

# Superconductivity, nonadiabaticity and strong correlation in the light of recent experiments

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**Abstract.** Recently a series of experiments in Scanning Tunneling Spectroscopy, angle-resolved photoemission spectroscopy (ARPES) and isotope effects have provided a great deal of information about the nature of the superconducting state, even though many questions are still open. In this paper we present a discussion of the various theoretical frameworks in the light of these new experiments. Strong correlations started as the possible path to an entirely novel physics but, in many recent versions, they are reduced to the modest role of just raising the coupling in a BCS gap equation with phonon mediators. We argue instead that a conceptual generalization of the Migdal-Eliashberg (ME) theory is necessary and we discuss the consequences arising from the breakdown of the adiabatic assumption. The Nonadiabatic Theory of Superconductivity represents a complex generalization of the ME theory which is natural and, in many respects, unavoidable. In fact Migdal's theorem is strongly violated in these materials for a variety of reasons. The quantification of these effects is technically complicated and it is rather model dependent. In this framework strong correlations can have an important role in locating the system in a favourable range of parameters (forward scattering). We present a critical discussion of these developments in the light of the recent experiments and we also propose some crucial tests.

## 1. Twenty Years of Challenge

Since the discovery of high- $T_c$  superconductivity (SC) in the Cuprates the possibility of interpreting this phenomenon within BCS theory with phonon mediators was immediately disregarded. This was due to a variety of reasons: first the value of  $T_c$  reaching about 150 K appeared too high with respect to the usual theoretical limits of BCS. Second the isotope effect was almost negligible for the optimal doping. Third, and probably most important, these materials are very far from optimal BCS systems because they are doped Mott insulators and the effective carrier density is very small [1]. This led to a riddle of proposals mostly based on electronic mediators or on more radical concepts like the separation of spin and charge (holons and spinons) and the Luttinger liquid picture instead of the usual Fermi Liquid.

The underdoped phase showed many forms of instability related to the lattice (stripes) and to the electronic properties. Such features, in general, become more pronounced by decreasing the doping, up to the final instability where the system becomes an antiferromagnet without metallic and superconductive properties. One line of reasoning was that these instabilities should correspond to a breakdown of the Fermi Liquid and, from this new state, the SC phase should appear. In addition the underdoped phase showed a marked evidence of a pseudogap which seemed to support this picture.

The basic idea was that one should first destroy completely the Fermi Liquid and enter in a new state and then, from this new state, one should study the SC instability. This led to a great attention to

all these instabilities which were considered as possible “smoking guns” from which the SC state should then appear [2].

On the contrary little attention was given to the overdoped phase in which these anomalies are much less evident. In fact one might also consider the opposite point of view: namely starting from the standard Fermi Liquid at large doping and approach the SC state from this side. In this perspective a perturbative scheme with respect to the right side Fermi Liquid appears as a plausible hypothesis.

## 2. Strong Correlation of Course

There is no doubt that strong correlations dominate the phase diagram of the cuprates. Only by doping the AF insulating state one obtains a poor metal and then the SC state. The Hubbard high energy physics is dominated by the large coupling  $U$  but superconductivity corresponds to much lower pairing energies and how the physics of  $U$  may reflect in the SC pairing is a highly nontrivial question which is basically unsolved.

One of the most popular schemes is to consider a canonical transformation where the Hubbard model is mapped into a  $t$ - $J$  model. In such a case the energy of the spin coupling would be  $J \approx 100$  meV. In principle a BCS instability based on the  $J$  interaction would be possible but problematic. First the question of avoiding the double occupation, which is a crucial one in the  $t$ - $J$  model, is not included in such a simplified picture. In addition it is not clear at all why the cuprates should be better than many other materials with a larger number of carriers and a coupling to some magnetic state arising from a different band like for example in the heavy Fermions. Third, recently the role of phonons has become more and more relevant as we are going to see later. Finally the idea that the new physics of the strong correlation state would reduce to a simple weak coupling BCS scheme with spin interaction does not appear very attractive from a conceptual point of view.

