Oxide Interfaces and Heterostructures
IV: Quantum Wells and Theory; Nonequilibrium and Devices

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Course made possible by Columbia-Sorbonne-Science Po-Ecole Polytechnique Alliance
Course schedule

Meetings: Wednesday 1:30-2:20 Lecture
         2:30-3:20 Lecture
         3:20-3:45 pause-cafe
         3:45-5:00 seminar

1. March 21: Introduction
   Seminar: J. Leseur (ESPCI) *seminar starts at 15:30*
2. April 4: Interfaces; magnetism and superconductivity
   Seminar: M. Gabay (Orsay)
3. April 11: Superlattices, Quantum Wells and Theory
   Seminar: M. Gibert (Geneve)
4. April 18: Superlattices (continued) and Devices
   Seminar: M. Bibes (Thales)
Oxide Interfaces Web Site
(under construction)

http://www.phys.columbia.edu/~millis/oxideinterfaces.html

Lecture slides
Bibliography (and some downloadable articles)
Links to major research groups (if you want your group here, send me the link!)
April 18
Superlattices and Quantum Wells

1. Theory: Continued
   • Theory: Methods
   • Theory vs Experiment
     • Propagation of order
     • Orbital polarization
     • Quantum well and metal-insulator transition

2. The ‘Mott’ transistor: concepts, results and need for nonequilibrium physics
Theory:
Many body physics of transition metal oxides (brief qualitative review)

Paradigm system: `ABO₃ perovskite`

B-site: transition metal with partly filled d-shell. Filling controlled by A-site

dont forget oxygen!
Transition metals and oxides

http://www.vertex42.com/Files/pdfs/1/periodic-table_color.pdf

‘Early’ transition metal oxides (TM from left side of row)

‘Late’ transition metal oxides (TM from right side of row)
Theory: how to go from periodic table and crystal structure to behavior
Theorists like simple models

Periodic table from J H Wood;
quoted in Z Fisk 2010 KITP talk

but how simple is too simple?
Can we test the simple models with better calculation

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Focus on single-particle properties: electron Green function

Green function: matrix in band/orbital indices

\[ G(k, \omega) = [\omega 1 - H_0(k) - \Sigma(k, \omega)]^{-1} \]

\[ H_0 = \sum_i \frac{P_i^2}{2m_e} + V_{ext}(r_i) \]

‘Self energy’ \( \Sigma(k, \omega) \)

Also matrix in band/orbital indices: parametrizes difference between propagation in reference potential (here, atoms) and in real material
Focus on single-particle properties: electron Green function

Green function: matrix in band/orbital indices

\[ G(k, \omega) = [\omega 1 - H_0(k) - \Sigma(k, \omega)]^{-1} \]

\[ H_0 = \sum_i \frac{P_i^2}{2m_e} + V_{ext}(r_i) \]

Density functional band theory (DFT) and DFT+U: specific static approximations to self energy

\[ G(k, \omega) \rightarrow [\omega 1 - H_0(k) - \Sigma_{DFT}(k)]^{-1} \]
Theoretically:

• DFT+U overpredicts order.
• Misses physics of doped Mott insulator
• No dynamics

Hartree-Fock
\(\leftrightarrow\) DFT+U for this model) predicts completely different phase diagram

C K Chan, P. Werner and AJM, PRB80, 235114 (2009).
How to go beyond?
Need dynamical part of self energy

\[ G(k, \omega) = [\omega 1 - H_0(k) - \Sigma_{DFT}(k) + \Sigma_{Dyn}(k, \omega)]^{-1} \]

Cant treat all components of self energy matrix dynamically

=> select subspace (‘correlated orbitals’) to be treated dynamically

In essence, solve ‘effective model’ (theory of interacting fermions on a lattice)
``Standard model” (of transition metal oxides)
d and p orbitals with only d correlated

\[
H = \sum_{a,\lambda} \varepsilon_d^\lambda d_{a\lambda\sigma}^\dagger d_{a\lambda\sigma} + U \hat{N}_{d,a} (\hat{N}_{d,a} - 1) + \ldots \\
+ \sum_{k,\nu} t_{pd}(k) d_{k\lambda\sigma}^\dagger p_{k,\nu\sigma} + H.c. + \varepsilon^\nu p_{k\nu\sigma}^\dagger p_{k\nu\sigma} + \ldots 
\]

\(t_{pd}, \epsilon_k\) etc determined by band theory.

