DESCRIPTION FOR GENERAL PUBLIC

After the formulation of the BCS theory (Bardeen-Cooper-Schriffer) in 1957 and its experimental verification the phenomenon of superconductivity (discovered in 1911) seemed to be fully explained. The important part of the BCS theory was the concept of an effectively attractive interaction between electrons which below the critical temperature can lead to the creation of the Cooper pairs (pairs of electrons). Due to the fact that Cooper pairs are not scattered on the crystal lattice ions there is no electrical resistance in the superconducting state. This together with other unique features of superconductors (such as the Meissner effect) makes those materials very attractive when it comes to possible application. For example they can be used in constructing strong magnets, sensitive magnetometers, superconducting processors, levitating trains, and in tomographic imaging. Unfortunately, due the destructive character of the thermal noise the transition to the normal state appears with increasing temperature. The critical temperatures of the first discovered superconductors were equal to only few Kelvins (0 Kelvin is equal to -273 Celsius degrees). However the discoveries made in the late 70s and 80s have shown that many materials can be in the superconducting phase in much higher temperatures. Unusual features of those high temperature superconductors cannot be described by the use of the BCS theory. Within this project the high temperature copper based materials are going to be analyzed. What makes those compounds even more interesting is the appearance of many other intriguing effects such as the Mott transition, charge and magnetic ordering as well as the puzzling pseudogap state. In spite of 30 years of extensive both theoretical and experimental research the complete theory which would explain the possibility of Cooper pair creation in high temperatures has still not been formulated.

According to one of concepts which is analyzed by the scientific community, in electronic systems with strong Coulomb repulsion the Cooper pair creation can appear due to collective effects without the effectively attractive interaction. This allows for the stability of the superconducting phase in significantly higher temperatures than in the conventional BCS superconductors. This theory of superconductivity in strongly correlated electron systems is a big challenge of the modern-day solid state physics. Due to high complexity of such description the theoretical analysis of the cuprates requires advanced computational techniques. Within this project, to properly include the correlation effects, the innovative *diagrammatic expansion Gutzwiller wave function* (DE-GWF) method, which was developed in recent years, is going to be applied. The DE-GWF approach is numerically effective and more accurate that other widely used methods. At the same time it is not limited to systems with small size.

An important aspect of the theoretical research of the high temperature superconductors is the formulation of proper mathematical model within which the description of the considered phenomena is possible. For the case of copper based systems this matter has not been completely settled and different scenarios are being considered. Recent experimental and theoretical reports have shown that the inclusion of the oxygen degrees of freedom is crucial for deeper understanding of the intriguing physics of the cuprates. Moreover, in spite of some successes resulting from the description based on the single-band models (within which the oxygen degrees of freedom are eliminated) it has not been possible yet to reproduce the complete set of principal experimental data within such approach. Therefore, the research oriented on the realistic 3-band description which takes into account the oxygen atoms in the Cu-O layers, together with the proper treatment of the correlation effects, is very important and is planned within this project. The results of the calculations are going to be compared with the available experimental data which will allow for the verification of the applied theoretical approach. The reproduction of the principal experimental observations within such approach would confirm the proper quasiparticle picture in the model and would constitute a significant step towards a complete theory of high temperature superconductivity in the cuprates.