Lecture notes on "Strongly Correlated" Transition Metal Oxides

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I. INTRODUCTION: BASIC CONCEPTS

In elementary condensed matter physics we consider the N-particle electron gas, with Hamiltonian H consisting of operators representing the 'kinetic energy' $\hat{K}$ and 'interaction energy' $\hat{U}$:

$$H = \hat{K} + \hat{U} \tag{1}$$

For the electron gas

$$\hat{K}_{el-gas} = \sum_{j=1...N} \frac{\hat{P}_j^2}{2m} \tag{2}$$

where P is the momentum operator. The electron-gas interaction energy operator (up to an irrelevant constant) is

$$\hat{U}_{el-gas} = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{\varepsilon \left(\vec{R}_i - \vec{R}_j \right)} \tag{3}$$

Here ε is a dielectric constant of the background material and we have not written the neutralizing uniform positive background explicitly. Because the kinetic and interaction energies do not commute, $\left[\hat{K}, \hat{U} \right] \neq 0$, the operators can not be simultaneously diagonalized and the physics is determined by a competition between the two.

If the interaction term vanishes ($\varepsilon \to \infty$) then the problem is non-interacting: the ground state is a simple Slater determinant of plane waves, and the excitations are simply particle-hole pairs. The order of magnitude of the energy per particle is $\sim K_0 = \hbar^2/(2ma^2)$ with a the mean spacing between the particles.

If the kinetic energy vanishes ($m \to \infty$) then the problem is one of classical electrostatics. The ground state is the ordered ('Wigner crystal') structure with the maximum interparticle separation. The ground state energy is a (small) constant times $\sim I_0 = e^2/(\varepsilon a)$. Very roughly the physics goes from being "kinetic energy dominated" for $K_0 > I_0$ to "potential

energy dominated" in the reverse limit. The parameter describing the crossover is the ratio r_s of the mean interelectron spacing a to the natural distance described by the constants in the problem.

$$r_s = \frac{I_0}{K_0} = \frac{2m\varepsilon e^2 a}{\hbar^2} \tag{4}$$

Observe that high density (small a) implies small r_s and hence kinetic energy dominated physics, whereas low density (large a) implies large r_s and hence potential energy dominated physics. Numerical study of the electron gas has established that metallic behavior persists up to quite large r_s, e.g. $r_s \sim 35$ in two dimensions. For r_s larger than this critical value the ground state is an insulating "Wigner crystal".

It is likely that the large r_s metallic behavior is in some respects unusual. However, it is generally accepted that for the free electron gas in two and higher dimensions, the metallic region even at large r_s has low energy physics described by "fermi liquid theory", which systematizes the idea that the low energy properties are in essence those of a weakly interacting electron gas, but with renormalized parameters.

These lectures discuss the electron gas in an important class of condensed matter systems, namely the transition metal oxides. These compounds have interesting (and potentially important) electronic properties including various forms of magnetic, charge and orbital ordering and unusual (for example high-T_c) superconductivity. In these materials "lattice" effects are strong, so that neither the kinetic nor potential energy are given by the simple electron gas forms [2,3] but it turns out that interaction energies are generically large relative to kinetic energies. The compounds are therefore termed "strongly correlated".

Materials and basic physics:

Transition metal oxides have crystal structures which are variants on the ABO_3 perovskite structure schematically depicted in Fig. 1. In the ideal perovskite structure the electronically interesting transition metal occupies the B-site, and is surrounded by (and strongly bonded to) 6 oxygen ions, which form an octahedron centered on the B-sites. A host of related compounds exist, for example involving layered ("Ruddlesden-Popper") structures in which one axis is stretched and the A-site structure is changed slightly, leading e.g. to La_2CuO_4, or different atoms are put on the B-sites (the "double perovskites" such as Sr_2FeMoO_6. The essential ingredient, however, is a transition metal octahedrally or tetrahedrally coordinated to oxygen ions.