Embedding issue: Hartree shift: \(\epsilon_d \rightarrow \epsilon_d + U \langle \hat{N}_d \rangle\)

part of this is included in any band calculation

must adjust \(\epsilon_d - \epsilon_p\)—but by how much??
Aside

Modern DFT+DMFT methods formulate problem entirely in terms of

$$G(k, \omega) = \left[ \omega 1 - H_0(k) - \Sigma_{DFT}(k) + \Sigma_{Dyn}(k, \omega) \right]^{-1}$$

without explicit reference to model system.

`Standard model’ still implicit in formalism and provides very useful language and physical picture
realistic and consistent embedding of correlated problem into band structure remains open problem.

Interesting for superlattices: band alignments determined by $e_p-e_d$ which depends on double counting and level occupancy
Parameters and Limits:

(1) Mott-Hubbard vs charge transfer:

Key parameter:

\[ \Delta = \varepsilon_d - \varepsilon_p \]

http://dmft.rutgers.edu/LDA/lmto/lmto_run.htm

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Parameters and Limits

(2) occupancy of partly-filled d-shells

Key parameter: # d-electrons/degeneracy of d-state

(a) Non-degenerate: cuprate
(b) 2-fold degenerate (e_g) Nickelate, Manganite
(c) 3-fold degenerate (t_{2g}) (titanate, vanadate,

Critical U, 1 orbital Hubbard model

C K Chan, P. Werner and AJM, PRB80, 235114 (2009).
Parameters and Limits

(2.1) Partly-filled d-shells: spin physics

Key parameter: Hunds coupling

\( J_H = 0 \)

\( J_H > 0 \)

High spin: half filled shell less metallic; partly filled shell more metallic

Parameters and Limits

(2.2) Partly-filled d-shells: orbital physics

Key parameter: orbital splitting (lattice distortion)

\[ J_H = \frac{U}{6} \]

reduce degeneracy relative to electron number: more insulating

Parameters and Limits

(3) band filling

(a) total electron count: ‘Mott’ insulator possible only if integer number of electrons per unit cell
(b) if local orbital high-spin: incoherent state.

J. Mravje, L. deMedici, A. Georges....

C K Chan, P. Werner and AJM, PRB80, 235114 (2009).
Parameters and Limits

(4) dimensionality

Lower dimension: insulating states easier to obtain

Simple argument:
--kinetic energy \( \sim \# \) directions for hopping, \( \sim \text{dim} \)

More refined argument:
--nesting (\( \Rightarrow \) fermi surface gapping) easier in lower d
How do we solve the many-body model
Direct diagonalization

$$\mathbf{H} = \sum_{\alpha,\beta} E^{\alpha \beta} \psi^{\dagger}_{\alpha} \psi_{\beta} + \sum_{\alpha \beta \gamma \delta} I^{\alpha \beta \gamma \delta} \psi^{\dagger}_{\alpha} \psi^{\dagger}_{\beta} \psi_{\gamma} \psi_{\delta} + \ldots$$

Dimension of Hilbert space: $2^M$

Direct diagonalization: exponentially difficult.

Present limit-- $M \sim 30$.

(and wont get much bigger)

Direct diagonalization becomes impractical before size gets big enough.
‘Optimized diagonalization’: density matrix renormalization group

Method of choice for ground state properties of 1d model system problems

Becoming important tool in quantum chemistry

d>1 remains a big challenge

??Excitations??

