Quasiparticle spectrum of superconducting heterostructures

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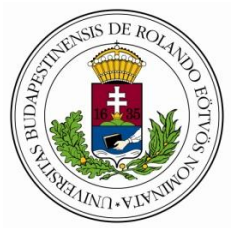

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1. Introduction

The physics of superconductor – normal metal heterostructures became a very intensively studied research field. The modern deposition techniques allows to create such high-quality thin films of solid. Interestingly, in the normal metal superconducting correlations are introduced by the so-called Andreev scattering, when an electron, with energy lying in the superconducting gap, arriving from the normal metal to the superconductor – normal metal (S/N) interface is retro-reflected as a hole and a Cooper pair is formed in the superconductor. This effect controls the transport properties of such systems and allows the understanding of the proximity-effect on a microscopic scale. It is also known that the Andreev reflection is the key effect behind the formation of Andreev bound states. While a great many theoretical works were dedicated to study the Andreev reflection and the Andreev bound states, it was done on model systems only, their material specific dispersion, their „band structure" has never been calculated (nor observed experimentally) to date. One of the main aim of the present dissertation is to make up this deficiency.

In those experiments, where the thickness of the superconductor is much greater than the normal metal's thickness, it was measured that the superconducting transition temperature decays linearly as a function of the normal metal's thickness.

However, if both the superconductor and the normal metal consist of only few atomic layers, a new phenomenon, the so-called inverse proximity effect can be observed. The superconducting transition temperature can grow if we add only few layers of normal metal to the ultrathin superconductor. In some sense this is an opposite of the well-known proximity effect (as the name suggests), and while it had been observed experimentally, only a few qualitative attempts have been made so far to explain it.

The main aim of the present dissertation to establish a method, which allows the quantitative and material specific description of these phenomena.

The density functional theory (DFT) was already generalized for the superconducting state (Kohn-Sham-Bogoliubov-de Gennes equations) and applied successfully in bulk superconducting systems. At present, this is the most accurate theory which allows the first principles calculation of the superconducting transition temperature. To describe only bulk systems, the LMTO (Linear Muffin-Tin-Orbital) method was also generalized for the solution of the Kohn-Sham-Bogoliubov-de Gennes equations.

The superconductor – normal metal hetereostructures can also be well described by these equations. The geometry of such systems can be built up from two-dimensional translational layers. By the generalization of the Screened Korringa-Kohn-Rostoker (Green function method) we can determine the dispersion relation, charge densities, density of states, energy of bound states, superconducting order parameter and many other physical properties of the superconducting system with arbitrary (e.g. semi-infinite) geometry. A fully ab-initio approach can also be constructed by taking into account the electron-phonon coupling (which can be obtained by the McMillan-Gaspari-Győrffy theory) within a simple approximation for the exchange functional.

2. Thesis Statement

1. The physics of superconductor – normal metal hetereostructures can be well described by the Kohn-Sham-Bogoliubov-de Gennes (KSBdG) equations. The scalar-relativistic form of the KSBdG equations was derived which takes into account the mass-velocity and Darwin terms (spin-orbit coupling is not included). The Screened Korringa-Kohn-Rostoker method was generalized, to properly describe the geometry of the heterostructures. The solution of the single-site scattering problem was determined by taking into account the Andreev scattering process. Formally, the generalized Faulkner-Stocks formula is the main result of this work, which defines the Green function of the KSBdG-Hamiltonian within Multiple Scattering Theory. Based on the new BdG-SKKR method a novel and unique computer code was developed for the non-magnetic, non-relativistic case, which allows us to study the nature of the Andreev bound states related to the proximity effect in normal metal – superconductor heterostructures. The basics of the spin-polarized fully relativistic formalism was also provided and it was shown that the functional form of the Faulkner-Stocks formula does not change.