The crucial electronic feature is a partially filled d-shell on the transition metal ion. The

d-orbitals are small, ($\sim 0.4A$) (cf Table 8.3 of J C Slater, Quantum Theory of Atomic Structure, v. 1); in fact the d-levels are 'inside' the 4s levels, so somewhat 'core-like'. The small size of the d-orbital enhances interaction effects (basically, one is squeezing several electrons into a small space) and decreases overlap with other orbitals (thus reducing the kinetic energy); this is why the correlations are strong. However, the role played by the small size of the d-orbital means that other atomic and solid-state physics effects (pertaining to the strong breaking of Galilean invariance, to the precise arrangement of electrons amongst the d-multiplet and to hybrization with other orbitals) are also important, so the electron gas analysis alluded to above cannot be carried over directly to the transition metal oxides.

II. KINETIC ENERGY

Goodenough-Kanamori hybridization rules. Orbital degeneracy. Kinetic energy Peierls phase and optics.

III. INTERACTION

Definition of U operator: Slater parameters. Screening by solid state effects. Mott vs charge transfer insulator. Optics as estimate of interaction scale.

Crucial electrons: Mn d-levels

–d-levels: weakly bound (so near fermi energy) but (esp 3d) but small in size .

–strong interactions=>energies depend on details of which spin and orbital states are occupied (cf Slater op. cit.) and Fig. 3.

–Key point: non-negligible 'Hunds coupling' favoring states with high spin.

–Key point: 'U' (coupling to total charge) strongly screened in solid.

Energetics of isolated Mn-O_6 octahedron:

–isolated $Mn - O_6$ octahedron: Mn d-levels and the O $2p$ levels.

–Define *zero of energy*: Mn in the d^5 maximal spin ($S = 5/2$) configuration and all of the O_{2p} states filled (so we have O^{2-}). (Note this does not correspond to any rare-earth manganese perovskite compound known to me). Choose spin quantization axis to be parallel to the direction of the $S = 5/2$, the ground state has $S = 5/2$ and $S_z = 5/2$.

–states which may be obtained from the ground state by removing one electron (adding one hole).

First neglect hybridization. => 17 one-hole states (electron removed from any of the 5 Mn d-levels (with spin necessarily parallel to the quantization axis) or to any of the 6 oxygens (in either spin state)).

Crystal electric field splitting: The 5 Mn levels are degenerate in free space, but in our cluster the Mn environment is not rotationally invariant (see fig 1); rather the presence of the 6 oxygen ions means that the Mn sits in an electric field with cubic symmetry, which separates the 5-fold degenerate d levels into two multiplets: one three fold degenerate (t_{2g}) and one two-fold degenerate (e_g). e_g lies higher.

(Determining how levels split in the presence of symmetry breaking fields is a problem of applied group theory. The most useful reference I have found is G. F. Koster and A. Dimmock, Table of the 32 Point Groups and Their Representations. I believe this book is out of print, but it contains, in tabular form, the answers to every problem of finite group theory).

A traditional and useful choice of basis for the t_{2g} levels is d_{xy}, d_{xz}, d_{yz} while the traditional choice of basis for the e_g levels is $d_{3z^2-r^2}$ and $d_{x^2-y^2}$. The *crystal electric field splittings* due to the electric fields of the O (and other) ions are in fact rather small, of order 0.3eV or less. For the rest of this discussion I neglect these level splittings

–define Δ as the difference in energy between adding a hole to the Mn (any state) or to the O.

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Problem: Estimate the magnitude of the crystal electric field splitting between the $d_{x^2-y^2}$ and d_{xy} levels in a cubic crystal field created by six O ions situated at the faces of a cube, whose center is the Mn ion, if the $Mn-O$ distance is $2A$ and the basic size of the Mn d-orbital is $0.5A$. For definiteness take the Mn-d wave functions to be proportional to

$$\psi_{xy} \sim xy e^{-r^2/2\lambda^2} \tag{5}$$

$$\psi_{x^2-y^2} \sim \left(x^2 - y^2\right) e^{-r^2/2\lambda^2} \tag{6}$$

with $\lambda = 0.4A$ (You will have to normalize the wave functions). I got about 0.3eV. Which state lies higher? (this needs no calculation)

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–Restore Mn-O hybridization.