U. Schollwoeck, RMP77 259

Standard method for exploring exponentially large configuration space:
Stochastic (Monte-Carlo) integration

Definition of expectation value
\[ \langle A \rangle_w = \frac{1}{Z_w} \int_C dx \ A(x)w(x) \]
Z=partition function

x=some configuration

w(x): "weight": contribution of x to partition function

For fermions: w(x) can be negative "sign problem"
Present state of the art:
Fermion calculations: exponential wall of computational complexity

Direct approaches: reach ‘wall’ before reach interesting system sizes, temperatures

If direct approach fails: take indirect approach: relate physics you want to properties of solution of simpler model.
Dynamical Mean Field Theory: indirect approach


Thomas Maier, Mark Jarrell, Thomas Pruschke, and Matthias H. Hettler, Rev. Mod. Phys. 77, 1027 (2005)


Modern interpretation

Parametrize self energy in terms of small number $N$ of functions of frequency

$$\Sigma^{\alpha\beta}(k, \omega) = \sum_{ab} f^{\alpha\beta}_{ab}(k) \Sigma_{ab}^{\text{DMFT}}(\omega)$$

parametrization function $f$ determines ‘flavor’ of DMFT (DFT analogue: LDA, GGA, B3LYP, ....)
Self energy functions $\Sigma^{ab}(\omega)$, obtained by solving a 0 (space) +1 (time) dimensional quantum field theory (``quantum impurity model’’).

Useful to view auxiliary problem as ‘quantum impurity model’ (cluster of sites coupled to noninteracting bath)

Important special case: ‘single site’ DMFT: no momentum dependence; one site per orbital

$\Sigma \rightarrow \Sigma^{ab}(\omega)$
Single-site DMFT, paramagnetic metal-insulator phase diagram:

Hubbard model

Critical interaction $U_c \sim 1.5W$

Carrier concentration (doping)

Correlated metal (fixed point conventional, but low energy scale)

Insulator

Normal metal

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Characterize approach to insulator

Increase interaction:
half filling

Vary doping--strong interaction

Key features: large (preformed) gap, in-gap states
Status of single-site approximation

Exact in infinite coordination number limit
Some information: 1 orbital Hubbard model $d=2,3$
Otherwise, very little known

``Far'' from insulator or (presumably) at very high temperature: approximation good.

2d Hubbard: $U=7t$ self energy zone face and diagonal
in d=2

Hubbard model
2d square lattice \( n=1 \)

No sign of 2 pole structure
3 dimensional Hubbard model
S. Fuchs, E. Gull, L. Pollett et al PRL 106 030401 (2011)

\[ U = 8t = 2W/3 \quad T = t/2 = W/24 \]

cluster sizes up to 100 sites

Probably worst-case comparison (in 3d)
approx not particularly good
However

except for the 1 orbital Hubbard model

**DFT+U**

and

**single-site DMFT (+DFT)**

are the only games in town

=> modelling of interface/superlattice systems is interesting and important challenge
Application to superlattices

Biscaras et al, Nature Communications 1 89 (2010)

Ishida and Liebsch, PRB77 115350 (2008)

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Ishida and Liebsch observe: LaTiO$_3$ grown epitaxially on SrTiO$_3$ has much smaller GdFeO$_3$ (rotation) distortion than bulk LaTiO$_3$

Pavarini et al: GdFeO$_3$ (rotation) essential for insulating state of LaTiO$_3$


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**LaTiO$_3$ on SrTiO$_3$**

**DOS: no rotations**

\[ n_{xy} = 0.14 \quad n_{zx} = 0.18 \]

Bulk but with substrate-imposed distortion

Band theory: cubic->tetragonal distortion imposed by substrate=> negligible orbital splitting (t$_{2g}$)

\[ n_{ag} = 0.23 \quad n_{ef} = 0.135 \]

Superlattice t$_{2g}$ bandwidth >bulk

Ishida and Liebsch, PRB77 115350 (2008)
Consequence for many-body physics

LaTiO$_3$ predicted to remain metallic up to much larger U in tetragonal superlattice than in orthorhombic bulk

Ishida and Liebsch,
PRB77 115350 (2008)
Experiment $\text{LaTiO}_3$/SrTiO$_3$

phenomenology same as for LAO/STO.

