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ELECTRON-LATTICE COUPLING IN THE CUPRATES

T. Egami
University of Tennessee, Knoxville, TN 37996, USA and Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

Abstract: This article summarizes the principal points of discussions at the Erice workshop on the relevance of electron-lattice coupling to high temperature superconductivity. While the majority in the field still believes that the phonons and lattice are irrelevant to the superconductivity in the cuprates, such a view is strongly challenged by recent experimental results, particularly in conjunction with the increasing evidence of intrinsic electronic inhomogeneity. It is likely that phonons are a vital component of the phenomenon through the unconventional electron-phonon coupling.

1. INTRODUCTION

It is now a widely accepted paradigm that the remarkable properties of transition metal oxides originate from the closely coupled interplay of spin, charge and lattice degrees of freedom. For instance the colossal magnetoresistance (CMR) in manganites is a consequence of an insulator-to-metal transition (IMT) induced by a magnetic field. In this system the IMT is concomitant with a ferromagnetic transition, and is determined by a precarious balance between the force to localize the charge (due to the electron-lattice interaction and spin correlation) and the force to delocalize the charge (due to the electron kinetic energy and elastic energy). When the

localization force is dominant charges are localized as spin-lattice polarons, and the system shows an insulating behavior. Thus the electron-lattice interaction is critically important, as first pointed out by Millis *et al*. [1] and was proven by further research.

In stark contrast, in the research field of the high temperature superconductivity (HTSC) the role of the lattice has been all but completely neglected by the majority. The conventional view is that it is a purely electronic phenomenon involving spin excitations, and is described, for instance, by the *t-J* model [2]. There are many reasons why the lattice has been dropped from consideration almost from the beginning, such as the near absence of the isotope effect on the critical temperature, T_C, and the linear resistivity. However, the arguments against the lattice involvement are less than perfect [3].

In the meantime evidence of significant lattice involvement has steadily been accumulating. The discussions at this workshop covered recent observations by ARPES, isotope effect and neutron scattering. At the same time recent theories suggest that the electron-phonon (*e-p*) coupling in the strongly correlated electron systems is unconventional, involving spins. Conventional arguments against the phonon mechanism are based on the *e-p* coupling in the Fermi liquids, and may not apply to the cuprates. For a long time since the discovery of the HTSC in 1986 the researchers who take phonons seriously have been a definite minority. However, while other theories have not been able to survive increased level of experimental scrutiny the relevance of phonons appears to be taking an opposite, rising trail. The majority may have made a premature decision on the phonon before important data were obtained.

2. EXPERIMENTAL OBSERVATION

A large amount of experimental results show, rather convincingly, that certain features of the local structure, not the average structure, respond to the superconductive transition or to the opening of a pseudo-gap [4]. The majority dismissed them as mere consequences of strong superconductivity, but more recent data provide more direct evidence of significant lattice involvement.

The recent results of angle-resolved photo-electron spectroscopy (ARPES) by A. Lanzara *et al*. show quite convincingly that the phonons,

most likely the zone-boundary oxygen LO phonons, interact strongly with electrons [5,6]. The position of the kink in the electron dispersion along the nodal direction (π, π) is largely independent on composition and the magnitudes of the gap and T_C, but changes with isotope substitution from ^{16}O to ^{18}O. Along the anti-nodal direction $(\pi, 0)$, they found that the electron dispersion shifts significantly with oxygen isotope substitution. Oxygen isotope substitution changes the volume very slightly, since ^{16}O has a larger zero-point phonon amplitude than ^{18}O. However, this volume effect does not appear to be large enough to explain the observed shifts. It is most likely that this shift is another evidence of strong *e-p* coupling. While the coupling along the nodal direction does not contribute to superconductivity the coupling along the anti-nodal direction does. This observation has increased the possibility that the phonons contribute to the HTSC phenomenon.

The superconductive penetration depth was found to depend strongly on the oxygen isotopic mass by the group of H. Keller, and the result was interpreted to represent the isotope effect on the electronic effective mass [7]. This observation ties in well with the ARPES observation mentioned above, and provides another piece of evidence for the strong *e-p* coupling and its relevance to the HTSC. While it may be argued that the observation provides a definite proof that the phonons significantly modify the electron dispersion, and may not directly prove that they contribute to the pairing, it is difficult to imagine that such a strong interaction does not have an important role in pairing.

The phonon branch that is suspected to interact strongly with the charge by the ARPES measurement, namely the zone-boundary Cu-O bond-stretching LO phonon branch (Fig. 1), was found by inelastic neutron scattering to show unusual temperature dependence [8].

