Illuminating the Strong Correlation Problem:
Optical conductivity of manganites, nickelates and cuprates

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Optical Conductivity

Spatially uniform transverse electric field

\[ \vec{E}(\Omega) \]

implies spatially uniform transverse current

\[ \vec{j}(\Omega) = \sigma(\Omega)\vec{E}(\Omega) \]

ratio of \( j \) to \( E \) defines conductivity \( \sigma(\Omega) \)
Why is it interesting?

• Essence of ‘strong correlations:’ inhibition of electron’s ability to move

• Electric field: tries to make electrons move

=> Conductivity: direct(?) measure of suppression of carrier motion by correlation physics.
Optical conductivity of a prototypical family of correlated materials

S. Uchida et al, PRB43 7942 (1991)
Optical conductivity of a prototypical family of correlated materials

Questions:

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• Why the gap at $x=0$?

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Questions:

• Why the gap at $x=0$?
• Interpretation of sub-gap absorption at $x=0$
• Doping dependence, $w<1\text{eV}$
• Functional form

S. Uchida et al, PRB43 7942 (1991)
Optical conductivity of a prototypical family of correlated materials

S. Uchida et al, PRB43 7942 (1991)

General idea: observed conductivity is related to the ‘strong correlations’ controlling the physics of high-Tc cuprates. This talk: survey of work on making the connection more precise
Outline

1. Introduction: optical conductivity
2. Theory (briefly)
3. ‘CMR’ manganites: temperature dependent spectral weight
4. Nickelates: energy scales and other transitions
5. Cuprates: what have we learned
6. Directions
A familiar example: the hydrogen atom

Light shined on hydrogen gas is absorbed at characteristic frequencies (here, dark lines)

http://stars.astro.illinois.edu/sow/spectra.html#absorption
Sequence of Understanding

1) Qualitative behavior

2) Inferences from Spectrum

3) Quantitative Understanding (Matrix Elements)
I: phenomenology

J. Balmer

Empirical formula for absorption energy

\[ \Omega = C \left( 1 - \frac{n^2}{m^2} \right) \]

http://www-history.mcs.st-andrews.ac.uk/PictDisplay/Balmer.html
II: energy spectrum

N. Bohr

Atomic states: principal quantum number $n$

$$E_n = -\frac{R_H}{n^2}$$

Absorption lines: Transitions between states of different energies

http://www-history.mcs.st-andrews.ac.uk/PictDisplay/Bohr_Niels.html
Wave functions and matrix elements

E. Schroedinger

$$\left( -\frac{1}{2m_e}\nabla^2 - \frac{e^2}{r} \right) \psi_n(r) = E_n \psi(r)$$

Equation

Coupling to light

$$\vec{J}_{n' n} \cdot \vec{A}$$

$$\vec{J}_{n' n} = \left\langle \psi_{n'} \left| -i \frac{\hbar}{m_e} \nabla \right| \psi_n \right\rangle$$

=> strengths of absorption lines

http://www-groups.dcs.st-and.ac.uk/~history/PictDisplay/Schroedinger.html
Condensed Matter Physics: Weakly correlated materials

Wave functions, energies and matrix elements known with reasonable accuracy

=> effective single particle (or few particle) problem: detailed understanding possible along ‘Schroedinger’ lines
Condensed Matter Physics: Strongly correlated materials

‘Intrinsic entanglement’ of single-particle states =>
--wave function formulation not useful;
--direct calculations a’la Schroedinger not (yet) feasible.

Field is somewhere between Bohr and Schroedinger: basic concepts established, inferences from spectrum obtained; now beginning to learn to calculate matrix elements, amplitudes.
Key strong correlation phenomenon: suppression of (low freq) charge response

Ex: \( \text{La}_2\text{CuO}_4 \):
- \( x=0 \): insulator (no low frequency charge response)
- \( x \) small: response ‘small’

H. Youngman question: response is small
??‘compared to what’??
Comparison: band theory

Schematic of band theory conductivity

0 energy: motion of free carriers: delta function of some weight $D_{\text{band}}$

higher energy: interband transitions.