Implication: few layers of LTO ARE insulating

Biscaras et al, Nature Communications 1 89 (2010)
Questions:

* Actual structure of LaTiO$_3$ on different substrates

* Is a mapping to a Hubbard model appropriate

* Reliability of single-site DMFT
Metal-insulator transition: quantum wells

SrVO$_3$ bounded by SrTiO$_3$ and vacuum

Carriers almost completely confined to SVO

suppress DOS, $n<8$; insulating $n=2,1$

In bulk: $d^1$, 3 degenerate orbitals: $d_{xy}$ $d_{xz}$ $d_{yz}$

Superlattice:

• Reduce dimensionality

• Lift orbital degeneracy

• Break symmetry

**?SrO or TiO$_2$ termination?**

<table>
<thead>
<tr>
<th>SrO</th>
<th>STO</th>
<th>TiO$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>Ti</td>
<td>O</td>
</tr>
<tr>
<td>O</td>
<td>Ti</td>
<td>O</td>
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<td>O</td>
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<td>O</td>
<td>Ti</td>
<td>O</td>
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<tr>
<td>O</td>
<td>Ti</td>
<td>O</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Vacuum</th>
<th>STO</th>
<th>TiO$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>Ti</td>
<td>O</td>
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<tr>
<td>O</td>
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<td>O</td>
<td>Ti</td>
<td>O</td>
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<tr>
<td>O</td>
<td>Ti</td>
<td>O</td>
</tr>
</tbody>
</table>

**Might think: termination affects level splitting of surface Ti**
Termination and occupancy

Simple model: Ti $d_{xz}$ hops to ``$O_{xz}$''

$d_{xy}$ does not notice capping layers
$d_{xz, yz}$ affected by presence or absence

Parameters $\varepsilon_d, \varepsilon_p, t_{pd}$
Result (H. Dang)

<table>
<thead>
<tr>
<th></th>
<th>Bulk</th>
<th>2 layers of V</th>
<th>1 layer of V</th>
<th>SrO both</th>
<th>SrO one</th>
<th>SrO none</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_{d,xy}$</td>
<td>0.33</td>
<td>0.32</td>
<td>0.31</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$n_{d,tot}$</td>
<td></td>
<td></td>
<td>0.27</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Net ‘orbital polarization’ small. Can go either way depending on termination.
Single-site DMFT phase diagram

- No crystal field $J=0.5$ eV
- SrO termination.
- $J=U/6 \sim 1$ eV

$U_c/U_{bulk}$ vs. $N^{-1}$

- d-only model

Metal insulator transition with layer thickness
=> how much `fine tuning' of interaction

Quasiparticle bands, 5, 6, 7..layers--See S. Okamot PRB 84 201305 (2011)

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Modelling Homometallic Superlattices

*(001) Superlattice of (AA’)BO₃ Perovskite*

Model:
*Define heterostructure: charge +1 at La site*
*electrons: move among B (Ti/Mn) sites*
*Interaction: + long range coulomb+on-site (Hubbard U or full Slater-Kanamori or ‘double-exchange’ J)*
Approximations

• **Long ranged coulomb: Hartree=>self consistent on-site potential**

\[
V(R_i) = - \sum_j \frac{e^2}{\epsilon |\vec{R}_i - \vec{R}_j^A|} + \sum_{j,\sigma} \frac{e^2 < n_{j,\sigma} >}{\epsilon |\vec{R}_i - \vec{R}_j|} 
\]

• **On site: dynamical mean field, or hartree/LDA(+U)**

\[
\Sigma(r, r', \omega) \rightarrow [\sum_{DMFT}(r, \omega) + V(r)] \delta(r - r')
\]
Results I:
Charge Profile, n-layer structure

Results robust: insensitive to magnitude of dielectric function, value of on-site U, orbital deneracy.

~3 unit cell wide “edge” where density drops
n>4 to get bulk-like (n=1) central region
Charge profile:
~3 unit cell wide ‘metallic edge’

Examine edge excitations in more detail

Important object: layer resolved spectral function
(observable in principle in photoemission)

\[ A(z, z'; k, \omega) = \lim_{z' \to z} \frac{1}{\pi} \text{Im} \, G(z, z'; k, \omega) \]
Layer Spectral Function
n=10 layer Hubbard heterostructure
U=16t>U_c ~ 14.7t
Layer Spectral Function

