放射光科学理論

Theoretical study on anomalous isotope effect of ARPES

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There is a long-standing debate concerning the role of electron-phonon (e-ph) interaction in the high-T_C superconductivity. Recent experiment [1] on $Bi_2Sr_2CaCu_2O_8$ shows that the isotopic substitution of ^{16}O by ^{18}O can give clear shift in the angle resolved photoemission spectra (ARPES), strongly suggesting that the electronic energy band is modified by the e-ph interaction.

To understand the mechanism of this isotopic change in ARPES, we calculate the ARPES based on the following model,

$$H = -\sum_{<l,l'>,\sigma} t(l,l')\left(a^{+}_{l\sigma}a_{l'\sigma} + a^{+}_{l'\sigma}a_{l\sigma}\right) + \frac{\omega_0}{2}\sum_{<l,l'>}\left(-\frac{1}{\lambda}\frac{\partial^2}{\partial q^2_{ll'}} + q^2_{ll'}\right) + U\sum_{l}(n_{l\uparrow}-\tfrac{1}{2})(n_{l\downarrow}-\tfrac{1}{2}).$$

Here, $t(l,l')$ is the electronic transfer energy between two neighboring Cu sites l and l', and modulated by the vibration of oxygen atom in between (see Fig. 1). The oxygen phonon is assumed to be of the Einstein type with a frequency ω_0 and a mass m. λ ($\equiv 1+\Delta m/m$) is the mass change factor of phonon due to the isotope substitution, and U is the Coulomb repulsion for electrons of opposite spins on the same site.

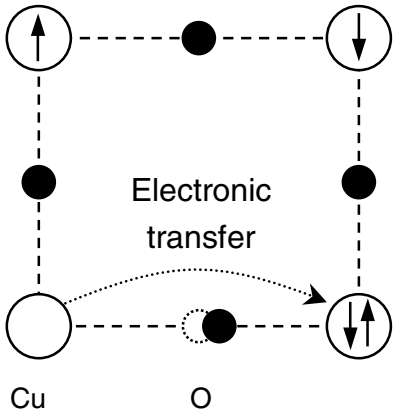

Fig. 1: A Schematic plot of CuO_2 conduction plane in cuprates.

Based on this model, we study the electronic band shift by the path-integral Monte Carlo and Hartree-Fork mean field methods. We confirm that the anomalous isotopic band shift is connected with the softening effect of oxygen phonon driven by the quadratic e-ph coupling. While the Coulomb repulsion partially suppresses this softening effect and reduces the band shift.

Reference

[1] G. –H. Gweon et al., Nature (London) 430, 187 (2004).