2. The new KSBdG-SKKR method was applied to Nb/Au heterostructures (where the superconductor's thickness is in the range of the coherence length, i.e. thick superconductor). simplified treatment of the electron-phonon interaction To model the superconducting properties at the interface, a simple step function was used to model the changes of the pairing potential (assuming the experimental value of the bulk gap in the superconductor). We showed that the quantum-well states (we found to exist in the normal state band structure calculations) become bound Andreev states due to Andreev scattering. The major result of our investigations is

the determination of the Andreev states' dispersion. We found that the proximity of a superconductor in the studied heterostructures induces the mirroring of the electronic bands, and opens up a gap at each band crossing. For those materials where no quantum-well states present, this simple picture is not applicable for the quasiparticle spectrum.

3. It was obtained that the induced gap (observed in the normal metal) remains constant for each layer for a given Au thickness, however, the size of the gap decays as a function of the Au thickness. the superconducting order parameter extends well into the normal metal and interestingly follows a $1/L$ decay. Nevertheless, the anomalous charge per layer (which is related to the superconducting order parameter) has shown the usual, layer-dependent property of the proximity effect. Moreover, it follows an $1/L$ decay in the normal metal, which was also obtained from one-dimensional model calculations by others. Calculations for more geometries (bcc and fcc gold) were also performed and the main conclusions do not differ for that case.

4. The dispersion relation was also obtained from the layer dependent anomalous spectral function . We showed that this function carries lot of informations about the Andreev scattering process, the electron-hole character and also about the proximity effect.

5. The role of the surface and interface state were also investigated in Nb/Au heterostructures. In the case of Au surface states, the gap does not appear in the energy spectrum of these states, probably, because they are localized to the surface and consequently do not take part in the Andreev scattering process. In contrast, the interface states do shift significantly upwards in energy and a larger gap can be observed than in the quantum-well states. The electron-hole character of these states were also investigated. We obtained that the surface states are purely electron - or hole-like, while the interface states consist almost equal parts of electrons and holes.

6. A simple phenomenological method was developed to predict the transition temperature of such heterostructures based on the solution of the KSBdG equations. The electron-phonon coupling was modeled with a step function. In the case of the Nb/Au system we found very good agreements with the experimental findings. The theory was also applied for different metal overlayers on a Nb host to predict the superconducting transition temperature.

7. If the superconductor is also ultrathin, the calculation of the electron-phonon coupling is necessary, which makes the theory fully first-principles. Therefore, the McMillan-Gaspari-Győrffy theory was extended to slabs and heterostructures and then it was connected to the exchange functional. The McMillan-Hopfield parameter was obtained from the Gaspari-Győrffy formula (using the SKKR method). While the layer dependent phonon spectrums were calculated with VASP by Dr. Stephan Schönecker. The KSBdG equations were solved self-consistently and the critical temperatue was obtained for two facets (bcc 100 and 110) of Nb slabs. While presently there is no first-principles way to calculate the effective Coulomb repulsion parameter directly, a procedure was developed to estimate this parameter. Different behavior was found for the two Nb facets. If the surface is more opened, the average phonon frequency is smaller on the surface, which results in large electron-phonon coupling for the surface and therefore the critical temperature is also greater.

8. The method was also applied to Nb/Au thin films where the inverse proximity could be observed (experimentally it was observed in Pb/Ag systems). The critical temperature grows if we add only one gold layer to the ultrathin niobium. It was shown that this effect is based on the changes of the effective electron-phonon coupling.

3. Publications related to the Thesis Statements

- Gábor Csire, Balázs Újfalussy, József Cserti, Balázs Győrffy, Multiple scattering theory for superconducting heterostructures Phys. Rev. B **91**, 165142 (2015).

- Gábor Csire, József Cserti, Istvan Tüttő, Balázs Újfalussy, Prediction of superconducting transition temperatures of heterostructures based on the quasiparticle spectrum, Phys. Rev. B **94**, 104511 (2016).

- Gábor Csire, Stephan Schönecker, Balázs Újfalussy, First-principles approach to thin superconducting slabs and heterostructures, Phys. Rev. B **94**, 140502(Rapid Communication) (2016).

- Gábor Csire, József Cserti, Balázs Újfalussy, First principles based proximity effect of superconductor – normal metal heterostructures, J. Phys.: Condens. Matter **28**, 495701 (2016).