Given this situation a number of different proposals have been formulated. However, all of them have met important difficulties up to now. For example the most recent scheme proposed by P.W. Anderson [3] is very interesting and provoking but it leads to the following problems. The link of the “hidden Fermi Liquid” to the SC instability is not specified with a gap equation. In this respect it is difficult to clarify the origin of the high- $T_c$  phenomenon and to compare it with the recent ARPES and STM experiments. For example the question whether the mediator would have energy of the order of  $J$  (not observed) or infinite has not been clearly discussed. Another general problem with this type of approaches is that they consider the particles as all identical. The ARPES data instead show that different portions of the Fermi surface have completely different properties and the SC state seems to arise only from the more Fermi Liquid (FL) portions.

Of course one can look at the glass as half empty or half filled in the sense that the key role for SC may be played by the non FL or by the FL features. Considering that a non Fermi liquid state is typically insulating, the fact that a transition between insulator and SC state as a function of temperature has never been observed, in our opinion suggests that the (partial) Fermi Liquid properties are positive for SC. The question is then why a “poor” Fermi Liquid can give advantages with respect to a normal Fermi Liquid and this is the basic point of view of our approach as we are going to see later.

## 3. Phonons are Back

A variety of isotope effects have been recently observed in the cuprates. Even if the optimal SC state shows a very small isotope effect on  $T_c$  much evidence has accumulated that, in general, these systems show important isotope effects on  $T_c$  (mostly in the underdoped phase) and also on properties that usually should not possess one, like the effective mass and the magnetic susceptibility.

A large amount of work on the isotope effect comes from the Keller’s group [4]. For various cuprate families one observes a rather general behavior of the isotope effect on  $T_c$  as a function of doping. At very low doping the isotope coefficient  $\alpha$  is very large (up to value 1). Upon hole doping it decreases gradually and for optimal doping it is almost negligible. This isotope effect refers

specifically to the in-plane oxygen. The isotope effect corresponding to apex or chain oxygen is very small for any doping.

An additional strong evidence of the role played by phonons came from the ARPES data, which show a well defined kink that naturally points to phonon self-energy effects [5]. The observation of a well defined isotope shift of the kink energy [6, 7] shows unambiguously that we are in presence of a Fermi liquid with a self-energy dominated by phonons. It is particularly important that this is so even at the optimal doping.

More recently the tunnelling data of the Davis group have identified a phonon (at 50 meV) as the mediator of the SC pairing [8]. In this respect it is particularly striking the relation (anticorrelation) between the phonon frequency and the SC gap. If confirmed these data show unambiguously that this phonon is the mediator of the SC and rule out the alternative interpretation of a spurious coupling in the scattering [9].

For additional evidence of the role of phonons in the cuprates see also various other contributions at this conference by Nagaosa, Cappelluti, Bianconi, Mihailovich, Shen and Balatsky.

#### 4. The Gap Equation and the Mediators

Despite the many attempts to introduce exotic concepts like the Luttinger liquid, holons, spinons and many others, to our knowledge no clear framework has been developed to link these concepts to a gap equation for superconductivity. So, at the moment, a discussion can only be made in terms of the two gap equations which are known, namely the Bose-Einstein Condensation (BEC) and the BCS-like.

The BEC mechanism implies the presence of preformed pairs above  $T_c$ . This is in contradiction with the observation of Fermi surface properties. Even invoking different kinds of states, the evidence is that coherent SC arises from the arcs which are more Fermi Liquid like. In addition the expression for  $T_c$  in BEC is inversely proportional to the effective mass of the pair which, for strong coupling, is rather large. This would imply rather low values of  $T_c$ .

The BCS like gap equation leads to an expression of  $T_c$ , which is dominated by two parameters, the energy of the mediator  $\Omega$  and the dimensionless coupling  $\lambda$ . This equation holds only for very small values of  $\lambda$ . For intermediate values one has to consider the Migdal-Eliashberg theory and the McMillan equation. For very large couplings another regime appears but then the system becomes unstable with respect to polaronic or other instabilities.