\( n=10 \) layer Hubbard heterostructure

\( U=16t \gtrsim U_c \sim 14.7t \)
Layer Spectral Function

$n=10$ layer Hubbard heterostructure

$U=16t > U_c \sim 14.7t$

Lower Hubbard band quasiparticle

Coherent
Layer Spectral Function

n=10 layer Hubbard heterostructure

$U = 16t > U_c \sim 14.7t$

question: are the midgap states just an artifact of the single-site DMFT
Cluster DMFT

Lead-induced in-gap states weaker, displaced from 0

Ishida and Liebsch, Phys Rev B82 045107 (2010)
Summary: charge profile

• \(~3\) unit cell wide transition region
• supports metallic behavior
• ‘metallic edge’ moderately correlated
• Question: does ‘edge’ support new magnetic (or superconducting?) behavior
Search for magnetism in LaVO$_3$/SrVO$_3$ superlattices

(LaVO$_3$)$_m$/(SrVO$_3$)$_1$

room temperature FM!

Density of states
bulk and superlattice

(a) Bulk DOS
(b) $m=3$ layer-DOS

H.T. Dang, unpub

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Magnetism?

Single-site DMFT
‘3 band’ model
U, J=0.5...

Estimate $T_c$ from inverse susceptibility

$m=3$ $T_c=-0.04$eV
$m=5$ $T_c=-0.1$eV

Modest tendency to ferromagnetism but no evidence for order
Orbital Order
Orbital Control:
Transition Metal Oxides

Orbital occupancy controls behavior:

Ex: CMR Manganites--orbital ordering=>magnetic structure

Nagaosa/Tokura Science 288 462
Orbital Control: Transition Metal Oxides

Orbital occupancy controls behavior:

Ex: Bulk CMR Manganites--carrier concentration $x$ controls orbital ordering $\Rightarrow$ conductivity

Nagaosa/Tokura Science 288 462

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Orbital Control: Transition Metal Oxides

Ex: CMR films--substrate-induced strain=>(putative) orbital ordering=>conductivity

Konishi et al., J. Phys Soc. Jpn 68 3790
Basic questions:

1. What controls the orbital splitting?
2. How much splitting can you get?
3. What achievable systems give the largest (or smallest) effect?
One strategy: ‘templating’

Manganites: staggered (2 sublattice) orbital order occurs in bulk:

Does order in 1 layer serve as a template for order in next layer.
Model for manganite multilayers

- Mn: cubic lattice. 2 (eg) orbitals, one $S=3/2$ “core spin”/site
- La: charge +1 rel. to Sr. Long ranged Coulomb (via hartree)
- Tight binding band structure (LaMnO$_3$)*
- Slater-Kanamori (U=J) interactions projected to eg manifold
- Jahn-Teller distortion of oxygen octahedra
- Unit cell (z-direction) expansion/contraction

C. Lin and AJM PR B78, 184405 (2008)
Method:
1 site DMFT, quasiclassical solver

Calculated bulk phase diagram

- Right phases, right sequence:
- T scale 3x too big

C. Lin and AJM PR B78, 174419 (2008)
Order Parameters

Note: superlattice growth along z
Key parameter: Charge confinement

Dimensionless parameter: Coulomb confinement energy in units of hopping $t$

$$\alpha = \frac{e^2}{a\epsilon t}$$
(LaMnO$_3$)$_4$(SrMnO$_3$)$_1$

Charge density determined by coulomb parameter; \( \sim \) indep. of temperature

Table: compares order on given plane to bulk order at that charge density

<table>
<thead>
<tr>
<th>Site label</th>
<th>( \alpha = 0.3 )</th>
<th></th>
<th>( \alpha = 0.09 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
<td>B</td>
<td>C</td>
</tr>
<tr>
<td>Charge density</td>
<td>0.99</td>
<td>0.99</td>
<td>0.52</td>
</tr>
<tr>
<td>(</td>
<td>\langle Q_x^a \rangle</td>
<td>SL [\tau])</td>
<td>1.17</td>
</tr>
<tr>
<td>(</td>
<td>\langle Q_x^a \rangle</td>
<td>Bulk [\tau])</td>
<td>1.18</td>
</tr>
<tr>
<td>(</td>
<td>\langle Q_z^a \rangle</td>
<td>SL [\tau])</td>
<td>-0.28</td>
</tr>
<tr>
<td>(</td>
<td>\langle Q_z^a \rangle</td>
<td>Bulk [\tau])</td>
<td>-0.32</td>
</tr>
</tbody>
</table>

