Report

Multiple scattering theory in superconductors

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The aim of the project was to match and compare two different methods (multiple scattering theory and the tight-binding formalism) which are able to describe the properties of superconductor-metal-ferromagnet heterostructures.

Earlier, based on first principles Bogoliubov-de Gennes (BdG) equations we developed a novel and unique computer code which allows us to study the role of the Andreev bound states related to the proximity effect in normal metal-superconductor heterostructures. For that purpose we have generalized the screened Korringa-Kohn-Rostoker method (SKKR) to be able to investigate the quasiparticle spectrum in superconductor-based heterostructures. We have applied this method for different superconducting heterostructures. These calculations were the first material specific calculations for a superconductor - normal metal heterostructure. The obtained results are the following: Formally the generalized SKKR method is the main result. We have calculated the quasiparticle band structure of a niobium-gold system. It was shown that the quantum-well states (which obtained from the normal state band structure calculation) determine the Andreev states which have dispersion now and form bound states. We found a k-dependent induced gap in the quasiparticle spectrum of the niobium - gold system and obtained its dependence on the size of the sample. The effect of different lattice structures was also investigated. We calculated the superconducting critical temperature using the McMillan formula and obtained very good agreement with the experiments. We also studied superconducting heterostructures composed from other materials and predicted the critical temperatures. We investigated the properties of the surface states and obtained that the gap does not appear in surface states because they do not take part in the Andreev scattering process.

I've presented and discussed the results in Bristol. We have talked over the possibilities of further developments: calculate electron-phonon coupling on the intefaces (investigating more accurately proximity effect), generalise the multiple scattering theory for the spin-polarised case (triplet order parameter, superconducting/ferromagnetic hybrid systems), work out the coherent potential approximation (CPA) for superconducting alloys, calculate transport quantities (with the generalisation of the Kubo–Greenwood formalism) and the full relativistic generalisation which is necessary to investigate Majorana fermionic systems. The evident and most interesting choice is to extend our code with the spin-polarised case. We have discussed in details how the BdG formalism can be generalized for Cooper pairs with $l > 0$. For triplet order parameters the size of the Hamiltonian is doubled and the potential must be nonlocal, however different correlation functions can be calculated from KKR which indicates the appearance of triplet states. I have learned this method from the tight-binding formalism used in Bristol which will be applicable in our code.

Our result are under the publication process, and further collaboration is expected in the topic of superconductor - ferromagnet heterostructures with Bristol group.