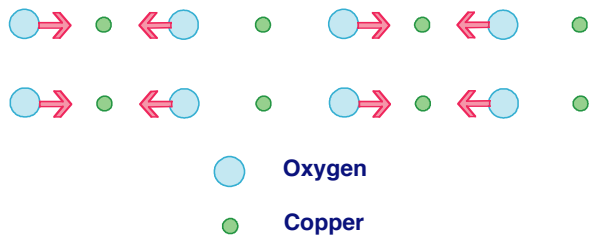

Figure II:1:1 Schematics of the Cu-O bond-stretching zone-boundary LO phonon (half-breathing) mode.

The intensity of inelastic neutron scattering from this branch changes with temperature just as the superconductive order parameter. At the same time other phonon branches with polarization along the c-axis, such as the apical oxygen mode and the buckling mode, do not show appreciable temperature dependence. This suggests that the zone-boundary oxygen LO phonons have a special significance to the lattice effect in the cuprates.

3. THEORETICAL PERSPECTIVE

The reason why the Cu-O bond-stretching phonons are important is not difficult to understand. The undoped cuprates are charge-transfer insulators [9]. The oxygen *p*-level and the Cu *d*-level form hybridized anti-bonding orbital states, and the gap lies between the filled *p*-like band and the empty upper Hubbard Cu-*d*-like band. When the Cu-O bondlength is modified the extent of the *p*-*d* hybridization is modified. This situation is somewhat similar to that of ferroelectric oxides, such as $BaTiO_3$. In $BaTiO_3$ the insulating gap is between the filled *p*-like state and the empty *d*-like state, and shortening the Ti-O distance increases the *p*-*d* hybridization, and thus results in the transfer of negative charge from the *p*-state of O to the *d*-state of Ti. A very rigorous and elegant theory was recently worked out by Vanderbilt and Resta [10,11], which relates this charge transfer to the electronic polarization in the compound that is as large as the ionic polarization, doubling the Born effective charge in many cases.

In the doped cuprate, as it turned out, shortening the Cu-O distance results in the transfer of ***positive*** charge, since the doped holes reside mostly on the oxygen *p*-like band. Thus the electronic polarization is antiparallel to the ionic polarization, greatly reducing the Born effective charge, or even changing its sign. As shown in Fig. 2 for the case of a one-dimensional Hubbard model, the effective charge strongly depends on the phonon wavevector, q, and becomes maximum in the middle of the Brillouin zone for the doping level, x = 1/4 [12]. This strong charge transfer results in the phonon softening [13,14], and strong *e*-*p* coupling.

It was found that because of the strong electron correlation the phonon-induced charge transfer depends on the spin. Consequently the phonon modifies the spin correlation and spin dynamics [12]. In the strongly correlated electron systems phonons interact not only with charge, but also with spins.

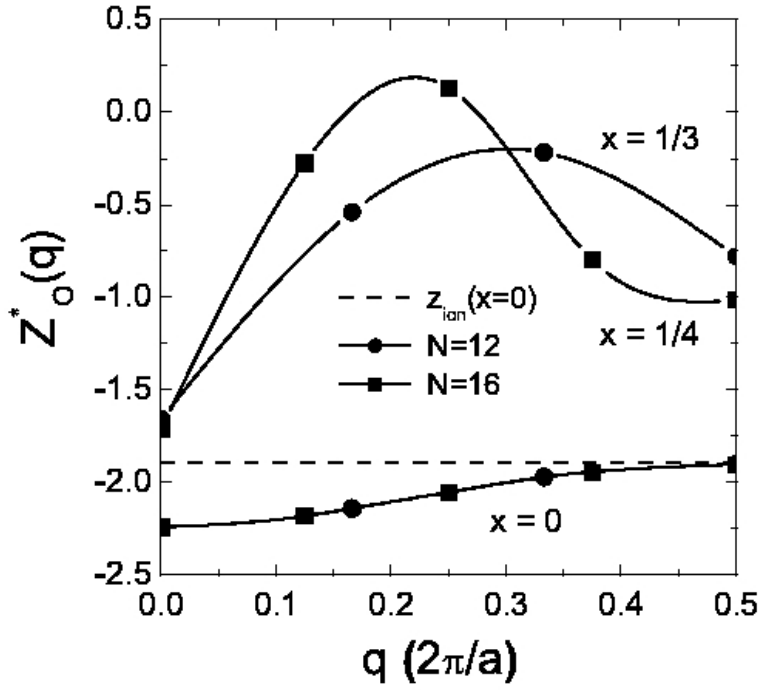

Figure II:1:2. The Born effective charge of oxygen calculated for the one-dimensional two-band Hubbard model with the Cu-O bond-stretching LO mode, calculated for N = 12 ring with doping level x = 0, 1/3 and for N = 16 ring with x = 0, 1/4. The dashed line correspond to the static (ionic) charge [12].

