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FORMATION, MOTION AND HIGH TEMPERATURE SUPERCONDUCTIVITY OF LARGE BIPOLARONS

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1. INTRODUCTION

Superfluidity and superconductivity are both associated with resistanceless flow at sufficiently low temperatures. The similarity of these two phenomena led (circa 1950-1960) to consideration of a common quantum-mechanical origin of these phenomena. In particular, superfluidity results from the Bose-Einstein condensation of mobile neutral bosons and superconductivity can result from the Bose-Einstein condensation of mobile charged bosons.[1] This form of superconductivity is now termed "bipolaronic superconductivity," since the charged bosons are presumed to be bipolarons. Bipolarons are electrons that pair as a result of the electron-lattice interaction.

Bipolaronic superconductivity requires two exceptional circumstances. First, at least some charge carriers must form bipolarons. Second, these bipolarons must be mobile (move coherently). However, beyond quasi-one-dimensional electronic systems, bipolarons have heretofore always been found to be "small." Small (bi)polarons are very compact (bi)polarons that localize rather than move coherently.[2] Thus, small bipolarons are not suitable carriers for bipolaronic superconductivity. However, in analogy with the case of large polarons, less compact bipolarons, "large" bipolarons, are expected to be mobile. These observations lead one to ask if and when large bipolarons can form in multi-dimensional electronic systems. Here the results of studies of the formation, motion

and superconductivity of large bipolarons are summarized.[3,4]

2. RESULTS

It is found that a two- or three-dimensional large bipolaron can only form in an ionic system with an exceptionally large ratio of the static to high-frequency dielectric constant: $\epsilon_0/\epsilon_\infty >> 2$. Remaining requirements for large bipolaron formation are less stringent in quasi-two-dimensional electronic systems than in three-dimensional systems. Furthermore, since the atomic displacement patterns associated with different bipolarons interfere with one another, there is an upper limit to the density of bipolarons that can be supported.

The coherent normal-state dc transport of a large bipolaron is characterized by both a large effective mass and a long scattering time. Above very low temperatures, the mobility associated with the coherent motion is inversely proportional to the temperature.[5] Thus, assuming a temperature independent carrier density, the resistivity is proportional to the temperature.

Interacting large bipolarons will display superconductivity below their Bose-Einstein condensation temperature, T_c. This temperature can be comparable to the transition temperatures observed in high-temperature superconductors. For example, with a density of 10^{21} cm^{-3} noninteracting bipolarons with isotropic effective masses of twenty free-electron masses, T_c is about 130 K. Since the Bose-Einstein condensation temperature is an increasing function of the density of bipolarons and bipolarons are destabilized beyond a maximum carrier density, T_c is a peaked function of the carrier density.

The transition temperature depends on the material's properties through their effect on the bipolaron's effective mass. The bipolaron's mass tends to be dominated by atomic displacements in the immediate vicinity of the electronic carrier. Therefore, with $\epsilon_0/\epsilon_\infty$ sufficiently large that the material is superconducting, T_c is only weakly affected by atomic substitutions away from the electronic carriers.

Within the CuO_2-based materials, the paired carriers are taken to lie primarily within the CuO_2 sheets. Thus, with an isolated CuO_2 sheet (as in La_2CuO_4), self-trapped electronic carriers have a disklike morphology. When CuO_2 sheets are contiguous (as in $YBa_2Cu_3O_{7-\delta}$), self-trapped electronic carriers are viewed as expanding to encompass the contiguous sheets. Since the bipolaron's mass varies inversely with its volume, increasing the thickness of such a bipolaron reduces its mass and increases T_c. Thus, T_c increases with the number of contiguous sheets until a limiting value is achieved. If a three-dimensional large bipolaron can exist, T_c will saturate at its three-dimensional value. If a three-dimensional large bipolaron cannot be supported, the large bipolaron and bipolaronic superconductivity disappears when the number of contiguous sheets exceeds its limiting value.

The dependence of the large bipolaron's mass on isotopic substitutions for the solid's atoms produces an isotope effect for T_c. In particular, the large bipolaron's effective mass depends on the mass of the atoms associated with the strain field of the bipolaron. If these strains primarily involve relatively heavy atoms, isotopic substitutions will only shift the bipolaron's mass and, hence T_c, by a small fraction of their values. Thus, a model for a p-type CuO_2-based superconductor in which the energy of a hole on an oxygen ion depends on displacements of the neighboring Cu ions yields a small isotope effect.

Upon Bose-Einstein condensation, a finite fraction of the bipolarons occupy their

groundstate. The groundstate of a low density of bipolarons is the ordered arrangement that minimizes their mutual Coulombic repulsion. The lowest energy excitation of this condensate is a long-wavelength density fluctuation that, because of the charge on the bipolarons, has plasmon character. The energy separation between the groundstate and this excitation is the gap for bipolaronic superconductivity. For the parameters of the previous example, the zero-temperature gap is ≈ 0.1 eV. With increasing temperature the number of bipolarons in the groundstate is reduced and the energy gap falls until it vanishes at T_c.

The groundstate provides the maximum dispersal of the positive charge of hole-like bipolarons. Therefore, the groundstate provides maximum shielding of the electrons of the (negatively charged) CuO_2 sheets from injected positrons. For bipolaronic superconductivity, the positron lifetime should increase with decreasing temperature below T_c as the occupancy of the groundstate is increased. This effect is observed in the novel superconductors but not in conventional (BCS) superconductors.

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