It is instructive to consider a simple argument to show the evolution from a BCS to a McMillan-like equation. Let us consider to this regard the bare electronic Green's function which enters in the BCS theory:

$$G(\mathbf{k}, \omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}}} . \quad (1)$$

In the spirit of a strong-coupling McMillan-like analysis, we can include many-body effects through the introduction of the self-energy  $\Sigma(\omega)$ , which, in general, gives rise to a coherent and an incoherent part of the Green's function,  $G(\mathbf{k}, \omega) = G_{\text{coh}}(\mathbf{k}, \omega) + G_{\text{inc}}(\mathbf{k}, \omega)$ . Only the coherent part contributes to SC. For the low-energy excitations, which are mainly involved in the SC pairing, we have  $\Sigma(\omega) = -\lambda\omega$ , and

$$G_{\text{coh}}(\mathbf{k}, \omega) = \frac{1}{Z} \frac{1}{\omega - \varepsilon_{\mathbf{k}}/Z}, \quad (2)$$

where  $Z = 1 + \lambda$  is the electron-phonon renormalization factor. Many-body electron-phonon effects affect thus the SC pairing in two different ways. On one hand they reduce the quasi-particle (QP) spectral weight by a factor  $1/(1 + \lambda)$ , which can be absorbed in the redefinition of an effective el-ph matrix element  $g_{\text{qp}} = g/(1 + \lambda)$ . On the other hand self-energy effects lead to a narrowing of the quasi-particle bandwidth and to a corresponding enhancement of the density of states (DOS),  $N_{\text{qp}}(0) = N(0)(1 + \lambda)$ . The effective total el-ph SC pairing results thus  $\lambda_{\text{eff}} = g_{\text{qp}}^2 N_{\text{qp}}(0) = \lambda/(1 + \lambda)$ , and the BCS expression results to be modified in the McMillan-like:

$$T_c \approx \omega_{\text{ph}} \exp\left(-\frac{1}{\lambda_{\text{eff}}}\right) = \omega_{\text{ph}} \exp\left(-\frac{1+\lambda}{\lambda}\right). \quad (3)$$

From this discussion it is clear that the attempt to reach high values of  $T_c$  by increasing the coupling is bound to a saturation effect and to the instability limits mentioned above.

So, in our opinion, since this path does not look very promising, one should try to go beyond this scheme and try to see how high values of  $T_c$  can be achieved without pushing too far the value of  $\lambda$ . In addition note that the high  $T_c$  superconducting materials are very bad in many respects in relation to the BCS scheme and the idea that some very high parameter may cure all these problems appears rather unlikely.

One can also discuss, in the same context, how electronic correlations can affect this el-ph framework in the same perturbative way. This discussion relates to those approaches in which the mediator is a phonon but it is argued that the electronic correlation can play a crucial role in enhancing  $T_c$ [10-12]. Within a perturbative context we can still consider an expression for the coherent Green's function as in Eq. (2), where the renormalization factor  $Z$  stems from the el-ph self-energy in the presence of electronic correlations. The important point to be stressed here is that, within this framework, electronic correlation does not affect the functional dependence of the SC pairing but it could only hopefully modify the value of the effective pairing  $\lambda_{\text{eff}}$ , in a McMillan context. A slightly modified scenario is proposed in some papers where it is argued that, for particular Jahn-Teller couplings, the special symmetry involved in the pairing can avoid the reduction of pairing due to the reduced quasi-particle spectral weight and profit only of the enhancement of the DOS. As a first comment, we would note that such a vision does not imply any enhancement with respect to BCS but just a reduction of the self-energy handicap. Secondly, in any case one would need a huge coupling to reach high values of  $T_c$ , which is a path that also meets the above problems in terms of instabilities. Finally one should note that such a path to high  $T_c$  is in any case a lower bound with respect to a simple Fermi Liquid with small interaction and therefore a high DOS.