Idea: compare absorption strength in some frequency range to that predicted by band theory
Spectral weight

\[ K(\Omega) = \int_{0}^{\Omega} \frac{2d\omega}{\pi} \sigma(\omega) \]

**f-sum rule:** \[ K(\infty) = \frac{ne^2}{m} \]. General (in this context so general as to be useless)

Thus ask: by how much is spectral weight in some low energy region reduced relative to band theory prediction.

ambiguity--interband transition
Tight binding, optical matrix element and kinetic energy

typical assumption in ‘correlated-electron’ materials: tight binding description ok

\[ H = - \sum_{i,j,ab} t_{i-j}^{ab} \left( c_{j,\sigma}^{\dagger} c_{i,\sigma} + H.c \right) + H_{int} \]

Couple to electromagnetic field: Peierl’s phase

\[ t_{i-j}^{ab} \rightarrow t_{i-j}^{ab} e^{i \frac{e}{c} \vec{A} \cdot (\vec{R}_i - \vec{R}_j)} \]

Equivalent to \( H^{ab}(k) \rightarrow H^{ab}(k - \frac{e}{c} \vec{A}) \)

if \( H_{int} \) is indep of \( k \)
Thus within tight binding approx:
spectrum=>optical matrix element

BUT

Two issues:
--interband transitions not included in tight binding model
--additional contributions to matrix element

See also Tomczak and Biermann, PRB80 085117 (2009)
tight binding model $\leftrightarrow$ `downfolding’, i.e.
projection of Hamiltonian onto chosen
(typically low energy) sector of Hilbert space

split Hamiltonian and wave function
into high and low energy sectors

$$\Psi = \begin{pmatrix} \psi_{\text{low}} \\
\psi_{\text{high}} \end{pmatrix} \quad \text{H} = \begin{pmatrix} H_{\text{low}} & H_{\text{mix}} \\
H_{\text{mix}}^\dagger & H_{\text{high}} \end{pmatrix}$$

$\Rightarrow$ Schroedinger equation becomes

$$\left( H_{\text{low}} - H_{\text{mix}}^\dagger \left[ E - H_{\text{high}} \right]^{-1} H_{\text{mix}} \right) \psi_L = E \psi_L$$
All ‘downfoldings’ make approximations equivalent to replacing $E$ on LHS by some average value

$$H_{\text{downfold}} = H_{\text{low}} - H_{\text{mix}}^\dagger [\bar{E} - H_{\text{high}}]^{-1} H_{\text{mix}}$$

current operator from downfolded $H$:

$$J_{\text{downfold}} = \frac{\partial H_{\text{low}}}{\partial k} - \frac{\partial H_{\text{mix}}^\dagger}{\partial k} [\bar{E} - H_{\text{high}}]^{-1} H_{\text{mix}}$$

$$- H_{\text{mix}}^\dagger [\bar{E} - H_{\text{high}}]^{-1} \frac{\partial H_{\text{high}}}{\partial k} [\bar{E} - H_{\text{high}}]^{-1} H_{\text{mix}}$$

$$- H_{\text{mix}}^\dagger [\bar{E} - H_{\text{high}}]^{-1} \frac{\partial H_{\text{mix}}}{\partial k}$$
Actual current operator

\[
\langle N|J|M \rangle = \frac{\partial H_{\text{low}}}{\partial k} - \frac{\partial H_{\text{mix}}^\dagger}{\partial k} [E_M - H_{\text{high}}]^{-1} H_{\text{mix}}
\]

\[
- H_{\text{mix}}^\dagger [E_N - H_{\text{high}}]^{-1} \frac{\partial H_{\text{high}}}{\partial k} [E_M - H_{\text{high}}]^{-1} H_{\text{mix}}
\]

\[
- H_{\text{mix}}^\dagger [E_N - H_{\text{high}}]^{-1} \frac{\partial H_{\text{mix}}}{\partial k}
\]

Note difference in energies: for higher energy transitions, downfolded model gets progressively worse, but as energy diff->0 model can be good.

