Electronic structure of correlated electron systems : theory and experiment Lecture 1,2

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Rough content of 5 lectures

• Lecture 1 and 2: Electronic structure of correlated and narrow band systems.

• Lecture 2 and 3: Electronic structure and theory of transition metal oxides (orbital, charge, spin and lattice degrees of freedom)

• Importance of non uniform polarizabilities Surfaces, interfaces of strongly correlated Oxides.

• Basic electronic structure and theoretical models of Fe Pnictides
Content Lecture 1,2

• Electronic structure of correlated electron systems
  – Why are TM compounds and rare earths special
  – Quasi atomic vs band structure approaches
  – A bit about DFT, LDA+U, DMFT, Model H exact diagonalization
  – A bit about Auger and ARPES
  – Spectral weight transfer arguably the most direct evidence for strong correlation
  – Models and curiosity’s
Some Old Historical milestones

• 1929-1931 Bloch Wilson theory of solids
• 1937 De Boer and Verwey (NiO-CoO breakdown of band theory)
• 1937 Peierls 3d electrons avoid each other (basically the Hubbard model)
• 1950 Jonker van Zanten - Zener Pervoskites double exchange
• 1959 Anderson superexchange (U>>W)
• 1964 Hubbard model-, Hohenberg Kohn DFT-Kohn Sham, Goodenough Transition metal compounds
Everyone claiming to work on real materials should be familiar with this

![Periodic Table of the Elements 2005](image-url)
Wide diversity of properties

- Metals: CrO2, Fe3O4 T>120K
- Insulators: Cr2O3, SrTiO3, CoO
- Semiconductors: Cu2O
- Semiconductor –metal: VO2, V2O3, Ti4O7
- Superconductors: La(Sr)2CuO4, LiTiO4, YBCO
- Piezo and Ferroelectric: BaTiO3
- Catalysts: Fe, Co, Ni Oxides
- Ferro and Ferri magnets: CrO2, gammaFe2O3
- Antiferromagnets: alfa Fe2O3, MnO, NiO ---
- Ionic conductors (batteries) LixNi1-xO
- Oxide fuel cells use Manganites and cobaltates

Properties depend in detail on composition and structure
Phase Diagram of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$

Uehara, Kim and Cheong

R: Rombohedral
O: Orthorhombic
(Jahn-Teller distorted)
O*: Orthorhombic
(Octahedron rotated)
Mizokawa et al. PRB 63, 024403 2001

Model for Charge, Spin and Orbital Correlations in Manganites

\[ \text{La}_{\frac{3}{7}} \text{Sr}_{\frac{4}{7}} \text{MnO}_3 \]

Mn$^{4+}$, d$^3$, $S=3/2$, No quadrupole; Mn$^{3+}$, $S=2$, orbital degeneracy

\[ S = 6 \times 2 + \frac{3}{2} = \frac{22}{2} \]
Ordering in strongly correlated systems

Stripes in Nd-LSCO

rivers of Charge—Antiferro/Antiphase

Charge inhomogeneity in Bi2212


Quadrupole moment ordering

$DQ_c \sim 1\ e$

$DQ_o \sim 0$

$DQ \sim 0.1\ e$

$DQ < 0.5\ e$
It’s the outermost valence electron states that determine the properties; Both the occupied and unoccupied ones
Two extremes for atomic valence states in solids

Where is the interesting physics?

Coexistence----Hybridization

Kondo, Mixed valent, Valence fluctuation, local moments, Semicond.-metal transitions, Heavy Fermions, High Tc’s, Colossal magneto resistance, Spintronics, orbitronics
# Characteristics of solids with 2 extreme valence orbitals

<table>
<thead>
<tr>
<th>R&gt;&gt; D</th>
<th>R&lt;&lt;D</th>
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<tbody>
<tr>
<td>• electrons lose atomic identity</td>
<td>• Valence Electrons remain atomic</td>
</tr>
<tr>
<td>• Form broad bands</td>
<td>• Narrow bands</td>
</tr>
<tr>
<td>• Small electron electron interactions</td>
<td>• Large electron electron interactions (on site)</td>
</tr>
<tr>
<td>• Low energy scale – charge fluctuations</td>
<td>• Low energy scale-spin fluctuations</td>
</tr>
<tr>
<td>• Non or weakly magnetic</td>
<td>• Magnetic (Hund’s’ rule)</td>
</tr>
<tr>
<td>• Examples Al, Mg, Zn, Si</td>
<td>• Gd, CuO, SmCo3</td>
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Many solids have coexisting R>>D and R<<D valence orbitals i.e. rare earth 4f and 5d, CuO Cu 3d and O 2p, Heavy Fermions, Kondo, High Tc,s , met-insul. transitions
Why are the valence 3d and 4f orbitals in transition metal and rare earth compounds special

- Lowest principle q.n. for that l value
- Large centrifugal barrier l=2,3
- Small radial extent, no radial nodes, orthogonal to all other core orbital's via angular nodes (snuggle up to the nucleus)
- High kinetic energy (angular nodes) compensates for the strong potential energy
- Relativistic effects
- Look like core orb. But have high energy and form open shells like valence orb.
Why does $E_n$ depend on $l$?

