev scattering that gives particle-hole symmetric spectra (equal spectral weights at positive and negative bias voltages), while experimentally one typically observes asymmetric spectra that match the asymmetry observed in the numerically calculated spectral function.<sup>51</sup> This implies the presence of a relaxation mechanisms (presumably due to phonons) that lead to a fast decay of excited states, so that the transport is actually dominated by the single-electron tunneling. The cross-over between these two transport regimes has been recently studied through scanning tunneling spectroscopy of magnetic adsorbates on superconductor surfaces using a tunneling microscope stabilized to two different temperatures.<sup>71</sup> In semiconductor quantum dots, it appears that the transport is dominated by the single-electron tunneling down to the lowest temperatures that can be achieved in dilution refrigerators.<sup>72</sup>

Recently a careful quantitative comparison between the theoretical predictions (as calculated using the NRG) and the experimental tunneling spectral (measured on InAs nanowires with Al contacts) has shown excellent agreement over two decades of the  $T_K/\Delta$  ratio.<sup>56</sup> This demonstrates the excellent tunability of modern quantum devices, as well as establishes the NRG results as the correct solution of the Kondo problem in the case of superconducting host.

### 3. BEYOND THE SIMPLE ANDERSON IMPURITY PROBLEM

Despite the successful description of a quantum dot coupled to superconducting contacts using the simplest Anderson impurity model with a single superconducting continuum, there are situation requiring more involved modeling.

#### 3.1 Normal-state Tunneling Probes

As previously described, a common technique to characterize quantum dot devices is tunneling spectroscopy involving an additional weakly coupled electrode. Ideally, such an electrode is expected to act as a non-perturbing probe that merely reveals the QD spectral function, but does not affect the system under study. There are, however, several caveats. A numerical study has shown that even a relatively weakly coupled tunneling lead can significantly shift the QPT line in the phase diagram.<sup>73</sup> Furthermore, in the case of the doublet ground state where the impurity remains unscreened, the continuum electrons in the tunneling probe can act as an additional screening channel and lead to the emergence of a Kondo resonance in the tunneling spectrum.<sup>73</sup> Using a superconducting lead as a tunneling probe provides no benefit in this regard: in this case one uses the Bogoliubov states at the edge of the continuum to probe the QD, again leading to Kondo screening, this time by the Bogoliubov quasiparticles.

### 3.2 External Magnetic Fields

An external magnetic field has a weak effect on the singlet sub-gap state, but it directly leads to Zeeman splitting of the doublet sub-gap state, as observed in experiments.<sup>74</sup> One spin direction will thus become favored compared to other states, hence the region in the phase diagram of the model where this state is the ground state will expand.<sup>73,75</sup> The exact behavior strongly depends on the  $g$ -factors of the impurity and of the host.<sup>76</sup> The standard theory neglects the  $g$ -factor in the host, which is a sensible approximation in system with very large (absolute value of) impurity  $g$ -factor, as is for example the case with InAs nanowires. More generally, the ratio of the  $g$  factors influences the phase diagram of the singlet-doublet transition as a function of the magnetic field and the  $k_B T_K / \Delta$  ratio.<sup>76</sup>

It is to be noted that in sufficiently strong external magnetic field a quantum impurity behaves increasingly like a classical, because the internal spin dynamics become frozen. Similar observation holds for the effect of the Weiss exchange fields in magnetically ordered systems. If the Néel relaxation time is longer than the typical experimental times, the mean-field decoupling is a perfectly valid approximation and theoretical description becomes simple. The most difficult theoretical situation is thus that of a small number (order 10) of coupled quantum impurities (see section 4), each of which is a dynamic object which couples with neighboring impurities.

Since the sub-gap states are spectroscopically very sharp, it is possible to very accurately measure the effective  $g$ -factor of the quantum dot. This value is reduced from the bare  $g$  value by the renormalization through Kondo exchange coupling, leading to an order  $\rho J$  correction. This provides a further way to extract the Kondo coupling strength from experimental measurements (although it has not been put to use so far).

### 3.3 High-spin Impurities

In quantum dots with specific geometry it is possible that several electron orbitals are partially occupied at the same time, leading to situations where the electrons form a high-spin many-body state. This is also the natural state of affairs in most adsorbed magnetic atoms and molecules on surfaces. In these systems the orbital moment is partially or totally quenched due to the broken spatial symmetry at the surface, while the spin degree of freedom persists but experiences magnetic anisotropy effects due to spin-orbital coupling. See section 3.4.