See also Tomczak and Biermann PRB80 085117
If tight binding estimate for optical matrix element is ok spectrum implies ‘restricted sum rule’

\[
\int_0^\infty \frac{2d\omega}{\pi} \sigma_{tb}(\omega) = - \sum_{ij,ab} t_{ij}^{ab} (R_i - R_j)^2 \left\langle c_{j,\sigma}^\dagger c_{i,\sigma}^b + H.c \right\rangle
\]

Thus: integral of conductivity associated with degrees of freedom in tight binding Hamiltonian gives you expectation value of hopping amplitude, weighted by how far you hop. If only nearest neighbor hopping, then you get ‘kinetic energy’


P. Maldague, PRB 16, 2437–2446 (1977)


A Moreo and E. Dagotto PRBB 42, 4786 (1990)
Simplest model system: (1 orbital) Hubbard model

Hamiltonian

\[ H_{Hubbard} = - \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Current operator

\[ j = - \sum_{k\sigma} \frac{\partial \varepsilon_k}{\partial k} c_{k\sigma}^\dagger c_{k\sigma} \]
To study

need method to

• access intermediate length, intermediate energy scale physics (lower than chemical bonding scales, higher than kT)
• treat intermediate correlation strengths
• capture dynamics

not involve a priori assumption of what correlations are important

Big step forward: dynamical mean field theory
Reference: Density Functional Theory

Basic Theorem (Hohenberg and Kohn): \( \exists \) functional \( \Phi \) of electron density \( n(r) \): minimized at physical density; value at minimum gives ground state energy

\[
\Phi[\{n(r)\}] = \Phi_{univ}[\{n(r)\}] + \int (dr)V_{lattice}(r)n(r)
\]

Useful because:

* Have uncontrolled (but apparently good) approximations to \( \Phi \)

* Have efficient way to carry out minimization
Dynamical Mean Field Method
Metzner/Vollhardt; Mueller Hartmann KOTLIAR/GEORGES

Standard many-body theory=>exists a functional of self energy
\[ F[\{\Sigma(p,\omega)\} = F_{univ}[\{\Sigma(p,\omega)\} + Tr \left[ ln \left( G_0^{-1}(p,\omega) - \Sigma(p,\omega) \right) \right] \]

extremized at correct self energy and from which ALL RESPONSE FUNCTIONS can be extracted.

Kotliar and Georges:

Approximation to \( F_{univ} \)

Method to carry out minimization
DMFT: approximation to self energy

\[ \Sigma_p(\omega) \rightarrow \Sigma_p^{approx}(\omega) = \sum_a \phi_a(p) \Sigma_a(\omega) \]

Different choices of basis function

=> different “flavors” of DMFT
(1-site, DCA, CDMFT....).

=> different computational complexity. ?different physics?
‘DCA’ version of multisite DMFT

\[ \Sigma_p(\omega) \rightarrow \Sigma_p^{approx}(\omega) = \sum_a \phi_a(p) \Sigma_a(\omega) \]

“DCA”: partition
Brillouin zone into “tiles”

\[ \phi_a(p) = 1 \quad \text{if p in tile `a’} \]

Here: 4 “tiles”

Severe approximation to self energy: piecewise continuous k-dependence
Clusters: trade off momentum resolution $\leftrightarrow$ computability

1-site: 

\[ \begin{array}{cc}
(0,\pi) & (\pi,\pi) \\
(\pi,0) & (0,0)
\end{array} \]

2-site 

\[ \begin{array}{cc}
(0,\pi) & (\pi,\pi) \\
(\pi,0) & (0,0)
\end{array} \]

3-site 

\[ \begin{array}{cc}
(0,\pi) & (\pi,\pi) \\
(\pi,0) & (0,0)
\end{array} \]

4-site 

\[ \begin{array}{cc}
(0,\pi) & (\pi,\pi) \\
(\pi,0) & (0,0)
\end{array} \]

