The role of phonons in high temperature superconductors - is there one?


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Introduction

- Conventional “Low-\(T_c\)” superconductors are phonon mediated
  - upper limit for \(T_c \sim 30 - 40\) K?
- Unconventional “High-\(T_c\)” mechanism is controversial
  - pairing mechanism not understood
  - large values for \(T_c\), other evidence argue against a phonon mechanism
    - debate has been rekindled
- Infrared active \((q \sim 0)\) modes observed in the \(a-b\) planes of electron and hole-doped cuprates - surprising!
  - modes are almost totally unscreened
  - no anomalies at \(T_c\)
    - implies little or no electron-phonon coupling
- Is there any role for phonons in high-\(T_c\)?
Phonons in High-$T_c$: the early days

- **Observed** along $c$-axis$^{(1)}$
  - poorly conducting
    - unscreened response
- **Not observed** in the $a$-$b$ plane$^{(2)}$
  - high conductivity: screened
  - linear resistivity, etc.
    - small $\lambda_{tr}$ ($\sim \lambda$), thus low $T_c$$^{(3)}$
  
  $$T_c \approx \frac{\Theta_D}{1.45} \exp \left[ \frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right]$$

  (\(\mu^*\) is a pseudopotential)

- **No clear role for phonons**

Unscreened lattice modes

- Carriers in an insulator are localized
  → strong interactions between cores
  → large splitting between the TO and LO modes
  → i.e., strong optic mode in alkali halide salts
  → strength of optic mode is related to LO-TO splitting
  → Model with a Lorentz oscillator

\[
\tilde{\varepsilon}(\omega) = \varepsilon_\infty + \sum_j S_j \frac{\omega_{TO,j}^2}{\omega_{TO,j}^2 - \omega^2 - i\gamma_j \omega},
\]

- Lyddane-Sachs-Teller:

\[
\frac{\omega_{LO}^2}{\omega_{TO}^2} = \frac{\varepsilon_0}{\varepsilon_\infty}
\]

\[
S_j \equiv \varepsilon_\infty \left( \frac{\omega_{LO,j}^2}{\omega_{TO,j}^2} - 1 \right)
\]
Screening in a Covalent or Metallic System

- Light couples to the induced dipole moment
  - determines optical strength
    - normally-active IR modes
- Metals & alloys: carriers are delocalized
  - free carrier response is fast relative to motion of ionic cores
  - carriers screen ionic cores
    - induced dipole moment is reduced
    - optical strength vanishes

\[ S_j \rightarrow 0! \]
Unscreened Lattice Modes

- In metals lattice modes are not observed due to screening effects.
- When $\omega_p \approx \sqrt{n/m^*} (\approx 1\,\text{eV}) > \omega_{TO}$, the Thomas-Fermi form of the dielectric constant is appropriate.

\[
\varepsilon_{TF}(\omega, q = 0) \approx 1 - \frac{\omega_{PD}^2}{\omega^2}
\]

\[
U(r) = \left(\frac{Z}{r}\right)\exp(-r/l_s)
\]

$\rightarrow$ The screening length is $l_s$ ($a_0$ is the Bohr radius).

$\rightarrow$ In Cu, $n \sim 8.5 \times 10^{22}\,\text{cm}^{-3}$ yields $l_s \sim 0.6\,\text{Å}$
  - which is much less than the n-n distance ($\sim 2.5\,\text{Å}$)
  - in good metals and alloys, phonons are screened

$\rightarrow$ in cuprates, $l_s < 1\,\text{Å}$, so the modes should be screened
  - consistent with early observations\(^{(1)}\)

Infrared spectroscopy

- Infrared spectroscopy has emerged as an important technique for probing fundamental electronic excitations
- Infrared region ~2 meV to 1 eV and beyond (optical and UV)
  - carrier dynamics, scattering rates
  - lattice modes, etc.
- Bruker IFS66v/S at NSLS U10A
  - Fourier transform interferometer
- Measure the reflectance of materials
  - near-normal angle of incidence
    - 10 K to above 400 K
    - ~ 20 to over 23,000 cm\(^{-1}\)
  - Kramers-Kronig analysis
    - \(\sigma_1(\omega)\), etc.