In conclusion we have seen that electronic correlation is unlikely to provide an enhancement if the mediator is a phonon. In the case of more radical hypothesis in which correlations should lead to properties which are not perturbatively related to the Fermi liquid these ideas are certainly interesting and challenging. However, in order to discuss them on a scientific basis their proponents should present some type of gap equation which permits to identify the reason for the eventual  $T_c$  enhancement and to compare them with experiments related to SC.

## 5. STM spectroscopy

Recently a number of important experiments based on the Scanning Tunnelling Microscopy have provided new important information. The Davis group data point very strongly to a phononic mediator of about 50 meV [8]. The key point for this conclusion is the anticorrelation between gap and phonon frequency. A new element of this type of experiments is the realization that local superconducting properties can vary appreciably from point to point in the surface of the sample. This is also the reason why previous experiments were unclear up to now. In addition the isotope effect clarifies the phononic nature of the mediator.

If confirmed these data leave little space to additional interpretations about the mediator. The objections that have been proposed to this interpretation, like the idea of P.W. Anderson that the key energy involved should be at a scale outside the experimental range, are very difficult to reconcile with the fact that there is a strong (anti)correlation between gap and phonon frequency [13].

From these STM data one can derive various other conclusions. First the fact that the gap is pinned on the chemical potential shows clearly the SC origin of the gap itself. The behavior of the gap as a function of doping resembles closely what has been usually discussed in terms of pseudo-gap.

However, the presence of coherence peaks in the spectra implies an instability of the Fermi surface with some type of low frequency excitations and it excludes condensation from preformed pairs which would lead to a dip without a coherence peak.

The detailed temperature dependence analyzed by the Yazdani group points then to a common origin between pseudogap and the real superconductive gap [14]. Different regions lead to different local gaps. When these regions reach a certain fraction of the total sample a coherent SC state extends through the whole system. The ratio  $2\Delta/T_c$  seems to give a universal value of 8 but this seems to refer to local values of the gap. If one uses the bulk value of the gap a more normal value of about 4 is obtained.

The fact that the largest values of the gap (or SC pseudo-gap) reach very large values ( $\sim 60$  meV), even larger than the energy of the phononic mediator ( $\sim 50$  meV) shows that we are in some sort of strong coupling regime.

## 6. Nonadiabatic Superconductivity: Status and Perspectives

The theory of Nonadiabatic superconductivity, that we have developed in the past years [15-17], represents an attempt to go beyond the BCS and Migdal-Eliashberg approach in a nontrivial way. It corresponds to a Complex Fermi Liquid in which one of the basic concepts of the usual many body theory, namely Migdal's theorem, does not hold any more.

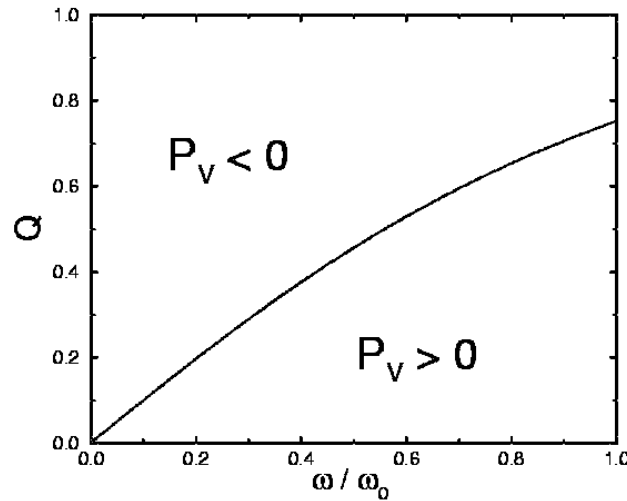
This is quite a natural path if one looks at the properties of the materials. In fact the basic assumption of Migdal's theorem, and therefore of the Migdal-Eliashberg and BCS theories, is that the Fermi energy should be much larger than the boson mediator (phonon). In a normal metal the carrier density is high and indeed the adiabatic condition is well satisfied. In high- $T_c$  materials instead the effective carrier density is very low, about twenty times less than in a normal metal and this leads to very low values for the Fermi energy. Actually this point of view creates a common link between apparently different materials. For Fullerene compounds the small Fermi energy arises from the band structure itself. For oxides a simple concept of band structure is not applicable because the undoped material is an antiferromagnetic insulator and the main energy in the system is the Hubbard repulsion  $U$ . Upon doping, however, one observes the development of metallic properties which are related only to the dopant carriers. These show poor metal properties and their propagating or localized nature depends on the position along the Fermi surface. There is evidence that superconductivity arises from the more metallic part of these states. Their Fermi velocity is rather small and the more so as they get close to the Van Hove singularity. Also for  $MgB_2$  one has a problem with the adiabatic assumption. In fact superconductivity arises essentially from the  $\sigma$  bands which are strongly affected by the zero point motion of the most coupled phononic modes.