5-site 

\[ \begin{array}{cc}
(0,\pi) & (\pi,\pi) \\
(\pi,0) & (0,0)
\end{array} \]

6-site 

\[ \begin{array}{cc}
(0,\pi) & (\pi,\pi) \\
(\pi,0) & (0,0)
\end{array} \]

7-site 

\[ \begin{array}{cc}
(0,\pi) & (\pi,\pi) \\
(\pi,0) & (0,0)
\end{array} \]

8-site 

\[ \begin{array}{cc}
(0,\pi) & (\pi,\pi) \\
(\pi,0) & (0,0)
\end{array} \]

Ferrero et al. PRB

Jarrell/Maier: 16, 32 sites

Gull, Lin, AJM (and many other groups)

Gull, AJM
At integer filling, find correlation driven insulating phase

Interaction strength required to stabilize insulating phase depends on method

Hubbard model
2d square lattice $n=1$

- $U^{(4)} \sim 5t$
- $U^{(8)} \sim 6.5t$
- $U^{(1)} = 12t = U_{c2}$

4-DCA  8-DCA  1-DCA
Single-site DMFT: no spatial correlations. Encodes Mott and Anderson’s original idea: insulator due to ‘jamming’ from strong repulsive interaction.

Phase diagram

Metal-insulator transition at $U=1.5x$ bandwidth

Paramagnetic insulator: entropy $\ln(2)/\text{site (free spins)}$
(N>1) ‘Cluster’ methods: incorporate some degree of spatial correlations

Insulating behavior at lower U: caused by short ranged order.

8 site: Neel AF

Gull...AJM PRB80 245102 (2009)
important question vis a vis materials

What is correlation strength with respect to $U_{c2}$

Is gap due to strong repulsion, or local correlations
1-site DMFT: optics

Rozenberg et al PRL 75 105 (1995)

$U < U_{c2}$: gap held up by AF
$U > U_{c2}$: paramagnetic insulator
=>$=>$different doping dependence
Quantify doping dependence: integrate up to about 1/2 of gap

‘Strong correlations:’ kinetic energy substantially suppressed relative to band value and strongly doping dependent

$U < U_{c2}$: extrapolation is to non-zero value
Cluster dynamical mean field:
k dependence of self energy=>‘vertex correction’
needed. We are still learning how to do this.

Paramagnetic insulating phase, 2D
Hubbard model, 4-site DMFT. Optics
including vertex correction. U=0.75U_{c2}.

Lin,Gull, AJM, PRB80 161105 (2009)
Summary so far

• If tight binding model appropriate, optics approximately measures ‘kinetic energy’ of correlated electrons
• If tight binding model appropriate, spectrum=>optical matrix elements
• Over suitable frequency range, comparison of optical spectral weight to band theory prediction quantifies reduction of motion of electrons by strong correlation physics
This is all very nice

BUT

What does it have to do with any real material?
Optical conductivity: Experimental aspects

$\sigma(\Omega)$: response to spatially uniform transverse field

$\Rightarrow$

infer $\sigma$: from reflection and transmission of light $\approx$ normally incident on high symmetry surface

surface sensitive probe: penetration depth

$\delta \sim \frac{1}{\sqrt{\sigma(\Omega)}} \sim 10^3 \text{Å}$
Sample and surface treatment issues are not trivial

Example: ‘CMR’ manganite:

Standard surface treatment technique (polishing) now known to produce wrong spectra for this compound

Moral:

Be careful about data
‘Colossal’ magnetoresistance manganites

Insulator at $x=0$

Doping produces a metallic state (and other interesting phases)
CMR manganites: the ‘kinetic energy’ idea works

$La_{1-x}Ca_xMnO_3$

Mn d-shell: holds up to 5 (x2 for spin) electrons

‘crystal field’: 5 --> 3 + 2

In $La_{1-x}Ca_xMnO_3$: 4 - x electrons all spins parallel

e_g: can move--but stays parallel to core spin

t_{2g}: Electrically inert

‘core spin’

