

Band crossover and magnetic phase diagram of superconducting $\text{Ba}_2\text{CuO}_{4-\delta}$

May 17 2022, by Zhang Nannan

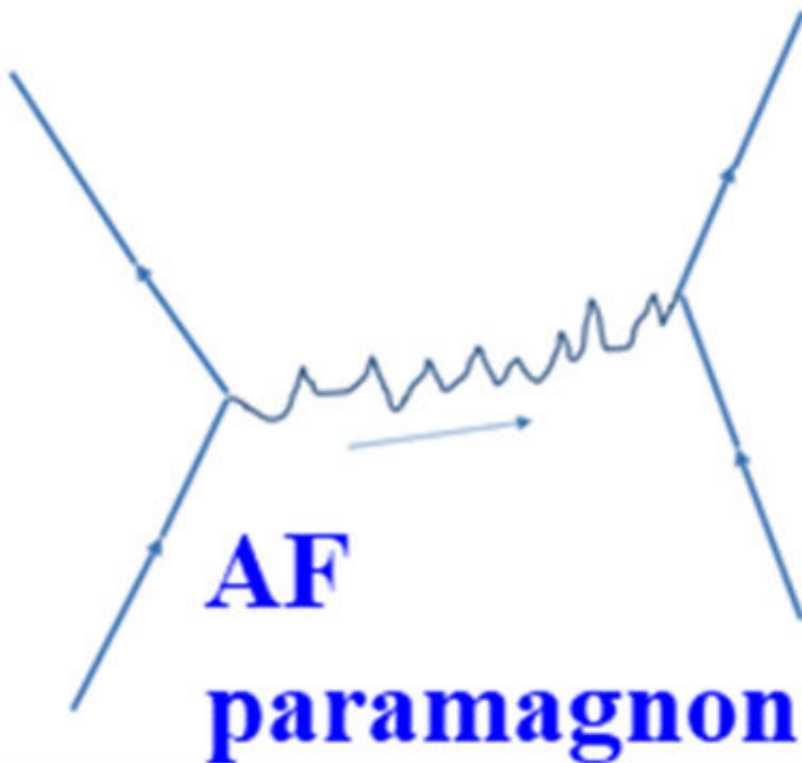


Fig. 1. An effective interaction mediated by exchanging an antiferromagnetic paramagnon. Credit: Bai Xiaocheng

Researchers led by Prof. Zou Liangjian from the Hefei Institutes of Physical Science (HFIPS) of the Chinese Academy of Sciences (CAS) have recently investigated the magnetic phase diagram of the high- T_c (critical temperature) superconducting compound $\text{Ba}_2\text{CuO}_{4-\delta}$ and its

superconducting pairing symmetry based on the spin-fluctuation mechanism. Results were published in *Physical Review B*.

It is well-known that two electrons in vacuum repulse each other. However, in [superconductors](#), two electrons near the Fermi surface form a Cooper pair by exchanging bosonic quasi-particles. These Cooper pairs with the same phase condensate the superfluid with zero resistivity. The pairing symmetry of Cooper pairs is an important feature for uncovering effective pairing interaction in superconductors.

A newly discovered cuprate superconductor $\text{Ba}_2\text{CuO}_{4-\delta}$ featured on high- T_c of 73 K, about two to three times higher than isostructural conventional cuprate $\text{La}_2\text{CuO}_{4-\delta}$. Also, it displays compressed CuO_6 octahedra, which is inverted to the CuO_6 octahedra or CuO_5 pyramids in the parent phases of conventional cuprates. This results in multiple orbitals contributing to superconducting properties in $\text{Ba}_2\text{CuO}_{4-\delta}$.

The phase diagrams of the previous cuprates superconductors showed antiferromagnetism in [close proximity](#), or in some cases coexisting, with superconductivity. Hence, it is proposed that the effective pairing interaction is mediated by spin fluctuation in the cuprates superconductors. To understand which mechanism contributes the effective pairing interaction in $\text{Ba}_2\text{CuO}_{4-\delta}$, it is crucial to investigate the magnetic phase diagram of it.

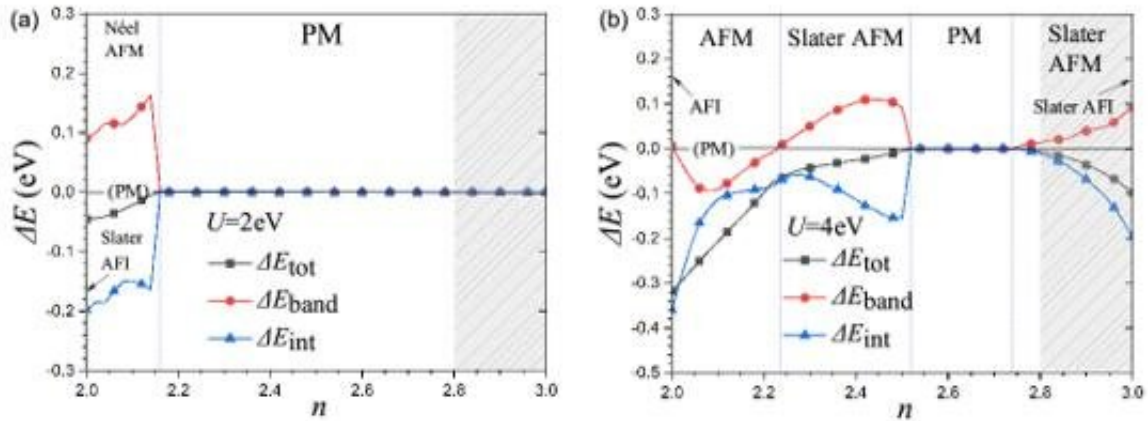


Fig. 2. The magnetic phase diagrams of $\text{Ba}_2\text{CuO}_{4-\delta}$ at $U = 2$ eV (a) and $U = 4$ eV (b). Credit: Bai Xiaocheng

In this work, using the rotationally invariant slave boson (RISB) method, the researchers investigated the magnetic phase diagram of the high- T_c superconducting compound $\text{Ba}_2\text{CuO}_{4-\delta}$. They also studied the superconducting pairing symmetry in its based on the spin-fluctuation mechanism within random phase approximation.

