Superconductivity in a Correlated $E\otimes e$ Jahn-Teller System

Takada Group

The competition of electron-phonon (e-ph) and electron-electron (e-e) interactions in the mechanism of superconductivity is an old issue in strongly correlated systems and it has been investigated mostly in a single-orbital system, like the Hubbard-Holstein model in which the e-ph interaction enhances charge fluctuations, inducing an s-wave superconductivity in the vicinity of a charge density-wave (CDW) phase, whereas the e-e interaction suppresses such charge fluctuations but enhances spin ones, leading to a d-wave superconductivity near a spin density-wave (SDW) phase. If the effect of the e-ph interaction is about the same as that of the e-e interaction, there appears a rather complex nature of the pairing, namely, the off-site pairing (leading to either the extended s-wave or the d-wave nature, depending on the lattice structure) composed of not the bare electrons but the (phonon fully-dressed) polarons [1].

Here we add a further complication to this correlated and strongly phonon-coupled system by including the orbital degree of freedom. More specifically, we consider a two-dimensional (2D) square lattice with each site made of an $E\otimes e$ Jahn-Teller (JT) center, namely, a site composed of doubly degenerate orbitals like the e_g orbitals in the d bands which are coupled to the doubly-degenerate JT phonons. At each center, we also consider the e-e interaction in an appropriate way to make this JT crystal as a prototype of the charge-spin-orbital complexes. Then the Hamiltonian H of this system is given by $H=H_0+H_{\text{e-e}}+H_{\text{e-ph}}$, where H_0 is the noninteracting part composed of the electron hopping term characterized by the nearest-neighbor and next-nearest-neighbor hopping integrals, t and t', respectively, with keeping the orbital symmetry and the degenerate-phonon term with the phonon energy Ω_0. The orbital degree of freedom will be described by pseudospin for analogy to spin degree of freedom and the pseudospin symmetry is conserved throughout the crystal in this choice of H_0. Other terms, $H_{\text{e-e}}$ and $H_{\text{e-ph}}$, consist of local-site terms written with the intra-orbital Coulomb interaction U, the Hund's-rule coupling J, and the JT coupling g.

Due to the SU(2) symmetry in spin space and the conserved symmetry in pseudospin space, the Cooper pairing state can be specified by three quantum numbers; S the total spin of the pair, L the total pseudospin, and L_y its y component, making it possible to write the anomalous self-energy as $\Delta^S_{LL_y}(k)$, where k is a combined notation of crystal momentum $\boldsymbol{k}$ and fermion Matsubara frequency $i\omega_n=i\pi T(2n+1)$ at temperature T with an integer n. Because of the rotational symmetry around the orbital-y axis, $L_y=\pm1$ states are degenerate and thus we treat only either $L_y=0$ or 1 here. The group theory determines the transformation property of $\Delta^S_{LL_y}(k)$ in $\boldsymbol{k}$ space; it transforms in accordance with Γ, one of the irreducible representation of the point group C_{4v} (A_1, A_2, B_1, B_2, or E). The Pauli exclusion principle dictates that $\Delta^S_{LL_y}(k)$ must be antisymmetric under two-electron interchange, indicating that Γ must be E for (S,L) equal to either (0, 0) or (1, 1); otherwise Γ must be either A_1, A_2, B_1, or B_2. With including this transformation property in Γ, we can easily write down the Eliashberg equation for $\Delta^S_{LL_y}(k)$ at $T=T_c$ with the pairing interaction $V^S_{LL_y}(q)$ containing the charge, spin, and orbital susceptibilities $\chi_c(q)$, $\chi_s(q)$ and $\chi_o(q)$, all of which are evaluated in the RPA with use of the irreducible susceptibility $\chi_0(q)$.

In Fig. 1, the phase diagram at $T=0.02t$ is plotted in the U-g plane for the typical case of $t'=0.125t$, $U=8t$, $J=t$, and $\Omega_0=0.10t$ at half filling. Two boundaries, denoted by L_{I} and L_{II}, indicates the lines where $\chi_o(q)$ and $\chi_s(q)$ diverge, respectively. In the close vicinity of these boundaries, those fluctuations are enhanced strongly enough to make the system enter into various superconducting phases, each labeled by $(\Gamma;S,L,L_y)$. Among them, we find (E;0,0,0) which is a novel chiral p-wave pairing state, $p_x(\boldsymbol{k})\pm ip_y(\boldsymbol{k})$, characterized by spin-singlet, orbital-singlet, and odd-parity in momentum space. This is a state very specific to the degenerate multi-orbital system and is induced by the cooperative effects of orbital and spin fluctuations that are, respectively, enhanced by e-ph and e-ph interactions [2].

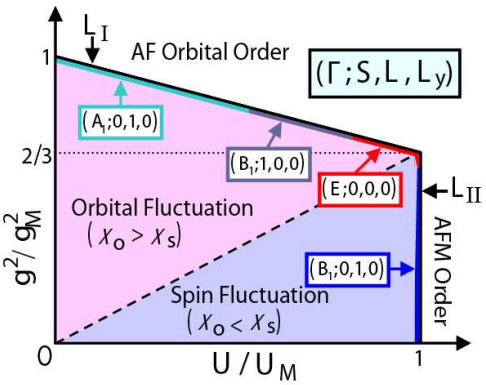

Fig. 1. Phase diagram in the U-g plane at half filling for $U/8=J=t$, $t'=0.125t$, and $\Omega_0=0.10t$ at $T=0.02t$. Units of strengths are so defined as $U_{\text{M}}=32/9\chi^0(\boldsymbol{Q},0)$ and $g_{\text{M}}^2/\Omega_0=1/\chi^0(\boldsymbol{Q},0)$, where $\boldsymbol{Q}$ [$=(\pi,\pi)$] is the momentum maximizing both $\chi_o(\boldsymbol{q},0)$ and $\chi_s(\boldsymbol{q},0)$.

The conservation of the pseudospin symmetry is assumed in this study, but it is not always the case. By some tentative works, we come to know that the perturbation breaking this conservation will enhance T_c for the iron pnictides, while it reduces T_c very much for the vanadium oxides. This is an issue to be studied further in the future.

References

[1] Y. Takada, J. Phys. Soc. Jpn. **65**, 1544 (1996).
[2] C. Hori, H. Maebashi, and Y. Takada, J. Supercond. Nov. Magn. **25**, 1369 (2012).

Authors

C. Hori, H. Maebashi, and Y. Takada