This is why we call the *e-p* interaction in the cuprates ***unconventional***. In addition, because the phonon induces charge transfer from O to Cu over the charge transfer gap of 2 eV, the effect of the phonon extends to high energy ranges [12]. The recent observation that the depression in the optical spectrum due to the gap opening extends to 2 eV was used as the basis for the argument for the electronic origin of the HTSC phenomenon [15-17]. However, it can be explained by the phonon-induced charge transfer [12].

Because of the topology of the CuO_2 plane this *e-p* coupling is anisotropic, strong along the $(\pi, 0)$ direction and weak along the (π, π) direction. The (π, π) mode is a full breathing mode that localizes charge on Cu. The kinetic energy penalty of localization makes this mode less strongly

coupled to charge. The (π, 0) mode, on the other hand, is "half-breathing", and allows charge to flow in the perpendicular direction, thus lowering the kinetic energy penalty. Because of this anisotropy the phonons are even capable of supporting the *d*-wave superconductivity [18], while the *s*-wave solution is usually preferred for the phonon mechanism.

4. RELATION TO SPATIAL INOMOGENEITY AND RELEVANCE TO HTSC

Even though the ARPES results show strong *e-p* coupling, the values of the *e-p* coupling parameter, λ, estimated from the ARPES data along the nodal direction, 1-2, is not large enough to bring about the HTSC. At the same time the spatial inhomogeneity of HTSC has long been suspected [19,20], and is now recognized as one of the common features of the HTSC cuprates as discussed in the other section in this volume [21]. Is it just an accident that the HTSC cuprates are inhomogeneous, or could it be a part of the mechanism? To answer this question we should examine the composition dependence of the pseudo-gap temperature, T_{PG}. This is a complex and confusing problem, but the T_{PG} line that lies above and covers the entire T_C dome seems to coincide with the start of local structural distortion [22]. In particular the fall of T_C on the overdoped side coincides with T_{PG}. This suggests that the spatial inhomogeneity of spin and charge and local lattice distortion associated with such inhomogeneity are the ***required*** conditions for HTSC. Without the phase separation the overdoped cuprate is just a regular Fermi liquid with a zero or vanishingly small value of T_C.

This is a very unique situation for superconductivity, since in the previous experience inhomogeneity is almost always harmful to superconductivity. Why is the superconductivity in the cuprates so different? While further research is clearly required to answer this puzzle, one possibility is that the spatial confinement produces the vibronic resonant state of phonon and charge that enhances HTSC [15,23]. The benefit of spatial confinement on HTSC has been strongly advocated for some time by Phillips with the idea of filamental superconductivity [24] and more recently by Bianconi [25] as the shape resonance effect. In both cases the effect arises due to the enhancement of the local density of states (DOS). An additional, and possibly more central, effect of confinement is to reduce the group velocity of electrons and bring it comparable to the phonon velocity, thus

making the non-adiabatic vibronic resonance possible [15,23]. While details need further scrutiny, the enhancement of the unconventional *e-p* coupling by spatial inhomogeneity appears to be the crucial element of the HTSC mechanism.

5. CONCLUDING REMARKS

Phonons have been discredited and ignored from the very early days of the HTSC research, particularly by theoreticians. However, such hasty dismissal always had a smell of avoidance for convenience without careful scientific examination, a guilty verdict without a due process. This is understandable since phonons are an old story, even called the "conventional mechanism". For theoreticians who thrive at the novelty of ideas working with phonons do not bring needed excitement and the possibility of glory. However, the experimental results have started to penetrate the cold wall of rejection and to chip away misgivings and misconceptions about the importance of the lattice effects. In addition it appears that the phonons in the cuprates are not "conventional" after all. They couple to spins, and may resonate with charge in a non-adiabatic vibronic manner due to magnetic and structural confinement. In this case we are not dealing with the old BCS mechanism any more, but with a drastically new and unexplored HTSC mechanism, worth a serious study. While the jury is still out on the relevance of the lattice to the HTSC mechanism, we may have succeeded in obtaining the court order for the stay of execution of the hastily issued, probably wrong, earlier verdict.

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