Role of Phonon Coupling in Cuprates

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Emergent States of Matter

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Abstract:

High temperature superconductors promises to usher in major technological advances. Cuprates in particular are an interesting called such because they are a class of compounds containing copper and oxygen that exhibit superconductivity. During the discovery of the cuprates theorist tried to use BCS theory to explain the pairing mechanism of the cooper pairs. They found that phonon-electron interactions do not entirely explain why cooper pairs form and additional studies need to be made to fully understand these superconductors outside a BCS model. Although this is not to say that phonons do not play any part in the formation of the cooper pairs in cuprates. In this article will explain what role the phonons have by examining ARPES and STM data.

Brief history

In 1908 Heike Kammerlingh Onnes became the first person to liquify helium using the Hampson Linde cycle. And in 1911 he broke history again with the first known discovery of superconductivity; by cooling Mercury via liquid helium and observed the resistance drop precipitously as shown in Fig. 1.



As more properties of a superconductor started to emerge so did the theories needed to explain them. From London calculations of the correlation length to Ginzberg Landau formulation which described most of the experimental observations with the introduction of an order parameter and the calculation of the approximate gap size of the superconductor by Cooper.

Brief intro to BSC theory

One of the great triumphs was in 1957 Bardeen -Cooper-Schrieffer published the BCS theory for superconductivity which articulated a mechanism for normal superconductors. In short they showed that the superconductor acts like a charged Bose Einstein Condensate. Electrons slightly above the fermi level couple together with the aid of a phonon and these pairs condense to an energy state lower than the fermi level. To visualize the cooper pairs imagine an electron traveling through the lattice. There is an attraction between the electron and the positive atoms dispersed in the background (jellium) which causes the atoms in the lattice to move slightly towards the electron. So, we see net positive ions clustered where the electron was and since the ions are much heavier their

timescale of their movement is much larger than that of the electrons. From the electrons' perspective the shifted ions are essentially standing still. Now if another electron follows in the wake of another electron they should both experience a long range attractive potential from the clustered positive ions. Below a certain temperature this potential becomes strong enough to cause a bond between the two electrons to form this is what we call a cooper pair.

As described above BCS theory articulated the glue to be caused by phonon electron interactions. This was a reasonable assumption since the isotope effect had shown that phonons played a role in superconductivity. The isotope effect was first demonstrated by Reynold et. al. 7 years before BCS theory was published. In Reynold's paper he showed that changing from mercury to one of its

$$\alpha = -\frac{d\ln[Tc]}{d\ln M} = \frac{1}{2}(1-\delta) \tag{1}$$

heavier isotopes changed the transition temperature as shown in Figure 3). Equation (1) describes the strength of the isotope effect[2]. For normal superconductors the ideal isotope coefficient α_{Tc} = .5 therefore δ tells you how much your superconductor differs from an ideal isotope effect, M is the ionic mass, and Tc is the critical temperature.



Figure 2. Transition temperature v. isotope mass.

Discovery of Cuprates

In 1986 newly fabricated materials with a high superconducting transition temperatures which could not be properly explained using BCS theory. So began the search to explain superconductivity in this class of compounds called cuprates. The materials consist of crystal planes composed of copper and oxygen atoms in a square lattice(fig.3a). Undoped cuprates have electrons stuck to the copper atoms and thus form an antiferromagnetic mott insulator. By p-doping the cuprate you allow electrons to hope from one empty site to the next; the more you dope the more freedom electrons have to move around. As you can imagine, if you keep doping the cuprate then you will eventually produce something that behaves like a metal with electrons freely flowing parallel to the CuO layers. But this is not the entire story as Figure 3b shows there are many different phases the cuprate can have if you hole dope it enough.



Figure 3. a) The lattice of a typical cuprate with stacked copper oxide planes and dopants in between[6]. b) Phase diagram of temperature v. hole doping [9].

It should also be mentioned that the d wave order parameter (a parameter used in Ginzberg Landau theory that shows whether your system is order across phase boundaries, in other words, it tells you whether your system is a superconductor) is not spherical symmetric unlike for normal superconductors. This is because the electrons are closer together resulting the electron coulomb repulsion to be stronger also in the low doping limit they are antiferromagnets with alternating spin up and spin down which corresponds to antisymmetric singlet. So spatially it must be symmetric but not spherically symmetric since the electrons would be too close to each other. To fulfill these qualifications angular momentum must to corresponds to 1=2 (has a node in the center). Therefore the cuprates will have a d wave order parameter which corresponds to a dumbbell shape in momentum space.