Usual 'Goodenough-Kanamori' rules (fig 4) $=>e_g$ levels couple to the $O_{p\sigma}$ orbitals and the t_{2g} levels couple more weakly to the $O_{p\pi}$ levels.

–Examine e_g electron coupling.

In fact the Goodenough-Kanamori rules imply that an electron in the $3z^2 - r^2$ state couples only to the two oxygens in the $\pm z$ direction; the $3x^2 - r^2$ couples only to the two oxygens in the $\pm x$ direction and the $3y^2 - r^2$ couples only to the two oxygens in the $\pm y$ direction. To write down the full Hamiltonian in the 'conventional basis' we must express the $3x^2 - r^2$, $3y^2 - r^2$ orbitals in terms of the $3z^2 - r^2$ and $x^2 - y^2$ orbitals.

General linear of the two basis orbitals as

$$\psi = \cos\theta|3z^2 - r^2 > +e^{i\phi}\sin\theta|x^2 - y^2 >$$

The linear combinations for all of the simple orbitals are given in the following Table (for all the simple orbitals $\phi = 0$)

Orbital	θ
$3z^2 - r^2$	0
$3y^2 - r^2$	$2\pi/3$
$3x^2 - r^2$	$4\pi/3$
$x^2 - y^2$	$\pi/2$
$x^2 - z^2$	$-\pi/6$
$y^2 - z^2$	$5\pi/6$

Hamiltonian: 1 hole, parallel spin

$$H_{1hole} = \sum_{a=3z^2-r^2,x^2-y^2} \varepsilon_d d_a^\dagger d_a + \Delta \sum_{i=1...6} p_i^\dagger p_i - t_{Mn-O} \sum_{i=1...6,a=3z^2-r^2,x^2-y^2} \cos\theta_{a,i} \left(d_a^\dagger p_i + H.c\right)$$

Notation: $p_i^\dagger$ creates a hole on one of the six oxygen $2p\sigma$ orbitals, with $i = 1,2$ the $\pm z$,

$i = 3, 4$ the $\pm x$ and $i = 5, 6$ the $\pm y$. the $\theta_{i,a}$ are given in the Table:

i/a	a=$3z^2 - r^2$	a=$x^2 - y^2$
i=1	0	0
i=2	0	0
i=3	$2\pi/3$	$-\pi/6$
i=4	$2\pi/3$	$-\pi/6$
i=5	$2\pi/3$	$\pi/6$
i=6	$2\pi/3$	$\pi/6$

Within this approximation we obtain four 'non-bonding' states at energy Δ, two 'antibonding' states at energy $E_+ = \frac{1}{2}\left(\Delta + \varepsilon_d + \sqrt{(\Delta - \varepsilon_d)^2 + 12t_{Mn-O}^2}\right)$ and two bonding states at energy $E_- = \frac{1}{2}\left(\Delta - \sqrt{(\Delta - \varepsilon_d)^2 + 12t_{Mn-O}^2}\right)$.

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Problem: Derive the results for $E_\pm$ and, for the parameters indicated, the result for the fraction of hole charge density which resides on the Mn

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Similarly, the t_{2g} levels couple to the $O_{p\pi}$ levels, but more weakly, leading to a smaller level splitting.

It is interesting to compare the results of these simple estimates to those obtained from band structure calculations. The left panel of Fig 5 shows the band structure of (hypothetical) cubic ferromagnetic $LaMnO_3$ calculated by V. Udovenko (Rutgers) using programs developed by S. Savrasov (NJIT). the right panel of Fig. 5 shows the same band structure, in a 'fat band' representation which highlights bands with a non-negligble content of a desired orbital–in this case the $Mn\ 3z^2 - r^2\ e_g$ orbitals. One sees fat bands at Γ-point energies of about 11.75 and 14.5eV representing the majority spin ('down, in the conventions of this calculation) and minority spin antibonding bands, and one sees at Γ-point energies of about 8.5eV bands with a smaller admixture of e_g states. We observe a band-center to band-center splitting of about $7eV$; also the center of gravity of the oxygen bands lies a bit below the middle of the e_g splitting. A rough fit of the calculated band theory to the simple model yields $(\varepsilon_d - \Delta) \approx 2.eV$ (but not very accurately determined) and

$\sqrt{(\Delta - \varepsilon_d)^2 + 12t_{Mn-O}^2} = 7 - 8eV$ implying $t_{Mn-O} \approx 2 - 2.5.eV$. For these parameters, in the one hole state a bit more than one half of the added hole resides on the Mn and a bit less resides on a linear combination of the surrounding oxygens. (Note: the 'fat band' representation is a bit misleading: the states in the bonding band are actually distributed over many oxygen bands so the fractional weights are relatively small).

