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Complex molecular structures

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(Summary)

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KEY-WORDS: *ferromagnetism, superconductivity, solid surface, contacts, interface, junctions, Andreev reflection, electric flow, tunneling, transistor effect.*

SUMMARY

1. Introduction. The scientific research in the Condensed Matter field is dominated in the recent years by two basic themes: nanostructures and the control of electrical circuits by spin polarization.

Between atomic scale (cca $1nm = 10$Å) and mesoscopic scale (cca $1\mu m = 10^4$Å) there exists large room ("there is plenty of room at the bottom" said Feynman as early as 1959), where new forms of matter aggregation occur: atomic and molecular clusters, nanowires, dots, surfaces, interfaces, junctions, contacts, with an infinite richness in electriocal, optical, magnetic, spectroscopic, chemical properties, opening new opportunities in the ultra-minaturization of the the control and command devices. On the other hand, multiple developments in the nanostructures field brought up again in discussion the question of matter aggregation: how do the ensembles of many atoms and molecules form, with more atoms than those in the usual molecules, what are their properties? What is the process underlying the nanoscopic binding, beyond the chemical bonds? This question received an important answer recently.[1]

Bringing into discussion the electron spin is for long an important wish, because it would give rise to use other degrees of freedom beside the electrical charge. New direction of research may appear in this context, with exotic names like "spintronics", or "moletronics", *i.e.* the electronics of spin, the electronics of the molecule, respectively. The magnetization associated to spin and, in general, the effects of the magnetic field on the electron motion (like the quantul Hall effect) are such as to bring surprising novelties in the control of the electrical current, like the giant magneto-resistance for instance (2007 Nobel prize, Fert si Gruenberg).

In the control of ultra-miniatural electrical circuits (meso and nanoscopic) there exists a fundamental problem: it is preferrable to have small currents and erlatively normal voltages. This would ensure a low power and an adequate control. Therefore, one needs a high resistance. In the ballistic transport, that dominates this nanoscopic region, thesituation is precisely the opposite: the current is high because the resistance is low. For getting out of this deadlock one must pay attention to the nature of the contcats, junctions, which must be carefully gauged, such as to ensure a convenient potential barrier.It is konwn for long that such a abrrier arises naturally at the normal metal-superconductor junction, by the effect called the Andreev reflection.[2, 3] The presence of the superconductor makes even more attractive such a junction. In addition, the Andreev reflection may depend on the electron spin orientation, which makes natural the interest for the ferromagnet-superconductor coupling. More, the ferromagnet may have the spin polarized, so that we may face the favourable opportunity of controlling effectively the electrical current through magnetization. In this context there have been carried out the studies that make the subject of the present doctoral Thesis. More specifically, we have tried to answer in this Thesis the question: is there possible a transistor-type effect at the feromagnet-sperconductor junction, and in what conditions? Obviously, the answer implies one main target:

the computation of the electrical resistance of such a junction as a function of magnetization. This is the main original result of the Thesis.

In order to get at this result a multitude of difficulties must have been overcome. In addition, being given the degree of difficulty and novelty of the subject a series of simplifying hyptheses were made, aimed at putting ourselves in a situation as close as possible to an ideal situation, while still preserving the main ingredients which ensure the degree of realism of the model , at least in principle.

2. Superconductivity. Therefore, we needed a convenient formulation of the classical tehory of superconductivity (Bardeen-Cooper-Schrieffer (BCS) theory). This is done in Chapter 2 of the Thesis, where we make a review ofthe pairingtheory, gap nad critical temperature equations, thermal properties, ultrasound attenuation, microwave absorption, ralaxation rate of the nuclear spin resonance, tunneling and Josephson current. Special attention is given to the Landau-Ginsburg theory, Meissner effect, quantization of the magetic flux,surface energy and, especially, the coherence length. In addition, this Chapter includes the general elements of the classical Andreev reflection. In particular, the tunneling, Josephson effect, coherence length, surface energy and the Andreev reflection are absolute requisitories for the effect envisaged.

3. The Magnetism of Matter. The second major problem was the characterization of the classical ferromagnet. As it is well-know, the magnetism of matter is an extremely rich field in physical phenomena and still the fundamental understanding of the ferromagnetism does not go, practically, beyond the mean field theory of Weiss. The profound cause of the ferromagnetic magnetism is still lacking (though important progress was made by introduction of the exchange integral by Heisenberg in the early time of Quantum Mechanics). This drawback may lead sometime to an inadequate tackling of the dynamics of the magnetisation. An instance for this point is provided by the study of this dynamics under the effect of the spin-polarized current, whic led recently to new results.[4] Therefore, Chapter 3 of the Thesis made a review of the magnetism of matter, including the paramagnetism, molecular field, quantum magnetism and exchange integral, Curie temperature, ferromagnetism, spin waves, ferromagnetic domains, antiferromagnetism and various sorts of diamagnetism. This review proved to be extremely useful in analyzing the main problem, because it assured us of the fact that an injection current with polarized spins is possible in ferromagnet and it is possible to work below the critical temperature of the ferromagnet which must lie below the critical temperature of the superconductor Of course, we havd in mind high-temperature superconductors (like those based on copper oxides, for instance ytrium-barium-copper-oxygen (YBCO)) and classical ferromagnets of manganese-compounds type (for instance lantan-strontium-manganese-oxygen (LSMO)).