This situation led us to reconsider the problem of the Migdal's theorem as a general fact potentially relevant for all these systems. Technically the first step is the study of the vertex correction diagram, which plays a similar role to the self-energy in the Migdal Eliashberg theory and the McMillan equation.

A detailed study of the vertex correction showed a rich structure not identified before in the  $\omega$  vs.  $\mathbf{q}$  space, as shown in Fig. 1, and it leads to a new scenario for the corresponding Complex Fermi Liquid in the normal and SC state. In particular the simplest possible effect would be to further substitute the coupling  $g_{qp}$  with an effective coupling  $g_v$  modified by the vertex function:

$$g_v = g_{qp} [1 + \lambda P_v(\omega, \mathbf{q})], \quad (4)$$

where the vertex function  $P_v(\omega, \mathbf{q})$  is positive for small values of  $\mathbf{q}$  and negative for large values (Fig. 1). This situation would imply raising or lowering of  $T_c$  depending on the properties of the material. Clearly the non-adiabatic phase space is much larger than the adiabatic one and the key point is then to identify the properties of the various regions. For example it is known that strong electronic correlations lead to forward scattering. Within our nonadiabatic framework this fact would enhance  $T_c$ .



**Figure 1.** Sign of the vertex function  $P_V(\omega, \mathbf{q})$  in the  $\omega$ - $\mathbf{q}$  space ( $Q=2q/k_F$ ).

So, in this perspective, the basic concept is nonadiabaticity but correlation would be also essential to locate the system in a favourable regime. However, important effects can be due also to Van Hove singularities and other properties.

In terms of the simple analysis we have made for McMillan we can also have an expression for the Nonadiabatic SC. Assuming to be in the favourable region where the vertex function is positive and  $P_V \sim 1$ , we can obtain a rough estimate for the effective el-ph coupling which include *both* the quasi-particle renormalization effects and the vertex corrections:

$$\lambda_{\text{eff}} = g_{\text{v}}^2 N_{\text{qp}}(0) = g_{\text{qp}}^2 (1 + \lambda)^2 N_{\text{qp}}(0) = \lambda(1 + \lambda), \quad (5)$$

and

$$T_c \approx \omega_{\text{ph}} \exp\left(-\frac{1}{\lambda_{\text{eff}}}\right) = \omega_{\text{ph}} \exp\left(-\frac{1}{\lambda(1 + \lambda)}\right). \quad (6)$$

One should note that this approach does not lead just to a reinterpretation of the value of  $g$  because different properties are affected in different ways within the extended theory. One important point is that, in order to achieve high  $T_c$  values, it is not necessary to have very large values of  $\lambda$ .

In addition we remark that in this generalized theory we have new pairing channels that can really provide an enhancement with respect to BCS [17,18]. Finally a conceptually important element of our approach is that it is possible to understand why a small density of carriers represents a positive ingredient for superconductivity.

The fact that the pairing is essentially dependent on the phonon frequency leads to a variety of unconventional isotope effects which are beyond Migdal-Eliashberg theory [19,10].

For example we predict an isotope effect on the effective mass of the electrons in the normal state and on the Pauli susceptibility. The observation of an isotope effect on the penetration depth is an indirect confirmation of this result. Of course direct measurements on the normal state would be very important. Also the observation of an isotope effect in the Pauli susceptibility in Fullerene compounds is an indication of nonadiabatic effects [21].