The results showed that in the intermediate correlation regime ($U \sim 2$ eV), the system behaved as single-band paramagnetic metal when $n > 2.4$, and had only one antiferromagnetic insulating parent phase.

In the strongly correlated regime ($U > 4$ eV) the system displayed two different antiferromagnetic insulating parent phases at $n = 2$ and 3 , corresponding to two-band and single-band nature, respectively.

Comparing the experimental spin coupling value of about 150 meV with the total-energy difference between the Néel antiferromagnetic and paramagnetic phases, the researchers estimated that $U \approx 2\sim 3$ eV in $\text{Ba}_2\text{CuO}_{3.2}$.

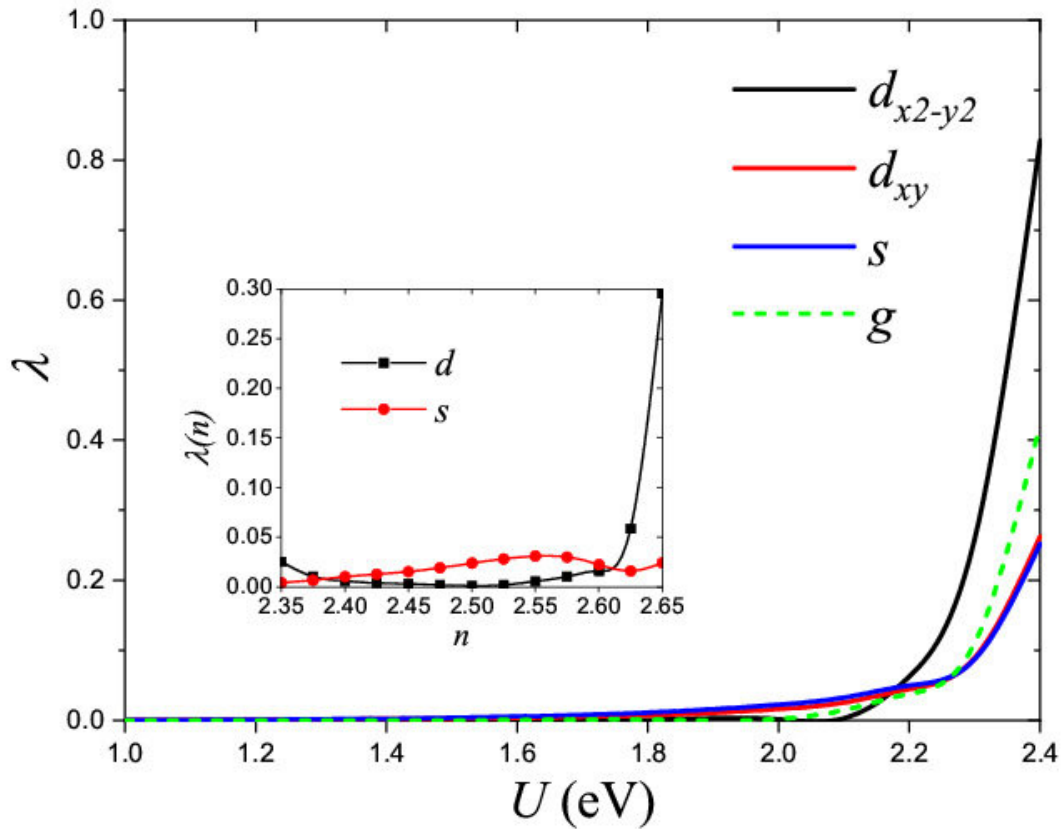


Fig. 3. The pairing strength λ of $\text{Ba}_2\text{CuO}_{4-\delta}$ with $\delta = 0.8$. Inset shows pairing strength λ for different doping at $U = 2$ eV. Credit: Bai Xiaocheng

They further studied the superconducting pairing symmetry in its based on the spin-fluctuation mechanism and found that the pairing strengths of s-wave and d-wave are nearly degenerate.

Results suggests that Cooper pairs in $\text{Ba}_2\text{CuO}_{3.2}$ are s+d –wave symmetric.

It's the first time that scientists theoretically illustrated the magnetic

[phase](#) diagram of $\text{Ba}_2\text{CuO}_{4-\delta}$, which suggested that Cooper pairs in $\text{Ba}_2\text{CuO}_{3.2}$ were s+d –wave symmetric provided that the effective pairing interaction is mediated by spin fluctuations.

More information: Xiao-Cheng Bai et al, Band crossover and magnetic phase diagram of the high- T_c superconducting compound $\text{Ba}_2\text{CuO}_{4-\delta}$, *Physical Review B* (2022). [DOI: 10.1103/PhysRevB.105.184506](#)

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