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Superconducting Order Parameter in Inhomogeneous Superconductors

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Superconductivity is the state of matter in which the electronic wave function spontaneously takes on a definite complex phase. The most fundamental ingredient in the theoretical description of this phenomenon is the superconducting order parameter. Modern computational methods and the corresponding computer codes allow the quantitative predictions of superconducting properties for realistic experimental settings involving not only bulk superconductors but also heterostructures. One major consequence is that it enables the accurate calculation of the superconducting order parameter in inhomogeneous systems, which has been limited so far due to the lack of an appropriate theoretical tool set, even though the superconducting order parameter is one of the central quantity of superconductivity. This is because the BCS theory of superconductivity, in its original formulation, is not easily generalized for heterostructures, especially in the relativistic domain

In this talk we attempt to provide a quantitative theory that takes into account the ab-initio band structure with its full microscopic complexity together with magnetism, effects from relativity, spatial inhomogeneity of the lattice and different orbital symmetries on the same footing. This can be achieved within the framework of Multiple Scattering Theory (MST), this time combined with the Bogolubov-deGennes (BdG) reformulation of the BCS theory. Similarly to the normal state, the central quantity of such an MST is the quasiparticle Green's function, which now carries information about the scattering of quasiparticles [1]. The main extra ingredient of such scattering events compared to the normal state Korringa-Kohn-Rostoker (KKR) formalism is the so called Andreev reflection. It occurs 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 formalism allows vast applications and we shall focus on the behavior of superconducting order parameter revealing its complexity and physical meaning in realistic systems. As an example, I will revisit the well known proximity effect, which is part of the standard textbook physics vocabulary and it is mostly understood within the quasiclassical picture. However, the real microscopic mechanism behind the proximity effect is the Andreev reflection. If one considers this microscopic picture for some artificial materials, often referred to as heterostructures it reveals the difference in important concepts, like the superconducting order parameter, pairing potential, superconducting gap, which are not well separated in the conventional BCS theory of bulk superconductors. We will use the example of Nb/Au heterostructures in the talk.

Then we will apply the approach to the complimentary problem, namely when a superconducting impurity cluster is embedded into a non-superconducting material. By doing so, we shed light on the build-up of the superconducting phase and its connection to the order parameter. As a testbed for our calculations, we consider superconducting Nb atoms surrounded by non-superconducting bulk Nb [2]. For a relatively small cluster of material with nonzero pair interaction parameter embedded in a normal metal, the superconductivity will be suppressed and the superconducting gap will be forced to close. However, the interesting question is what happens when the size of the cluster reaches the same order as the corresponding superconducting coherence length. Here one should remember that the Cooper pairs are extended in real space, since Cooper pairs are formed in momentum space and not in real space. In fact our local pairing model is the analog of conventional BCS theory, where Cooper pairs are formed by electrons with different quantum numbers **k,**↑ and –**k,**↓ in which states from the region of the gap around the Fermi level are mixed. The coherence length is the extension of these wave packets in real space given by the BCS theory.

When a magnetic impurity or a cluster of magnetic impurities is introduced into a singlet *s*-wave time-reversal invariant superconductor, there is a pair-breaking effect due to the spin-dependent scattering, and the superconducting transition temperature decreases as the impurity concentration increases. Yu, Shiba and Rusinov revealed that local states (referred as YSR states) appear within the BCS energy gap due to multiple scattering between conduction electrons and magnetic impurities. Later, it was realized theoretically that one can engineer nanostructures, where hybridized YSR states form a topological fully gapped quasiparticle spectrum. For magnetic impurities an especially rich internal structure of the superconducting order parameter can be calculated from the local Green's function as non-zero elements in the electron-hole off-diagonal block. It will be demonstrated, that the complexity of the ab-initio electronic structure allows the appearance of an exotic local triplet state in magnetic ***s***-wave time-reversal symmetry breaking superconductors. Furthermore, we also show how topological superconductivity is manifested in the structure of the superconducting order parameter.

References

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