The above discussion refers to an analysis on the nonadiabatic effects only considering the vertex correction term. This is analogous to the self-energy discussion in relation to ME theory and the McMillan expression. On the other hand we have also studied nonperturbative approaches to this problem by using Dynamical Mean Field Theory [20]. The result was that the two approaches are in very good agreement in the appropriate regime and it seems that real materials are reasonably within

the perturbative region. One problem with this nonperturbative approach, however, is that the important  $\mathbf{q}$  dependence cannot be included.

The properties of the vertex function have been studied also by other authors with a somewhat different starting point. One delicate point to be considered is that the full momentum and frequency dependence requires an appropriate approach with respect to the mathematical properties of the diagram. For example if only simple limits ( $\omega \rightarrow 0$ ;  $\mathbf{q} \rightarrow 0$ ) are considered the results are not representative of the full behavior [22,23]. In addition the band filling can also play an important role.

A particularly interesting case is the role of a van Hove singularity in the density of states which is very relevant for the cuprates. A naive interpretation of this situation would be to argue that the singularity raises the density of states and this may lead to an enhancement of  $T_c$ . However, this picture is not realistic because the singularity implies an intrinsic violation of Migdal's theorem because as soon as you approach it the energy range for scattering is intrinsically reduced, independently on the width of the original band. Therefore this problem requires necessarily a nonadiabatic theory [24,25]. The result is that the main effect is not the apparent enhancement of the density of states, but rather the fact that, near the singularity, the scattering is limited to small values of  $\mathbf{q}$ .

We have mentioned that electronic correlations tend to favour small  $\mathbf{q}$  scattering. A detailed study of this effect shows that this limitation is due to the correlation hole which is associated to each carrier [26-28]. In this case one has also to consider the problem of the coherent and incoherent part of the propagator and the SC instability refers only to the first one. An additional effect of correlation is that there is a residual repulsive interaction at large values of  $\mathbf{q}$ . This situation can naturally lead to anisotropic SC like d-wave [29].

## 7. Local Properties in real and $\mathbf{k}$ space

Since some time the ARPES data provided clear evidence for a Fermi surface even though of rather complex nature. In particular the properties of these systems are strongly non homogeneous along the Fermi Surface. The arc regions have reasonably well defined metallic properties while near the antinodal points the electronic states appear to be essentially localized. Doping increases the size of the Fermi liquid arcs and coherent SC seems to be related to these arcs. Of course we are in presence of a complex Fermi Liquid and the standard theoretical framework cannot be applied.

From the STM studies one also learns that the SC properties are strongly position dependent. The origin of this effect has to be found in the role played by the dopant oxygen ions which are randomly distributed in the system. From the various experiments the following picture emerges. The pseudo-gap seems related to the SC instability in a local sense but not necessarily leading to a coherent SC state. On the other hand, upon cooling, when these gapped regions reach a certain fraction of the total volume, a coherent gap establishes through the system.

Clearly we are in presence of an inhomogeneous superconductivity. Up to now these properties have been studied for bilayer systems which are symmetric in terms of charge density. It has been shown that, if one has three or more layers in the unit cell, the charge distribution among the various layers is not any more homogeneous. Namely the central layers are depleted with respect to the outer layers [30]. It would be very interesting to study these type of systems for two reasons. First to analyse the effect of the different charge filling in terms of the corresponding gaps. Second the central layers should be much less affected by the disorder of the doping ions.

From a theoretical point of view this space inhomogeneity has been studied up to now in terms of a fully coherent superposition of the different regions [31]. This means that the system is considered essentially as if it would have many bands with different couplings and bosonic energies. The result is a sort of effective medium theory in which each point of the system is coupled to its neighbours but the phase is uniform. We can see instead that the properties of the systems are more complex with respect to the phases as shown for example by the behavior of the local gap or pseudo-gap with respect to the bulk. This suggests, in our opinion, that the appropriate framework should be in the direction of granular superconductivity with Josephson couplings between the grains.

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