Fig 6 shows more comprehensive decompositions of the bands: The left panel shows all of the e_g levels and the right panel shows one of t_{2g} levels (the others have very similar bands). One can see that the t_{2g} bands are less strongly hybridized with the oxygen than the e_g; this 'ligand field splitting' is the reason why the low energy physics of manganites involves mainly the e_g levels. We observe, however, that within the local spin density approximation the minority spin t_{2g} band goes slightly below the fermi sruface near the Γ point, so that in this approximation the material is not a half-metal. Of course, interaction effects not included in band calculations might change this physics, in particular by adding a 'U' which might push the t_{2g} levels up in energy.

Important open question: where are the t_{2g} levels in the actual materials? Is there an energy range in which they are of dynamical importance?

Important open question: significance of the admixture of O states. One point of view is that we should simply remember that the object which we call an e_g electron is really a linear combination of Mn and O states; another is that the O states constitute an important dynamical degree of freedom.

Interaction effects.

Let us now consider spin 3/2 states obtained by removing two electrons from the filled shell configuration. To simplify the discussion I treat only the e_g levels and the combinations of oxygens which couple to them. We have four such states, which I denote by the number of holes removed from the reference configuration (recall in present notation the operatores

create holes)

$$
\begin{array}{cc}
\text{State} & \text{Occupancy} \\
|A> & d^{\dagger}_{3z^2-r^2}d^{\dagger}_{x^2-y^2}|0> \\
|B> & d^{\dagger}_{3z^2-r^2}p^{\dagger}_{x^2-y^2}|0> \\
|C> & p^{\dagger}_{3z^2-r^2}d^{\dagger}_{x^2-y^2}|0> \\
|D> & p^{\dagger}_{3z^2-r^2}p^{\dagger}_{x^2-y^2}|0> \\
\end{array}
$$

Within this subspace the Hamiltonian is a 4×4 matrix with entries

$$
H_{2holes} = \begin{pmatrix}
2\varepsilon_d + U & \sqrt{3}t_{Mn-O} & \sqrt{3}t_{Mn-O} & 0 \\
\sqrt{3}t_{Mn-O} & \varepsilon_d + \Delta & 0 & \sqrt{3}t_{Mn-O} \\
\sqrt{3}t_{Mn-O} & 0 & \varepsilon_d + \Delta & \sqrt{3}t_{Mn-O} \\
0 & \sqrt{3}t_{Mn-O} & \sqrt{3}t_{Mn-O} & 2\Delta
\end{pmatrix} \tag{7}
$$

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Problem: derive H_{2holes}

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The interesting quantity is the difference in energy between the two-hole ground state with $U = 0$ and with $U \neq 0$. This is plotted in Fig 8. We see that the effects of a repulsive U are very small– as shown in Fig 9 the wave function simply readjusts to avoid the repulsive interaction. For negative U (for holes) we see that the initial effects of U are very small–the *effective U* (defined as the difference between twice the one-hole groundstate energy and the two hole ground state energy) is less than $1/3$ of the 'bare U'.

Important open question: what is the value of U_{eff} relevant to real materials??

Non-maximal spin states: Hunds coupling J_H.

–Definition–energy change if flip a spin, keeping all orbitals fixed.
–band theory (fig 4,6) $J_H \approx 2.5eV$
–Similar values from 'screened atomic' calcs (Fig 2) exc for d^5 which is a little larger.

Important open question: what is the value of J_H relevant to real manganite materials??

Jahn-Teller coupling

–even parity volume preserving distortions of MnO_6 octahedron couple to splitting of e_g levels.