Ramirez et al PRL 75 1336
CMR: continued

Ramirez et al PRL 75 1336
CMR: continued

FM order: hopping easy

Ramirez et al PRL 75 1336
CMR: continued

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Ramirez et al PRL 75 1336
CMR: continued

FM order: hopping easy

AFM order: hopping suppressed

Ramirez et al PRL 75 1336
CMR: continued

FM order: hopping easy

AFM order: hopping suppressed

Ramirez et al PRL 75 1336
CMR: continued

FM order: hopping easy

AFM order: hopping suppressed

Ramirez et al PRL 75 1336
CMR: continued

FM order: hopping easy

No order: spins at ~90 degrees

Ramirez et al PRL 75 1336
CMR: continued

FM order: hopping easy

No order: spins at ~90 degrees

Ramirez et al PRL 75 1336
CMR: continued

No order: spins at ~90 degrees

Hopping reduced by $\sim \frac{1}{\sqrt{2}}$
CMR: continued

No order: spins at ~90 degrees

Hopping reduced by $\sim \frac{1}{\sqrt{2}}$

Magnetic order controls kinetic energy

Ramirez et al PRL 75 1336
Data: obvious T-dependence to K w<3eV

Quijada,...Drew...AJM PRB58 16093 (1998)
Weight lost between 0 and 3eV reappears only at $w>12eV$

Conductivity

Change in spectral weight with temperature

Rusydi et al PRB78 125110
Modest dependence on material

<table>
<thead>
<tr>
<th>Ion</th>
<th>K(3eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sr</td>
<td>0.28</td>
</tr>
<tr>
<td>Ca</td>
<td>0.24</td>
</tr>
<tr>
<td>Nd</td>
<td>0.22</td>
</tr>
</tbody>
</table>
Doping dependence not much studied (!) but apparently weak

La$_{1-x}$Sr$_x$MnO$_3$

$x=0.3$

K(3)=0.28eV

PRB58 16093 (1998)

$x=0.175$

K(3)=0.24eV

PRB60 16093 13011 (1999)
Band structure

Near fermi surface bands (LSDA) of hypothetical ferromagnetic LaMnO$_3$ including GdFeO$_3$ rotational distortion

- $e_g$-derived bands well separated from others
- t.b. (1st and 2nd neighbor) not bad fit
- band-narrowing effect of GdFeO$_3$ rotations studied

C. Ederer and AJM PRB76 155105 (2007)
T.B. fits at $x=0.3$ imply

<table>
<thead>
<tr>
<th>Ion</th>
<th>$K(3\text{eV})$</th>
<th>$K_{\text{band}}$</th>
<th>spectral weights close to band theory values. Differences between materials: differences in amplitude of GdFeO$_3$ rotation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sr</td>
<td>0.28</td>
<td>0.29</td>
<td></td>
</tr>
<tr>
<td>Ca</td>
<td>0.24</td>
<td>0.26</td>
<td></td>
</tr>
<tr>
<td>Nd</td>
<td>0.22</td>
<td>0.23</td>
<td></td>
</tr>
</tbody>
</table>
x-dependence, La-Sr material  
(note GdFeO$_3$ rotation is x-dependent)

<table>
<thead>
<tr>
<th>x</th>
<th>K(3eV)</th>
<th>$K_{\text{band}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>0.28</td>
<td>0.29</td>
</tr>
<tr>
<td>0.18</td>
<td>0.24</td>
<td>0.27</td>
</tr>
</tbody>
</table>

Spectral weights close to band theory values.  
x-dependence: compensation of increase in GdFeO$_3$ rotation and doping dep of band KE
Temperature dependence: too big for simple theory

No order:

Data: reduction more like 60%

Hopping reduced by $\sim \frac{1}{\sqrt{2}}$
Extra physics: fluctuating (bond) density wave order in high T phase

q-scan

E-scan: ‘central peak’ + spin wave

CMR transition: first order because of high T short ranged ordered ‘phase’
Manganites: summary