These systems can be described using a multi-orbital Anderson or high-spin Kondo impurity system, similar to the Hamiltonian in section 2, but with electrons carrying a further orbital quantum number. As in the single-orbital situation, the impurity spin degrees of freedom will be screened by the itinerant electrons in a generalized Kondo effect.<sup>77,78</sup> As a rule, a single “channel” of conduction band electrons (carrying a specific value of the orbital momentum) can screen a spin-1/2 unit of spin, thus a spin- $S$  impurity will be fully compensated if it is coupled to  $2S$  different channels. Here, in the context of quantum dots, a “channel” means a linear combination from one or several conduction leads which couples to one of the orbitals of the impurity. To each of these channels one can assign a corresponding Kondo exchange coupling constant  $J_i$ . In turn, each of these defines a different Kondo temperature  $T_{K,i}$ . If  $J_i$  are unequal, as is usually the case, the temperatures  $T_{K,i}$  will be (exponentially) different. In a normal-state situation (none of the leads superconducting), the Kondo screening will then proceed in several stages as the temperature is reduced.<sup>79</sup> If some of  $T_{K,i}$  are much lower than the experimental temperature, the moment is partially unscreened and the impurity remains magnetic. When the leads are superconducting, the (partially) screened Kondo states will become discrete sub-gap many-particle states.<sup>80</sup> In the presence of  $c \leq 2S$  channels, the original spin- $S$  is screened to  $c$  different spin- $(S - 1/2)$  states,  $\binom{c}{2}$  spin- $(S - 1)$  states,  $\binom{c}{3}$  spin- $(S - 3/2)$  states, etc. Some (or most) of these states will be merged with the continuum and will hence be non-observable: only those with  $T_{K,i} \sim \Delta$  will be sufficiently inside the gap to play a role. Furthermore, only those that differ by  $\Delta S = \pm 1/2$  from the ground state spin will be spectroscopically observable in tunneling experiments at zero temperature, while at finite temperature additional peaks will become observable, corresponding to the transition between thermally excited states coupled by the same  $\Delta S = \pm 1/2$  selection rule.

### 3.4 Magnetic Anisotropy Effects

In the presence of spin-orbit coupling and reduced spatial symmetry (notably on surfaces) the spin multiplets will be split.<sup>81</sup> This can be described using a Hamiltonian such as

$$H_{\text{aniso}} = DS_z^2 + E(S_x^2 - S_y^2), \quad (6)$$

where  $D$  is known as the longitudinal anisotropy and  $E$  is the transverse anisotropy. The directions  $xyz$  are here determined as the principal axes of the magnetic anisotropy tensor. For axial anisotropy,  $D < 0$ , the absolute value of  $S_z$  is maximized and the impurity behaves as an Ising variable. For planar anisotropy,  $D > 0$ , the fermion parity determines the resulting state: for integer spin, the non-magnetic state  $S_z = 0$  will be the ground state, while for non-integer spin, the Kramers doublet  $S_z = \pm 1/2$  emerges. For axial anisotropy, the transverse anisotropy is particularly important: for integer spin, it leads to “quantum spin tunneling”, Rabi oscillations between the  $S_z = +S$  and  $S_z = -S$  states.

When an impurity is coupled to a superconductor, the magnetic anisotropy splittings are directly visible in tunneling spectroscopy.<sup>80,82</sup> All spin multiplets are split, and those connected by  $\Delta S_z = \pm 1/2$  (for  $E = 0$ ) are spectroscopically well visible. At finite temperatures, the weights of the spectral peaks depend on the occupancy of the levels and make it possible to distinguish the splitting in the ground state from that in the excited state. This fact allowed to experimentally confirm the presence of magnetic anisotropic splitting of the  $S = 1$  state in magnetic molecules adsorbed on a superconductor surface.<sup>83</sup>

### 3.5 Thermal effects

Strictly at zero temperature, and in the absence of environment noise, the sub-gap states in  $s$ -wave superconductors should be true  $\delta$  peaks with vanishing intrinsic line-width. In reality, there is a number of mechanisms that lead to a finite line-width. In hybrid semiconductor-superconductor devices, the induced gap is “soft” in the sense that the density of states inside the gap is not zero, but there is instead a finite concentration of quasiparticles. This mechanism is absent in systems of magnetic adsorbates on thick superconducting substrates which have “hard” gaps. There the broadening is due solely to thermal effects, most likely linked to thermally excited vibrational degrees of freedom which are probably extrinsic to the impurity and rather located in the substrate.<sup>71</sup> It is presently unclear whether the electron-electron interaction may intrinsically lead to finite width of YSR peaks at finite temperatures. Delicate NRG calculations suggest that this might be the case.<sup>84</sup> In magnetically anisotropic Kondo impurities the presence of a continuum of excitation inside the gap at finite temperatures has been shown analytically using a perturbative expansion which is a good approximation in the limit of weak Kondo coupling constant.<sup>85</sup>

