

INTER-BAND THEORY OF SUPERCONDUCTORS: RESOLUTION OF OBSERVED S AND D-WAVE TUNNELING WITH ISOTROPIC S-WAVE PAIRING

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A fundamentally different, yet conceptually and computationally simple theory is presented for high temperature superconductivity. We assume the existence of two bands, one with predominantly planar $d_{x^2-y^2}$ character on the copper sites and the other with predominantly p_z character with lobes pointing normal to the CuO planes on the oxygen sites. An attractive phonon coupling across the bands is assumed with a purely isotropic (s-wave) attraction. Thus, a Cooper pair consists of a $k \uparrow$ electron from one band and a $-k \downarrow$ electron from the other band. Due to the different masses of the two bands, Cooper pairs can carry current, or equivalently, are not invariant under time-reversal. This leads to a dramatic change in the standard picture of Josephson tunneling. Inter-band pairing makes the orbital nature of the bands contribute to the tunneling current. It is shown that the four key experiments designed to measure the phase of the gap: 1.) YBCO tri-crystals (d-wave) by Tsuei et al., 2.) YBCO-Pb corner junctions (d-wave) by Wollman et al., 3.) hexagonal YBCO junctions (s-wave) by Chaudhari et al., and 4.) YBCO-Pb c-axis tunneling (s-wave) by Dynes et al., are all a natural consequence of inter-band pairing. Finally, the temperature dependence of the Knight shifts in YBCO₇ and YBCO_{6.63} and their completely different c-axis optics are qualitatively explained by the matrix element for electric-dipole transitions between the two bands.

1 Inter-Band Pairing Model

Assume an attractive coupling *across* two bands one with predominantly $d_{x^2-y^2}$ character on the Cu sites and the other with predominantly p_z character with lobes pointing normal to the CuO planes on the O sites. The bands are assumed to occupy the same phase space and have coincident Fermi surfaces at optimal doping. This assumption can be relaxed, but in this paper we will see how far we can go with the simplest possible assumptions about the bands.

Then, the possibility exists of optical absorption down to $\omega = 0$ from one band to the other so long as the relevant electric-dipole matrix element is non-zero. Experimentally, such optical absorption exists for light polarized along the c-axis for the “lower” T_c materials, YBa₂Cu₃O_{6.63} and La_{2-x}Sr_xCuO₄ but not for fully doped YBa₂Cu₃O₇. No strong absorption exists for light polarized in the CuO planes for any of these materials.

The d and p bands above can explain these facts with the added assumption that for YBCO₇ there is very little to no p_σ character of the $d_{x^2-y^2}$ on the O sites and no d_{xz}, d_{yz} character of the p_z band on the Cu site. The creation of oxygen vacancies in the chains causes some hybridization making the matrix element non-zero.

The key difference between inter-band pairing and BCS-like intra-band pairing is that inter-band Cooper pairs are *not* invariant under time-reversal although the complete Hamiltonian is time-reversal invariant. This dramatically alters the interpretation of Josephson tunneling. With intra-band pairing, the single electron tunneling matrix element gets mod-squared because both the electron and its time-reversed partner tunnel together. Thus,

all phase information determining the supercurrent is contained in the phases of the gap functions on both sides of the junction.

With inter-band pairing, the single electron tunneling matrix elements are different for the two electrons since they come from different bands leading to a phase contribution from these matrix elements on top of the contribution from the gap functions. We define the simplest possible phases for the band wavefunctions and assume an isotropic s-wave attraction. This leads to a pure s-wave gap. Thus, the Josephson supercurrent is controlled solely by the phases of the band orbital matrix elements.

The four key tunneling experiments,¹⁻⁴ two leading to an “s-wave” gap and the other two to a “d-wave” gap can all *simultaneously* be explained by inter-band pairing. For the hexagonal YBCO (s-wave) of Chaudhari et al.,³ the key feature leading to an s-wave result is the mismatch of the CuO planes across the grain boundary due to the use of a MgO seeding layer for the YBCO hexagon. This naturally leads to the dominant tunneling of d electrons to p electrons and p to d electrons. The single electron matrix element thus get mod-squared and we are left with “s-wave” behavior. On the other hand, for the YBCO tri-crystal experiment of Tsuei et al.,² the CuO planes align across the grain boundary forcing tunneling of d to d and p to p. In this case the d-d orbital overlap simulates the effect of a “d-wave” gap.

The temperature dependence of the Knight shift can be understood by essentially the same matrix elements that we used to understand the low-energy optical absorption. This is due to the orbital (Van Vleck) paramagnetism. Usually the orbital paramagnetism is temperature independent because the energy differences with non-zero matrix element in the expression for the orbital paramagnetism χ are either very small compared to kT or else very large compared to kT . With inter-band pairing as we have assumed this is no longer the case and the contribution to the Knight shift from the nuclear orbital coupling can be temperature dependent. It is not hard to see from the expression for χ that the shift must increase with increasing temperature as experimentally observed.

Finally, for YBCO₇ all of the relevant matrix elements will be zero for the same reasons as the optics. For YBCO_{6.63} and LASC0, the matrix elements are zero for magnetic fields along the c-axis and non-zero for fields in the CuO planes as observed.

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