• T=0 spectral weight reasonably consistent with band theory. Main differences: structural effects
• Weight is spread over several eV=>form of conductivity requires interaction
• Temperature dependent decrease: confirms association: KE and conductivity
• ‘Lost’ spectral weight transferred to very high energies
• Temperature dependence too big for simple spin orientation argument
See also

Jan M. Tomczak\textsuperscript{1,2} and Silke Biermann\textsuperscript{3,2}

PHYSICAL REVIEW B 80, 085117 (2009)

\begin{center}
\begin{tikzpicture}
\begin{axis}[
width=\textwidth,
height=\textwidth,
set layers=false,
axis lines=middle,
tick style={draw=none},
xlabel={$\omega$ [eV]},
ylabel={Re $\sigma(\omega)$ [10$^3$ (Ω cm)$^{-1}$]},
legend style={at={(0.5,0.9)},anchor=north},
]
\addplot+[no markers,smooth] file {data/total.dat};
\addplot+[no markers,smooth,mark=*,mark options={black}] file {data/t2g_to_t2g.dat};
\addplot+[no markers,smooth,dashed] file {data/t2g_to_speg.dat};
\addplot+[no markers,smooth,dotted] file {data/speg_to_t2g.dat};
\addplot+[no markers,smooth,dashed,dotted] file {data/speg_to_speg.dat};
\addplot+[no markers,smooth,loosely dashed] file {data/Experiments.dat} node{Experiments};
\legend{total, $t_{2g} \rightarrow t_{2g}$, $t_{2g} \rightarrow s,p,e_g^\sigma$, $s,p,e_g \rightarrow t_{2g}$, $s,p,e_g \rightarrow s,p,e_g^\sigma$, Okazaki et al., Qazilbash et al.}
\end{axis}
\end{tikzpicture}
\end{center}

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LaNiO$_3$

ReNiO$_3$ materials: metal insulator transition

Zhou et al PRB67 020404
Chaloupka/Khaliullin: use LaNiO$_3$ to design a new high-$T_c$ superconductor

Idea:

Bulk LaNiO$_3$ Ni [d]$^7$ (1 electron in two degenerate eg bands).

In correctly chosen structure, split eg bands, get 1 electron in 1 band—”like” high-$T_c$
Question:
how strong are the correlations?
Question: how strong are the correlations?

Optical conductivity: good samples have been difficult to make. Recent success with films

Stewart et al UCSD

Ouellette et al UCSB

ArXiv:1005.3314

Unpub.
Question: how strong are the correlations?

Optical conductivity: good samples have been difficult to make. Recent success with films.

Data are different!
Here: discuss SB data
S. Stemmer, J. Son (samples)
D. Ouellette, J Allen, (measurements)
S.Lee, L. Balents AJM calc

Unpub.
Question:
how strong are the correlations?

Optical conductivity: good samples have been difficult to make. Recent success with films

‘Drude’ peak and 0.5-3eV absorption

Ouellette et al UCSB

Unpub.
LaNiO$_3$--continued

Near fermi surface states: 2 orbital tight binding model (as in manganites). Compare spectral weight to that in tight binding model (called ‘theory’ in fig).
Comparison of oscillator strength

ratio of areas: Drude peak in data less by ~factor of 3-5 than band calc.
Conductivity over wider range?

Comparison of tight binding and LDA (Wien2K; LDA +U) calc. of optical conductivity

\[ \sigma(\omega) \quad (\text{eV}) \]

J. Rondinelli and AJM unpub; see also arXiv:1005.3314 (Haule)
Conductivity over wider range?

Comparison of tight binding and LDA (Wien2K; LDA +U) calc. of optical conductivity

$t_{2g}/O_{p\pi}$ states near fermi level

J. Rondinelli and AJM unpub; see also arXiv:1005.3314 (Haule)
LaNiO$_3$: summary

This is work in progress but a few points are clear:

• ‘Drude’ mass enhancement not small

• analysis of higher energy transitions requires more sophisticated (beyond simple tight-binding) understanding of matrix elements--and raises the question of correlation effects on interband transition

• nearby states=>$vitiates$ analogy to high Tc
High $T_c$ Cuprates

One approach:

Compare optical oscillator strength at $w<1\text{eV}$? $2\text{eV}$? to band theory value
Spectral weight, integrated over low (red) and intermediate (black) frequency range.