### 3.6 Mesoscopic superconducting islands

Recently it has become possible to attach a small mesoscopic superconducting island to a quantum dot.<sup>86</sup> In this case the superconductor has a finite charging energy,  $H_{SC} = E_c(\hat{N} - N)^2$ , where  $\hat{N}$  is the electron number operator while  $N$  is a parameter which is proportional to the applied gate voltage. This problem is thus a superconducting generalization of the Kondo quantum box problem. Since the continuum becomes interacting in this case, it would seem that the problem is beyond the scope of the NRG method. One can, however, apply a technical trick. By introducing a charge operator of the electron box, one can track the particle transfers between the quantum dot and the reservoir. The reservoir can then again be considered as noninteracting and the only price is the introduction of an additional auxiliary local degree of freedom, which can however be handled in the NRG calculations.<sup>87</sup>

An example is considered in Fig. 3. A quantum dot is coupled to a superconductor with a moderate value of charging energy  $E_c = U/10$ . It is observed that the charging of the superconducting islands affects the charging of the dot. The charging diagram has the appearance of the honeycomb and it is not unlike the charging diagram of double quantum dot structures in its appearance. The modulation of the charging of the charge box also affects the sub-gap states in the quantum dot, leading to a periodic pattern. This model may provide a microscopic interpretation of the results in Ref.<sup>86</sup> In that work an ad-hoc picture in terms of a fixed-energy bound state was introduced to explain the repetitive pattern observed in the Coulomb diagrams. Instead, the repetitive structures find a natural explanation in terms of charging of a mesoscopic charge reservoir (which here happens to be superconducting).

## 4. MULTIPLE-QUANTUM-DOT DEVICES

Nanostructures constructed out of several quantum dots can be considered as tunable artificial molecules. They make it possible to study the inter-impurity interactions induced by tunneling electrons, such as the formation