(1 eV ~ 8065 cm\(^{-1}\))
Model system: $\eta$-Mo$_4$O$_{11}$

- 2D electronic properties (b-c planes)
  - incommensurate charge density wave (CDW) transitions at $T_{c1}$ (110 K) and $T_{c2}$ (85 K)
- Fermi surface partially gapped, but material becomes more metallic with decreasing temperature
- Expect 47 infrared-active modes
  - these modes are totally screened above $T_{c1}$
- Below $T_{c1}$ modes suddenly appear
  - material is still metallic!
- Formation of CDW
  - modes no longer screened

Hole-doped systems

**Oscillator fits at 295 K**
(all units in cm$^{-1}$, except $S_j$)

<table>
<thead>
<tr>
<th>$\omega_{TO,j}$</th>
<th>$\gamma_j$</th>
<th>($\omega_{p,j}$)</th>
<th>$S_{d,j}$</th>
<th>$S_{d,j}/S_{u,j}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>582</td>
<td>23</td>
<td>(479)</td>
<td>0.68</td>
<td>1.33</td>
</tr>
<tr>
<td>359</td>
<td>12</td>
<td>(460)</td>
<td>1.64</td>
<td>1.06</td>
</tr>
<tr>
<td>275</td>
<td>20</td>
<td>(378)</td>
<td>1.89</td>
<td>2.22</td>
</tr>
</tbody>
</table>

$S_j = \frac{\omega_{p,j}^2}{\omega_j^2}$

- **Surprise:** phonons in Cu$_2$O planes almost **totally** unscreened!
- Ion cores are **unscreened**: opposite of earlier results$^{(1)}$
- No anomalies below $T_c$ (i.e., Holstein modes...)

Electron-doped systems

What are the nature of these vibrations?
- do the originate in the conducting CuO$_2$ planes?

Oscillator fits at 10 K
(all units in cm$^{-1}$, except $S_j$)

<table>
<thead>
<tr>
<th>$\omega_{TO,j}$</th>
<th>$\gamma_j$</th>
<th>$(\omega_{p,j})$</th>
<th>$S_{d,j}$</th>
<th>$S_{d,j}/S_{u,j}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>16</td>
<td>(364)</td>
<td>0.53</td>
<td>0.55</td>
</tr>
<tr>
<td>338</td>
<td>6</td>
<td>(348)</td>
<td>1.06</td>
<td>0.93</td>
</tr>
<tr>
<td>306</td>
<td>4</td>
<td>(739)</td>
<td>5.83</td>
<td>0.85</td>
</tr>
</tbody>
</table>

$$S_j = \frac{\omega_{p,j}^2}{\omega_j^2}$$
Vibrational analysis

- Normal coordinate analysis of two systems (valid for $q=0$)
  - non central forces: angle bend, interactions

<table>
<thead>
<tr>
<th></th>
<th>Pr$<em>{1.85}$Ce$</em>{0.15}$CuO$_4$</th>
<th>YBa$_2$Cu$<em>3$O$</em>{6.95}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ellab $(E_u)$</td>
<td>Pr-O(1) 490</td>
<td>Cu(1)-O(2) 583</td>
</tr>
<tr>
<td></td>
<td>Pr-O(2) 331</td>
<td>Ba-O(1) 359</td>
</tr>
<tr>
<td></td>
<td>Cu-O(1) 304</td>
<td>Ba-O(4) 275</td>
</tr>
</tbody>
</table>

- Vibrations of the CuO$_2$ planes are different for these materials
  - clearly unscreened

Role of phonons

- Phonons are unscreened, despite small $l_s$
- Fluctuating charge inhomogeneities in CuO$_2$ planes?
  - alter/disrupt screening currents, or
  - diffusive transport - long wrt phonons
    - ion cores effectively unscreened
    - phonons are excellent local probes...
- No apparent anomalies at or below $T_c$!
  - no new phonon structure (Holstein modes)$^1$
    - observed in Nb “single bounce” geometry$^2$
    - typical of strong-coupling systems
  - absence implies small $\lambda$, poor coupling
    - consistent with transport (linear resistivity), no isotope effect$^1$
- Phonon-mediated superconductivity unlikely

2. J.J. Tu (private communication); this conference.
Summary and continuing work

- Phonons are observed in the conducting CuO$_2$ planes
  - little or no screening in hole and electron doped systems
  - fluctuating charge inhomogeneities?
    - disrupts screening currents

- Phonons are excellent local probes

- Role of phonons in superconductivity?
  - No new structure below $T_c$
    - usually observed in systems with strong coupling
  - other evidence for small coupling
  - probably spectators, but…
    - sensitive to charge dynamics!

- Try and connect IR and ARPES…