Comanac...AJM Nat Phys 4
Spectral weight, integrated over low (red) and intermediate (black) frequency range.

Focus on intermediate range
Spectral weight, integrated over low (red) and intermediate (black) frequency range.

Spectral weight on scale of 1/2 gap does not extrapolate to zero at zero doping.
Spectral weight, integrated over low (red) and intermediate (black) frequency range.

Compare to calculation
Spectral weight, integrated over low (red) and intermediate (black) frequency range.

Implication: on the scale of \( \sim 1/2 \) gap, materials are strongly correlated, but \( U < U_{c2} \)
Spectral weight, integrated over low (red) and intermediate (black) frequency range.

Note: data for both electron and hole doped materials included.
Spectral weight, integrated over low (red) and intermediate (black) frequency range.

Note: data for both electron and hole doped materials included.

Implication: correlations about the same for both material classes
Spectral weight, integrated over low (red) and intermediate (black) frequency range.

Focus on low frequency range
Spectral weight, integrated over low (red) and intermediate (black) frequency range.

Spectral weight integrated to 0.2eV does extrapolate to zero at zero doping
Spectral weight, integrated over low (red) and intermediate (black) frequency range.

Spectral weight integrated to 0.2eV does extrapolate to zero at zero doping

Implication: extra correlations, on lower frequency scale, ‘know’ the material is becoming an insulator
Temptation: relate observations to cluster DMFT calculations for Hubbard model

Calculation: short (but not 0) range antiferromagnetic correlations => gap at $x=0$; evolution with doping similar to expt

4 site DMFT

$U=0.75U_{c2}$

Lin, Gull, AJM, PRB80 161105 (2009)
More refined picture:
8 site DMFT calculation

Lin, Gull, AJM, PRB in press
Scattering rate analysis

\[ \sigma_1(\omega) + i\sigma_2(\omega) = \frac{K}{-i\omega(1 + \lambda_{\text{opt}}(\omega)) + \Gamma_{\text{opt}}(\omega)} \]

Data

Lin, Gull, AJM, PRB in press
Reasons not to ‘declare victory’ just yet

‘Interesting’ electrons embedded in complex crystal structure

Basic unit: CuO$_2$ plane

\[
\begin{array}{ccc}
\text{Cu} & \text{O} & \text{Cu} \\
\text{O} & \text{O} \\
\text{Cu} & \text{O} & \text{Cu}
\end{array}
\]

charge transfer insulators: $e_p$-$e_d$ plays role of $U$
Reasons not to ‘declare victory’ just yet

‘3 band’ model: studied by similar techniques (so far, 1-site DMFT)

Wang, deMedici, Capone, AJM PRB80 054401 (2009)

see also:
Weber, Haule, Kotliar

[arXiv:1005.3100
arXiv:1005.3095
arXiv:0804.151]

Upper hubbard band: d-like
Lower Hubbard band: p-like
3 band model: orbital (p/d) character depends on energy, doping, interactions

Implications for many body effects; optical matrix elements

Holes: larger self energy than electrons

Conductivity: ~similar for both

Change in matrix element compensates for change in self energy

Wang, deMedici, Capone, AJM PRB80 054401 (2009)
Charge transfer insulator:

Theoretical near gap edge conductivity too small
By~2eV, 1 band model matrix element badly wrong

Wang, AJM to be published

Interesting new idea: other orbitals important. Weber et al ArXiv: 1005:3001
Summary

qualitative understanding: effect of correlations on optics: reduce spectral weight

Information from spectra: model systems coming under control

Theory of wave functions, quantitative account of conductivity not yet there for interesting cases.