Result: very weak “proximity effect”
Summary: manganites

- Physical properties (including orbital/magnetic ordering) controlled by layer charge density: negligible proximity effect

- Status of theory: single-site DMFT and d-only model. Are these approximations adequate?
Orbital polarization: late transition metal oxides

Superlattice: $\text{La}_2\text{AlNiO}_6$

LaAlO$_3$ layer: insulating barrier

Question (Khalliulin): how much orbital polarization can we get?

$$P = \frac{n_{x^2-y^2} - n_{3z^2-r^2}}{n_{x^2-y^2} + n_{3z^2-r^2}}$$

MJ Han, X Wang, C. Marianetti and A. J. Millis
PRL 107 206804 (2011)
Band theory of $\text{La}_2\text{NiAlO}_6$ heterostructure:

Degeneracy of $e_g$ bands lifted: $3z^2-r^2$ band moves up

Hansmann et al PRL 103 016410 (2010)
Band theory of $\text{La}_2\text{NiAlO}_6$ heterostructure:

$\text{La}_2\text{NiAlO}_6$

2d fermi surface

$\text{LaNiO}_3$

3d fermi surface

Hansmann et al PRL 103 016410

Hamada J Phys. Chem Sol 54 1157

No qualitative difference
Add interactions: Standard approach

Map conduction bands to (multiple-orbital) Hubbard model
Solve by standard approximation.

e.g. Hansmann et. al.: 2 orbital hubbard model, DMFT

Dispersion from band theory

\[ \varepsilon^2_{k} = -2(\cos k_x + \cos k_y) \begin{pmatrix} 0.45 & 0 \\ 0 & 0.17 \end{pmatrix} + 2(\cos k_x - \cos k_y) \times \begin{pmatrix} 0 & 0.28 \\ 0.28 & 0 \end{pmatrix} - 4(\cos k_x \cos k_y) \begin{pmatrix} 0.09 & 0 \\ 0 & 0.03 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0.15 \end{pmatrix}. \]

Interaction: phenomenological

\[ \hat{H}_{\text{int}} = U \sum_{i\sigma} n_{i\sigma}^{\uparrow} n_{i\sigma}^{\downarrow} + \sum_{i > m \sigma' \sigma} (V - \delta_{\sigma, \sigma'} J)n_{i\sigma}^{\sigma} n_{i\sigma'}^{\sigma'}, \]

and Phys. Rev. B 82, 235123 2010
Result: Proximity to Mott insulator $\Rightarrow$ enhanced polarization

Interactions enhance ‘orbital polarization’

Interactions drive ‘orbitally selective metal-insulator transition’


Phys. Rev. B 82, 235123 2010

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But Ni is a ‘late’ transition metal oxide: charge transfer physics is important

Repeat same exercise, using ‘standard model’ with oxygen states

Find: interactions decrease orbital polarization

Hubbard model is fundamentally misleading

Double Counting

Band theory: electron moves from O to Ni, configuration is $d^8\bar{L}$.

Interaction $\frac{U}{2} N_d (N_d - 1)$ acts to change d occupancy.

$\Rightarrow$ ‘double counting’ question: as one adds ‘$U$’ to a model do you (a) reduce $N_d$ (b) shift d-level energy to keep $N_d$ fixed.

La$_2$InNiO$_6$
Two dimensional parameter space:
U and d-level energy

Phase Diagram

Here--vary correlation strength by considering two trajectories in parameter space:
$N_d$ constant or $E_d$ constant

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Fermi Surface

Phase Diagram

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Spectral function and orbital polarization

Spectral functions

Phase Diagram

Columbia University
L’Ecole Polytechnique
Compare Fermi Surface

Hubbard: Hansmann et. al.
PRL 103, 016401 (2009)
PRB 82 235132 (2010)

‘Hubbard’
(no ligand)

U=4eV

Realistic: MJ Han, X Wang, C. Marianetti and A. J. Millis,PRL 107 206804

‘Realistic’
(include ligand)