–Definition of distortions (Fig 10)

–Coulomb effect: point charge model–for a basic distortion δ of $0.1A$ I find about $0.6eV$ splitting between up and down states.

–change in hybridization–similar magnitude

–*Pseudospin representation for e_g orbitals*

$$'up' = |3z^2 - r^2 > \tag{8}$$

$$'down' = |x^2 - y^2 > \tag{9}$$

The net result of these considerations is a Hamiltonian (for the e_g) level splitting of the for

$$H_{JT} = \lambda \left(\tau_z Q_3 + \tau_x Q_2 \right)$$

where $\tau_{z,x}$ are Pauli matrices.

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Write a formal expression for the Coulomb contribution to the Jahn-Teller splitting, within a point charge model. Linearize this in the bond-length change and estimate the resulting level splitting.

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Fits to band theory for the distorted structure (fig 12) imply $\lambda = 1.4eV/A$ (Ahn and Millis, PRB^1 13545 2001).

Summary of energies–maximal spin states

The energies expected for $LaMnO_3$ (in the absence of hybridization) are summarized in Fig. 11. We expect that the d^4 configuration is the lowest energy. The d^3 energy would be equal in the absence of interaction effects, and is presumably higher (positive U for holes) because there is no evidence of phase separation.

The ordering of the levels in the actual materials (relative positions of upper d^4 JT level, $d^{3,5}$ and minority spin d^4) are not well established.

Band theory:

nearest neighbor (nn) tight binding.

$$H_{band} = \frac{-1}{2} \sum_{i\delta ab\alpha} (t(\delta)^{ab} c^+_{i+\delta,a,\alpha} c_{ib\alpha} + H.c.) \tag{10}$$

where δ is a vector connecting site i to a nearest neighbor. t^{ab} orbital dependent hopping. Fourier transform; Pauli matrix notation:

$$\varepsilon = \varepsilon_0(p) + \vec{\varepsilon}(p) \cdot \vec{\tau} \tag{11}$$

with $\vec{\tau}$ the usual Pauli matrices, b the lattice constant,

$$\varepsilon_0(p) = -t(\cos(p_x b) + \cos(p_y b) + \cos(p_z b)) \tag{12}$$

and $\vec{\varepsilon}(p) = (\varepsilon_x(p), 0, \varepsilon_z(p))$ with

$$\varepsilon_x(p) = -\frac{\sqrt{3}t}{2}(\cos(p_x b) - \cos(p_y b)) \tag{13}$$

$$\varepsilon_z(p) = t(\cos(p_z b) - \frac{1}{2}(\cos(p_x b) + \cos(p_y b))) \tag{14}$$

The energy eigenvalues are

$$E_\pm = \varepsilon_0 \pm \sqrt{\varepsilon_x^2 + \varepsilon_z^2} \tag{15}$$

Note that along the zone diagonals ((1,1,1) etc) $\varepsilon_{z,x} = 0$ so the two bands are degenerate and along the line to any cube face ((1,0,0) and equivalent) one of the two bands is dispersionless. These two features occur, to a high degree of accuracy, in the calculated band structure, lending support to the nearest neighbor tight binding modelling.

The best fit to the calculated band theory leads to $t = 0.67eV$. This, for example, implies that at band filling $n = 0.7$ the density of states is $0.57eV$ which reproduces almost exactly the band theory approximation to the specific heat coefficient $\gamma = $ quoted for $x = 0.3$ manganite in[?]. (Note also that[?] contains a misprint[?] in the value of the Drude plasma frequency $\Omega_p = 1.9eV$. The correct band theory value is very close to the $\Omega_p = \sqrt{4\pi e^2 D/b} = 3.1eV$ which follows using $t = 0.67eV$ in Eq. 18 below).

