Microscopic theory of fulleride superconductors

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Strongly correlated electron systems with multiple orbital degrees of freedom show a variety of intriguing phenomena and are realized in a wide range of materials. The alkali-doped fullerides are the typical cases where the strong correlation effects with multiple (t_{1u}) molecular orbitals are relevant. This material shows the superconductivity with a high transition temperature of ~40K. While the mechanism is identified as the electron-phonon interaction, the superconducting dome in the temperature-pressure phase diagram is found to be located near the Mott insulator, featuring the typical behaviors of strongly correlated superconductors [1].

In the Mott insulating phase, the electrons are localized in each molecule. Because of the coupling between electrons and anisotropic molecular vibrations (Jahn-Teller phonon), the imbalance of the occupancy in t_{1u} orbitals appears and leads to the deformation of the fullerene molecule. Interestingly, such behavior is observed also in the metallic phase near the Mott insulator, and this anomalous electronic state is called the Jahn-Teller metal [2].

To clarify the origin of these intriguing behaviors, we have analyzed the multiorbital Hubbard model which describes the correlated electron systems. Here, the Hund's coupling becomes effectively antiferromagnetic by the coupling to phonons, which is characteristic for fullerides. We show that the property of the Jahn-Teller metal is consistently explained by a previously unrecognized phenomenon: the spontaneous transition of multiorbital systems into an orbital-selective Mott state [3,4]. This symmetry-broken state, which has no ordinary orbital moment, is characterized by an orbital-dependent two-body operator (the double occupancy) [3,5].

For more quantitative analysis, we need to include the electron-phonon interaction directly. To this end, we have also analyzed the multiorbital Jahn-Teller-Hubbard model which takes account of the anisotropic molecular vibrations. Based on the Eliashberg approach, the superconducting properties are quantitatively explained [6]. In the presentation, we will discuss these theoretical advancements on fulleride superconductors in detail.

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