U=6eV

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Key point: Ni-O covalency

Band theory: electron moves from O to Ni, configuration is \( d^8 \bar{L} \)

\( d^8 \) is high spin: both orbitals occupied
Take-away: Interactions decrease orbital polarization

Nickelate (d$^8$L) is not cuprate (d$^9$)

d$^8$ is high spin: both orbitals occupied
Some experimental support

Benckiser et al, Nature Materials 10 189 2011

negligible orbital polarization in 4-LNO-layer structures

To be definitive: fewer LNO layers
Summary: theory

Basic Issues:

--Band alignments: within reach
--Orbital polarization: importance of correlations, coupling to ligands. plausibly within reach
--Metal-insulator phase boundary severe test of theory
--Magnetic order severe test of theory
Applications (very sketchy)

Bolometers: a use for the metal-insulator transition

Spintronics: exploiting high spin states

‘Multiferroics’: E-field controlled magnetism

‘Motttronics’: prospective metal-insulator transition based devices
Bolometers: thick films

VO2: thermally driven metal-insulator transition

Wu et al, Nanoletters 6 2313 (2006)

Tune device to critical temperature. Small amount of absorbed heat => large change in resistance
VO₂ proposed for actual use

(12) United States Patent
Grossman et al.

(10) Patent No.: US 6,323,486 B1
(45) Date of Patent: Nov. 27, 2001

(54) METHOD AND APPARATUS FOR BIAS AND READOUT OF BOLOMETERS OPERATED ON A HYSTERETIC METAL-INSULATOR TRANSITION

(75) Inventors: Erich N. Grossman, Boulder; Carl D. Reintsema, Nederland, both of CO (US)

(73) Assignee: The United States of America as represented by the Secretary of Commerce, Washington, DC (US)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 0 days.

(21) Appl. No.: 09/365,113

OTHER PUBLICATIONS

(List continued on next page.)

Primary Examiner—Constantine Hannaher
Assistant Examiner—Albert Gagliardi
(74) Attorney, Agent, or Firm—Greenlee, Winner and Sullivan, P.C.

ABSTRACT

This invention consists of a bias and readout scheme for resistive bolometers. It is chiefly intended for use with bolometer materials which exhibit a phase transition that is hysteretic. A preferred bolometer material is vanadium dioxide, which has a metal-semiconductor phase transition at 68°C and a hysteresis of typically 5°C, depending on material preparation. The existence of hysteresis precludes
Hysteresis is a problem

`Spintronics’

Example: ‘spin valve’

Desiderata: high spin polarization, good interfaces
Rare earth manganites: ?promising candidates?

Example: $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$

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

‘crystal field’: 5→3+2

In $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$: 4-x electrons all spins parallel

‘Colossal’ magnetoresistance!

Ramirez et al PRL 75 1336

Columbia University L’Ecole Polytechnique

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But performance at room T is not good

Challenge: identify materials/interfaces with high spin pol. at room T

Lu et al PRB54 8357 (1996)
Multiferroic response

‘Simple’ ferromagnet CoFe grown on top of thin film of ‘multiferroic’ BiFeO$_3$

E-field, applied to BaFeO$_3$, changes phase of magnetoresistive response of CoFe

Heron et al PRL 107 217202 (2011)
‘Mott-tronics’

Idea: voltage across Mott insulator causes it to become metallic.

Change of state => large increase in mobile carrier density

Newns et al APL 73 780 (1998)
Increase of conductance with bias voltage is observed

Chae et al Physical B369 76 (2005)
What is going on

Question: is the Mott state reconstructed or just doped
One orbital Hubbard model: 1-site DMFT

Hint of collapse of Mott insulating state at high voltage

More results: driven Mott insulator

Hubbard model (cubic lattice) in presence of field $F$ along body diagonal. Single-site DMFT. NCA/OCA ‘solver’.

Transient feature, then `steady’ state with constant current, increasing double occupancy

Eckstein et al. PRL 105, 146404 (2010)
Summary

• Many interesting phenomena

• Meaning and reliability of approximate method of solution

• New nonequilibrium questions associated with Mott metal-insulator devices

Lots to do!