Density of states (Fig 14)

$$D(\epsilon) = \frac{\partial n}{\partial \mu} \tag{16}$$

'kinetic energy' per site $K = -\frac{<H_{band}>}{N}$ (N is the number of sites) given by

$$K = \frac{1}{2N} \sum_{\delta a \sigma i} t^{ab}(\delta) < c_{ia\sigma}^+ c_{i+\delta a\sigma} + H.c. > \tag{17}$$

and the 'Drude weight' D which for a spin polarized system and current flowing in the z direction is

$$D_z = b^3 \int \frac{d^3 p}{(2\pi)^3} \sum_{\lambda=+,-} \left(\frac{\partial E_\lambda(p)}{b^2 \partial p_z} \right)^2 \delta(E_\lambda(p) - \mu) \tag{18}$$

Figure 14 shows the kinetic energy (divided by 3 to facilitate comparison to optics) and Drude weight, plotted against particle density for a fully spin polarized gound state.

A. Conductivity

Need coupling between the electric field and the electronic states.

Represent the electric field by a vector potential A and adopt the *Peierls phase approximation*, $t_{i-j} \rightarrow t_{i-j} e^{i\frac{e}{c}\vec{A}\cdot\vec{R}_{ij}}$

Widely used. Accuracy not yet clear.

$$\hat{J}_z \equiv \frac{\delta\hat{H}}{Nb^3\delta A_z} = -\frac{2te}{b^2} \left(\sin(p_z b) - \frac{eb}{c} A \cos(p_z b) \right) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{19}$$

The expectation value of the term in J proportional to A gives the total oscillator strength, $S(\infty)$ in the conduction band contribution to the optical conductivity (see[?][?][?] for details). We have

$$S(\infty) = \frac{e^2}{3b} K \tag{20}$$

The conductivity is

$$\sigma(\Omega) = \frac{S(\infty) - \chi_{jj}(\Omega)}{i\Omega} \tag{21}$$

with χ_{jj} the usual Kubo formula current-current correlation function evaluated using J evaluated at $A = 0$.

B. Spin Wave stiffness

To compute the $T = 0$ spin wave stiffness we follow the standard procedure outlined in[?][?] We compute the energy cost of a small amplitude, long wavelength rotation of the order parameter away from the fully polarized ferromagnetic state, which we take to be aligned with the z axis. The calculation is most easily carried out by locally rotating the spin quantization axis to align with the local spin direction, so that the $T = 0$ Hamiltonian becomes

$$H = -\frac{1}{2} \sum_{i,\delta,a,b,\alpha,\sigma,sigma'} t^{ab}(\delta) c^+_{i+\delta,a,\sigma} c_{i,a\sigma'} R^+_{i+\delta\sigma\alpha} R_{i\alpha\sigma'} + H.C. \tag{22}$$

where R are the usual $S = 1/2$ rotation matrices. We find two terms. The first one arises from the term in $R^+ R$ proportional to the square of the deviation, $\vec{m}_q$ of the magnetization from its ordered state value and is (K is the kinetic energy defined above in Eq 17).

$$E^{(1)} = \frac{K}{24} (qa)^2 \, \vec{m}_q \cdot \vec{m}_{-q} \tag{23}$$

while the second one arises from inserting the expression for the term in $R^+ R$ which is linear in $\vec{m}_q$ into the familiar second order perturbation theory expression, and is

$$E^{(2)} = - (qa)^2 \, \vec{m}_q \cdot \vec{m}_{-q} I_{SW}(J) \tag{24}$$

with

$$I_{SW}(J) = \sum_p t^2 \sin^2(p_z) \left(\Psi_+(p) + \Psi_-(p) \right) \tag{25}$$

where (note we have suppressed the momentum labels to avoid clutter in the equations)

$$\Psi_+ = \frac{f(E_-) \left(J \cos^2(\theta) + \cos^4(\theta) \sqrt{\varepsilon_x^2 + \varepsilon_z^2} \right)}{2J \left(J + \sqrt{\varepsilon_x^2 + \varepsilon_z^2} \right)} \tag{26}$$

$$\Psi_- = \frac{f(E_+) \left(J \sin^2(\theta) - \sin^4(\theta_p) \sqrt{\varepsilon_x^2 + \varepsilon_z^2} \right)}{2J \left(J - \sqrt{\varepsilon_x^2 + \varepsilon_z^2} \right)} \tag{27}$$

and $\tan(\theta) = \varepsilon_x / \left(\sqrt{\varepsilon_x^2 + \varepsilon_z^2} + \varepsilon_z \right)$.

