Giant oxygen isotope effect in high-T_c metal-oxide superconductors

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The theory of polaron superconductivity is shown to admit large values of the isotope effect, $\alpha > 0.5$. The oxygen isotope effect in $YBa_2Cu_3O_{7-x}$ can be anomalously large.

The first experiments[1] on the isotopic replacement of oxygen in the recently discovered high-T_c superconductors (YBCO and LSCO) showed that the value of the isotopic constant is relatively low:

$$\alpha = -\frac{d\ln T_c}{d\ln M} \lesssim 0.2. \tag{1}$$

This result was interpreted in several studies as evidence of the presence of soft modes,[2] anharmonicity, and Coulomb interaction or as an indication of the dominant role played by the nonphonon carrier-pairing mechanism (see, e.g., Ref. 3). Here M is the mass of the oxygen atom.

On the other hand, the energy-band calculations[4] and analytic calculations,[5] a comparison of the tunnel characteristics with the neutron vibration spectra,[6] the temperature dependence of thermal conductivity,[7] and several other experiments[8] have shown that the carriers of the high-T_c metal-oxide superconductors interact strongly with the clearly indentifiable hard vibration modes of the light oxygen anions and that this interaction, in principle, should lead to a more pronounced isotope effect.

The low values of α in the experiments[1] on the replacement of O^{16} by O^{18} may stem from the fact that O^{16} does not leave the crystallographic positions in the copper planes and the primary candidate for a replacement is the more mobile oxygen in the copper chains and in the Ba neighborhood, whose isotopic state affects T_c only slightly. These conclusions have been confirmed by the recently obtained results[9] on the synthesis of YBCO from the basic oxides which generally do not contain an O^{16} isotope:

$$\alpha \approx 2.5. \tag{2}$$

This result corresponds to a decrease in T_c from 92 K in O^{16} samples to 59 K and 77 K in samples which were synthesized identically from O^{18} and O^{17} isotopes, respectively. The giant isotope effect (2) is five times larger than the limiting value predicted by the BCS theory for a weak and strong electron-phonon coupling.

In this letter we offer an explanation of the anomalous isotope effect[9] on the basis of a polaron model of a high-temperature superconductor,[2] according to which a sufficiently strong electron-phonon interaction ($\lambda \geqslant 1$) leads to the formation of small heavy bipolarons with an effective mass m^{**} which condense to a charged superfluid Bose liquid at the temperature[10]

$$T_c = f(p)/m^{**}, \tag{3}$$

where $f(p)$ is the concentration function of the carriers p, which does not depend on the mass of the isotope. At low concentrations ($\hbar = k_B = 1$) we have

$$f(p) \approx 3.3\,(p/2)^{2/3}. \tag{4}$$

According to Aleksandrov and Kabanov,[11] in the simple case of an interaction with a dispersion-free vibration mode with a frequency ω we have

$$m/m^{**} = 2T_{ij}\,\Delta^{-1}\,M(1.1 + \Delta/\omega,\ 2g^2), \tag{5}$$

where $\Delta = (2_g^2\omega - V_c)$ is the bipolaron binding energy which does not depend on the isotope mass, V_c is the Coulomb repulsion potential, g is the Fröhlich dimensionless coupling constant, T_{ij} is the integral which describes the hopping in the rigid lattice and which determines the band mass m, and $M(a,c,z)$ is a confluent hypergeometric function.

Assuming $\omega \sim M^{-1/2}$ and $g^2 \sim M^{1/2}$, we find from (3)–(5)

$$\alpha = g^2\,F(\Delta/\omega, 2g^2), \tag{6}$$

where

$$F(x,y) = 1 + M^{-1}(1,1+x,y)\,(M(1,2+x,y) - (x/y)\,dM(1,1+x,y)/dx)$$

varies from $F(0,y) = 1$ to $F(\infty,y) = 2$.

As we can see from expression (6), the bipolaron superconductivity theory[10] thus gives us the conceptual possibility of producing an isotope effect $\alpha > 0.5$, with values of $g^2 \gtrsim 1$, which account for the existence of a small-radius polaron.[10] The value (2) corresponds to $g^2 = 1.25$–2.5, in agreement with the estimates[2] of the bipolaron effective mass obtained from T_c, the magnetic field penetration depth, and the electron specific heat of $YBa_2Cu_3O_{7-x}$.

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