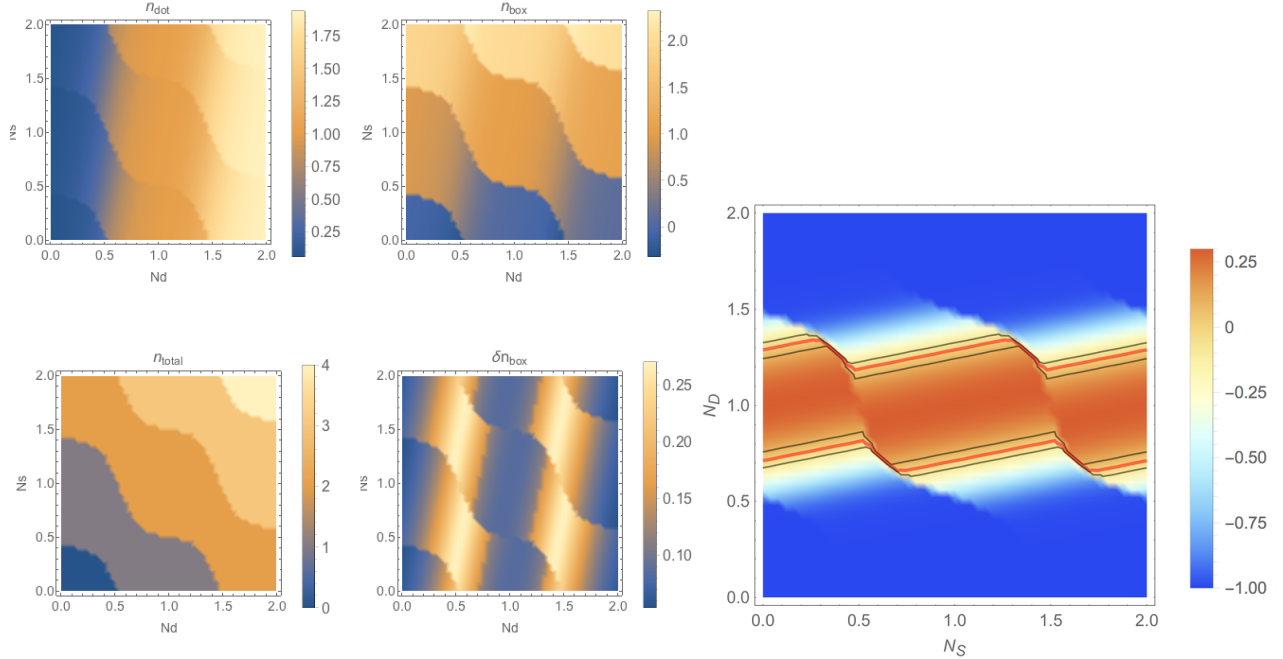


Figure 3. Quantum dot coupled to a small superconducting island with sizable charging energy. (a) Electron filling (occupancy) of the quantum dot,  $n_{\text{dot}}$ , superconducting island,  $n_{\text{box}}$ , their sum,  $n_{\text{total}}$ , and charge fluctuations on the superconducting island,  $\delta n_{\text{box}}$ . The axes correspond to gate voltages applied on the dot,  $N_D$ , and on the reservoir,  $N_S$ , expressed in dimensionless units of charge/occupancy. (b) The energy difference between the singlet and doublet states. Positive value corresponds to a doublet ground state, negative value to a singlet state. Red line is the singlet-doublet transition line and the gray lines indicate the width of the transition region. Model parameters are  $U = 1$ ,  $\Gamma = 0.1$ ,  $E_c = 0.1$ ,  $\Delta = 0.01$  in units of the superconductor half-bandwidth.

of molecular-orbital levels via hybridisation of electron states in individual dots, as well as the exchange coupling that leads to spin alignment of confined electrons. These effects were intensely studied in a variety of different realisations of double quantum dots (DQDs) with normal-state leads.<sup>88–90</sup> More recently, the interest in the same phenomena resurged in the context of sub-gap states,<sup>91,92</sup> where it is equally interesting to determine the fate of YSR states in extended systems. The YSR states are known to hybridize when their wavefunctions overlap, a question of particular importance for the search of Majorana edge states in topological superconductors. In addition, there is the super-exchange interaction that is predicted to lead to different spin states of the collective many-particle state. Controlled experiments of this type required the development of tunable devices with multiple (finger) electrodes. These are now available. They allow independent tuning of several model parameters, e.g. the on-site potentials on the dots, coupling to the superconductors as well as that between the dots. At the same time, the refinement of algorithms and the availability of powerful computers made it possible to simulate these systems with increasing accuracy.

In a recent experiment, a DQD was coupled to a single superconductor. The properties of the device were characterized by sweeping the potentials of each dot, thereby changing the electron occupancy of each dot between 0 and 2, and measuring the differential conductance using an additional weakly-coupled electrode.<sup>72</sup> In particular, the zero-bias differential conductance was mapped as a 2D diagram in all charge states. For weak coupling to the superconductor, one obtains results similar to that for normal-state DQDs, the so-called “honeycomb diagram”, where the lines of high conductance correspond to charge degeneracy, i.e., to many-body states with different occupancy being degenerate in energy. In the superconducting case, the lines of high conductance correspond to the YSR states crossing zero frequency in the spectra, but the interpretation is essentially the same: different YSR sub-gap states become degenerate. The lines thus delineate the different regimes of singlet or doublet ground states. As the coupling to the superconductor is increased, however, the diagrams change their appearance



completely: the singly-occupied charge state (a spin-doublet at weak coupling) on the dot directly coupled to the superconductor is becoming increasingly screened. In other words, the YSR singlet drops in energy until it becomes the ground state in that part of the phase-diagram. This leads to a characteristic shape and topology of the transition lines. This behavior was fully captured in theoretical calculations based on a simple approximation of the superconductor with a single electron orbital (the so-called “zero-bandwidth approximation”), as well as in full NRG simulations.<sup>72</sup>

## 5. CONCLUSION

Nanostructures constructed out of quantum dots coupled to superconductors have in addition to their potential utility as building blocks of topological quantum computers a more fundamental scientific value: the superconducting gap namely opens a window to directly observe and study the competing many-body states that manifest as spectroscopically sharp spectral features, while they are otherwise masked by the continua of excitations in normal-state systems. As the control of the devices is further increased (improvements in lithography, harder gaps with reduced residual density of states in the gap, better control over the gate electrodes, multi-finger electrode geometries) and the resolution in spectroscopy is improved (microwave spectroscopy), it is expected that some of the interesting details that are presently still elusive will eventually be observed. Some prominent examples are the triplet YSR states in multiple-quantum-dot structures,<sup>72,92</sup> as well as the multiple singlet states in two-channel-Kondo-effect structure incorporating mesoscopic superconducting islands, indicating the non-Fermi-liquid nature of the ground state.<sup>93</sup>

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