Phonon pairing mechanism

In the advent of these new high temperature superconductors researchers had great interest in explaining them within the lens of BCS theory. As they quickly found out the theory was ill-equipped to predict much of the experimental findings. One such experiment was done by L. C. Bourne et. al. in his study of the isotope effect in Y-Ba-Cu-O [1]. They did this by replacing O^{16} in YBa₂Cu₃O₇-delta with one of Oxygen's isotopes O^{18} . Then they measured sample resistance vs. temperature. As figure 1 displays there were no measurable differences between the transition temperature before and after the isotope exchange. This would imply a zero isotope coefficient α . However this is not sufficient evidence to claim phonons play no part in the pairing of electrons. One claim by Pringle et. al. is that since the intrinsic isotope coefficient (isotope coefficient independent of doping) for YBa₂(Cu_{1-x}Ni_x)₄O₈ is so small (α_{Tc0} = .04). Equation 2 shows the relationships

$$\alpha_{\rm Tc} = \alpha_{\rm Tc0} \left(1 - \frac{dln[F(z)]}{dln z} \right)$$
⁽²⁾

This tells us that the isotope effect coefficient gets a small contribution α_{Tc0} which is a function of the gap size. Therefore the pairing mechanism is mostly nonbosonic since most of the contribution comes from the pseudogap states[4].



Figure 4. Transport measurements for $YBa_2Cu_3O_{7-\delta}$ show no change in the transition temperature when oxygen 16 is replaced with oxygen 18 [1].

Current studies of electron phonon interactions

More recent studies emphasize the role phonons play in high superconductivity. Angle-resolved photoemission spectroscopy (ARPES) studies of cuprates allow a unique perspective into electron interactions. The technique involves exposing your sample to coherent light with spot sizes on the order of 1mm. When the light is at sufficiently high energies the electron will escape the surface of the material and be measured by an analyzer. You can then plot the binding energy versus the momentum parallel to the surface to find the electron dispersion. Using this technique researchers could see a ubiquitous signature in the quasiparticle dispersion[8]. Figure 5 the quasiparticle dispersion plotted for various cuprates at different doping and different temperatures.



Figure 5. Quasiparticle dispersion with doping δ dependence of a) LSCO at 20 K b) BI2212 at 20 K c) and Bi2201 at 30 K all taken in the nodal direction(0,0) – (π , π). d) LSCO optimally doped with blue below T_c and red above T_c e) BI2212 optimally doped with blue and light blue below T_c and red above T_c f) estimates the coupling constant λ for different samples as a function doping. Arrows show the location of the kink for each plot [8].

They found a kink in each plot which appeared when the sample was above and below the transition temperature. The kink what observe at energy range 50-80 meV for LSCO, Bi2201, and Bi2212. Since the gap sizes are different for each of these cuprates but the energy range of the kink is similar it does not make sense to attribute the kink to a gap opening. Also the 41 meV neutron mode (obtained from neutron scattering measurements) is ruled out since it only appears when the material is superconducting [9] and the "kinky" behavior was seen at temperatures above and below T_c . Furthermore, inelastic neutron scattering has shown that a phonon mode appears at 70 meV in LSCO which is in the range of the kink in figure 5a). Therefore when can conclude that the large kink is most likely due to electron – phonon interactions.



Figure 7. There are seven scans along $(3+q_x, 0, 0)$ at 10 K. There is a peak in each plot at 70 meV which corresponds to the oxygen bond-stretching mode (phonon mode) [11].

Scanning Tunneling Microscopy Studies

Another tool that can be used to investigate phonon electron interaction is scanning tunneling microscopy (STM). Most systems rely on a constant current of tunneling electrons from an atomically sharp tip to the sample (although systems can use constant height mode), any slight change in the current will cause the feedback to move the tip in the direction which opposes that change. Due to the tunneling properties of electrons the transmission coefficient is an exponential decay as a function a of distance. So a small change in distance produces a large change in current and thus cause the tip to move up or down. This is the property that allows STM to resolve feature with the resolution on the order of angstroms. Jinho Lee et. al. utilized STM to not just see small features but also to see density of states and phonon modes [12]. By using equation 3 where the Δ is the gap

$$\Omega(r) = \prod(r) - \Delta(r) \tag{3}$$

 \prod is the bias energies where peaks in the $\frac{d^2I}{dV^2}$ occur and Ω is the boson energy. Lee et. al. obtained \prod and Δ from their measurements with the STM as Figure 8 shows below. The sample measured was Bi2212. They then plotted



Figure 8 shows the differential conductance spectrum on the left and the second derivative with respect to voltage on the right. Energies corresponding to the largest peak in the right graph are considered \prod .

histogram of Δ and Ω measured from 5 samples at different dopings. Although Δ and \prod both changed significantly the difference between them Ω remained fairly

constant with a measured value of 52 meV [12]. This energy is within the range of the kink that was observed via ARPES. So it lead credence to the idea claim that the observation of the kink is an electron phonon interaction.

Conclusion

As we see with our data from ARPES and STM the initial claim that phonon exhibited no effect on superconductive cuprates is false. The data shows that the effect of phonons on the quasiparticles is strong and should be taken seriously as contributing to the glue of a cooper pair.

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