Symmetry of superconductivity in the vicinity of the SC-AF transition in $NH_3A_3C_{60}$

Yoshihiro ASAI
Research Institute for Computational Sciences
(RICS-AIST)
Umezono 1-1-1, Central 2, Tsukuba,
Ibaraki 305-8568, Japan
and
Department of Chemical System Engineering,
The University of Tokyo
7-3-1, Hongo, Bunkyo-ku, Tokyo, 113-8656, Japan

We have studied possible change of the superconducting pairing symmetry in the ammonia intercalated fullerides by using a multiband electron-phonon model. The change is induced by lifting the t_{1u} orbital degeneracy, which may be realized close to the boundary between the superconducting (SC) and the antiferromagnetic (AF) phases of these materials, where reduction of the crystal symmetry is expected.

The doped C_{60} sometimes called fulleride forms a unique family of materials which range from superconductor, antiferromagnet to ferromagnet. The conduction bands are derived from C_{60} molecular orbitals which are degenerated due to the high symmetry of the molecule. Owing to the large intermolecular separation and the high frequency molecular vibration, the nonadiabatic parameter ω/W where ω is the vibrational frequency and W is the band-width is not small. Fullerides are the overlapping and narrow band system.

The electron-intramolecular-vibration (e-MV) couplings have turned out to play the most important role in the mechanism of superconductivity in this family of materials. The interband e-MV coupling constant originating from the kinetic energy exchange between the molecular vibration and electron beyond the Born-Oppenheimer (BO) approximation has been estimated to be rather large as well as the standard intraband Holstein e-MV coupling constant.[1,2] Because the nonadiabatic parameter is not small, vertex corrections beyond the Migdal approximation become non-negligible in this system.[3,4] We have to take all of these into account.

The phase transition between the superconductivity and the antiferromagnetism in the ammonia intercalated fulleride may be accompanied with the symmetry reduction of the crystal and the subsequent lifting of the t_{1u} band degeneracy.[5] The lifting of the degeneracy diminishes the interband e-MV coupling constant.[1,2] The ammonia intercalated doped C_{60} is a suitable system to study details of the interband e-MV couplings. Keeping these in mind, we study the two-band e-MV model that includes both the intra- and inter-band e-MV couplings. Corrections to the Migdal approximation which have been successful in explaining some experiments were included.

It has turned out that while the nonadiabatic corrections to intraband e-MV coupling favor anisotropic pairings, the corrections to the interband e-MV coupling favor the isotropic pairing symmetry. Lifting the band degeneracy diminishes the latter coupling and only the effect of the anisotropic pairing potential remains. This is clearly shown in Fig.1. The change may be observed close to the phase boundary between the SC and the AF phases.

References

1. Y. Asai and Y. Kawaguchi, Phys.Rev.B46, 1265 (1992).
2. Y. Asai, Phys.Rev.B49, 4289 (1994).
3. E. Cappelluti, C. Grimaldi, and L. Pientronero, Phys. Rev. B64, 125104 (2001).
4. A. Perali, C. Grimaldi, and L. Pientronero, Phys. Rev. B58, 5736 (1998).
5. T. Takenobu, T. Muro, Y. Iwasa and T. Mitani, Phys. Rev. Lett. 85, 381 (2000).

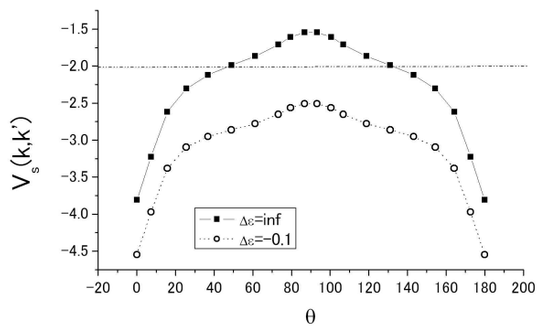

Fig.1 The pairing potential $V_S(\vec{k},\vec{k}')$ of the two-band e-MV model. $\Theta = \arccos\left(\vec{k}\cdot\vec{k}'/|k||k'|\right)$ in degree. Θ is 0 when the momentums are parallel, while it is 90 when the momentums are orthogonal to each other. $\Delta\varepsilon$ denotes the energy difference between the band centers. The broken line at -2.0 denotes the potential without corrections. $V_S(\vec{k},\vec{k}')$ below -2.0 denotes the attractive correction, while that above -2.0 denotes the repulsive correction. The corrections in the single band case ($\Delta\varepsilon = \infty$; closed squares) is anisotropic, while the correction in the multiband case ($\Delta\varepsilon = -0.1$; open circles) is attractive everywhere.