The spin wave stiffness D_{SW} as conventionally defined is given by twice the total coefficient of $(q)^2 \, \vec{m}_q \cdot \vec{m}_{-q}$ divided by the ordered moment, i.e.

$$D_{SW} = \left[\frac{K}{12} - 2I_{SW}(J) \right] b^2 \tag{28}$$

Fig. 14.

Standard model: band theory +Hunds +JT+U....

Tests;–parameter values: Optics

–general theory–see appendix)

LaMnO3: tight binding–calc results (17) in poor agreement with data (Fig 18) . Question–accuracy of Peierls phase approx.(Figs 16,19).

Possible alternative: much large U so 'tb model' transition is not visible below oxygen band. Observed 1.6eV feature an onsite d-d transition combined with lattice distortion (Perebeinos) (Fig 20).

Metallic manganites: temperature dependence. Need method of calc. Digression–DMFT (Appendix and Figs 21-25).

Double exchange 'blocking' of transport

Interesting result (Michaelis): for J which approx reproduces T_c, spin wave stiffness, theory implies only small change in kinteic energy between T_c and $T = 0$. (Figs 26,27). Suggestion–double exchange is not the crucial physics????

Summary:

Value of T_c and spin wave stiffness (+quantum chemistry) suggests intermediate J, U Data suggest larger J and U???

C.   Overview

To evaluate the properties of H we use the dynamical mean field method[?][?][?][?] This method is extensively described and justified elsewhere, and is relevant here because the principal interactions are local. In brief the central approximation is to the electron Green function. For the band structure of present relevance the electron Green function is written in general as

$$\mathbf{G}(z, p) = (z - \mathbf{\Sigma}(p, z) - \varepsilon(p) + \mu)^{-1} \qquad (29)$$

with $\Sigma(p, z)$ the self energy. In the dynamical mean field method one takes Σ to be p−independent, i.e. to depend only on z. The important quantity is then the momentum integrated green function

$$G_{mom-int}(z) = b^3 \int \frac{d^3p}{(2\pi)^3} \mathbf{G}(\mathbf{z}, \mathbf{p}) \tag{30}$$

The local Green function, being a function of frequency only, may be derived from a local quantum field theory, which is specified by a partition function Z_{loc} given in terms of a mean field function $a(\tau)$. This is in general a matrix in orbital and spin indices (which we do not explicitly write here)

$$\begin{aligned} Z_{loc} &= \int \mathcal{D}c^+ c \, Exp[\int d\tau d\tau' c^+(\tau) \mathbf{a}(\tau - \tau') c(\tau') \\ &+ \int d\tau H_{int}] \end{aligned} \tag{31}$$

From this action one may extract a local Green function G_{loc} and self energy Σ via

$$G_{loc}(\tau) = \frac{\delta ln Z_{loc}}{\delta a(\tau)} = (a - \Sigma)^{-1} \tag{32}$$

The mean field function a is fixed via the constraint that the local Green function calcuated from Z_{loc} is identical to the momentum integrated Green function obtained from Eq 30, using the local self energy defined in the second equality in Eq 32, i.e.

$$G_{loc}(z) = G_{mom-int}(z) \tag{33}$$

In the present problem the two orbitals are degenerate so it is not necessary to consider orbital indices in G_{loc}. For T=0K a ferromagnetic core spin configuration yields a spin dependent but frequency independent $\Sigma_\sigma = \sigma_z J$. For $T > T_c$ Eq 33 is an integral equation for Σ, which is solved by numerical iteration.

In the dynamical mean field approximation there are no vertex corrections for the current current correlation function[?][?] , so it is given by

$$\chi_{jj}(i\Omega) \qquad = \qquad T \sum_{\omega_n} \int \frac{d^3p}{(2\pi)^3}$$
$$Tr\left[\mathbf{J_z}\mathbf{G}(p, i\Omega + i\omega_n)\mathbf{J_z}\mathbf{G}(p, i\omega_n)\right] \tag{34}$$

with G given by Eq. 29 using the momentum-independent self energy from the final solution of Eq 32.