4. Transport. Since the main question was the computation of the electrical resistance at the ferromagnet-superconductor junction, the transport theory was another prerequisite. The more so as the theory of the ballistic transport and the transition from the ballistic transport to the diffusive transport are less known. Consequently, a series of results were included in Chapter 4 of the Thesis, regarding the phonon and electron thermal transport, with special emphasis on the electrical transport. In all situation we have given special attention to the transition from the ballistic transport to the diffusive transport. The calculation of electrical resistance has been formalized in various situations, in order to employ these formulae for the ferromagnet-supeconductor junction. In contrast to the two previous Chapters, where, probably, there are not many orginal results, this Chapter contains several original results regarding the transport in matter, mostly unpublished. On such a basis there has been obtained recentlty an important result regarding the quanta of electrical conductance.[5]

5. Ferromagnet-Superconductor Junction. Finally, the last preparatory Chapter, Chapter 5 in Thesis, deals with one of the most difficult problem regarding the main question, namely the nature and properties of the ferromagnet-superconductor interface, contact, jonction. In investigating this problem we employed largely the knowledge achieved recently in the theory of the aggregation of the nanostructured mater.[1, 6, 7, 8] Two similar solids form up an ideal contact, as it is easy to imagine; in the limit, two identical solids form up no contact, in the sense that their separation surface is as homogeneous as the two solids. In practical situation, this is far to be fulfilled. In the other limit, where the two solids are very different in their structural and electronic properties, an important diffusion occurs at their contact, which evolves in time, such that we have a spatially extended junction, with properties different than the two solids; it is as if the junction is formed by three solids. In contrast to the ideal contact, the tunneling barrier has an imporatnt effect, the only convenient aspect being its slow variation in space, both structurally and electronically. Conseqeuntly, it is favourable to have a junction formed up between two solids with as much alike properties as possible. Often, inpractice the contact is formed by a controlable deposition of a film, for instance a metalic oxide. In any case, in all realistic situations the junction works in time, which entails its degradation and the loss of the control on the electrical conduction. In ideal situations, like those described above, the ferromagnet-superconductor Andreev reflection is affected to a small extent, by an additional tunneling factor. In the present Thesis we have assumed this factor equal to unity, as for a perfectly ideal junction. In the presence of an extended junction the Andreev reflexion may still be maintained, but one may lose the ferromagnetic and superconducting effects, by the so-called proximity effects. For this reason, it is little doubt that the results presented in this Thesis can be applied to such a situation.

6. Electric flow through a ferromagnet-superconductor junction. Chapter 6 in Thesis presents the main result: the computation of the electrical resistance at the ferromagnet-superconductor ideal junction as a function of magnetization. Thios computation is based on partial results derived in the previous Chapters. First, we formulate explicitly the spectrum of the electronic elementary excitations in ferromagent, by means of which we can express the spin-polarized injected current, making use of the results presented in Chapter regarding the transport theory. Then, we reformulate the theory of the Andreev reflection for the spin-polaried injected current, *i.e.* the Andreev reflection at the ferromagnet-superconductor ideal junction. Next, we identify the two transport regimes, ballistic and diffusive, and compute the electrical resistance as a function of magnetization. For a variable magnetization (by changing for instance the ferromagnet temperature below its critical temperature - and much below the critical temperature of the superconductor) the two currents with opposite spins pass from the ballistic transport regime to the diffusive one. Two such modes of ballistic-diffusive passing are identified. The electrical resistances have different forms in the two regimes, so that the total resistance exhibits a jump, either positive or negative, (depending on the two ballistic-diffusive passing moeds). This is the main result : it tells us that we may have a transistor-like effect at the ferromagnet-superconductor junction, controlled by magnetization.

7. Conclusions. The Thesis contains five main original results: the spectrum of the electronic elementary excitations in ferromagnet and their electrical transport; the theory of the Andreev reflection for spin-polarized currents; definition of the structural character of the contact between two solids; computation of the electrical resistance on passing from the ballistic to diffusive transport regime; transistor-like effect at the ferromagnet-superconductor junction. All these ersults are published in Refs. [9, 10, 11, 12].

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