Atomic hydrogenic, $E_n = \frac{m_2 z^2 e^4}{2\hbar^2 n^2}$

$l$ comes in relativistic effects

$E = \sqrt{p^2 c^2 + mc^4} = mc^2 + \frac{p^2}{2m} - \frac{1}{2} \left( \frac{mc}{m c^2} \right)^2$

From $<p^2> \propto l (E_n^0 + z e^2 <\frac{1}{r}>)$

$\Delta E = -\frac{1}{2mc^2} \left( <E_n^0>^2 + 2 E_n^0 z e^2 <\frac{1}{r}> + 2 z^2 e^2 <\frac{1}{r^2}> \right)$

$<\frac{1}{r}>$ independent of $l$; $\frac{2}{a_0 n^2}$

$<\frac{1}{r^2}> = -\frac{2}{a_0^2 n^2 (2l + 1/2)}$

$\Delta E_{\text{ion}} = \frac{<z^2 >}{n^2} \left( \frac{n}{2e/\hbar^2} - \frac{3}{2} \right) E_n^0 \left( \frac{a_0^2 e^2}{\hbar^2} \right)$

For $3d$ (3s) energy $\sim 120 \text{ eV}$

$\frac{3p_{1/2}}{3d} \text{ eV} \sim 10 \text{ eV}$

$E_{\text{ion}}$ can be larger than $E_n$ if we include larger Coulomb repulsion.
Special place for transition metal and rare earths

Note that the 4f states are not full or empty for the rare Earths and yet they are well inside other occupied orbitals!!
Hubbard
For 4f U as large as 12eV
# Band Structure approach vs atomic

<table>
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<tr>
<th><strong>Band structure</strong></th>
<th><strong>Atomic</strong></th>
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<tbody>
<tr>
<td>• Delocalized Bloch states</td>
<td>• Local atomic coulomb and exchange integrals are central</td>
</tr>
<tr>
<td>• Fill up states with electrons starting from the lowest energy</td>
<td>• Hunds rules for the Ground state  -Maximize total spin-  Maximize total angular momentum-total angular momentum $J = L - S &lt; 1/2$ filled shell , $J = L + S$ for $&gt; 1/2$ filled shell</td>
</tr>
<tr>
<td>• No correlation in the wave function describing the system of many electrons</td>
<td>• Mostly magnetic ground states</td>
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<td>• Atomic physics is there only on a mean field like level</td>
<td></td>
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<tr>
<td>• Single Slater determinant states</td>
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Recall that the ground State has few properties. It is the excited states that determine the response to external perturbations such as fields.

\[ \Phi = \frac{1}{\sqrt{n!}} [\phi_1 \cdots \phi_n] \quad (\text{Slater det.}) \]

\[ \phi_n \text{ are one electron Bloch states} \]

No correlation in \( \Phi \) but in \( \mathcal{H}_{\text{eff}} \)

\[ \left[ -\frac{1}{2} \nabla^2 + W(\mathbf{r}) + V_V(\mathbf{r}) + V_{\text{xc}}(\mathbf{r}) \right] \phi_n(\mathbf{r}) = \epsilon_n \phi_n(\mathbf{r}) \]

One particle problem

\[ V_V = \int d^3 \mathbf{r} \mathbf{V}(\mathbf{r}-\mathbf{r}') \phi(\mathbf{r}') \]

\[ V_{\text{xc}} = \int f(\langle \phi(\mathbf{r}) \rangle) \phi(\mathbf{r})^2 d\mathbf{r} \]

\[ 2\varepsilon = \frac{\partial E_{\text{xc}}}{\partial \epsilon} \]

exchange-correlation potential

- Hohenberg-Kohn
- Exact for \( E_0 \neq 0 \) (ground state)

\[ \phi, \epsilon \neq \epsilon_c \text{ have no physical meaning!} \]

Math. functions to get \( E \neq 0 \).
\( \psi_0^{\text{off}} \) also has no physical significance

\( E q \) is exact \( \phi(r) \) is exact but

\( H_{\text{exact}} \neq E q \psi_0^{\text{off}} \)

\( H_{\text{exact}} = \frac{2}{2m} \left[ -\frac{1}{2} \nabla^2 + W(r) + \frac{1}{2} \gamma \frac{e^2}{4\pi \hbar^2 (r_2 - r_1)} \right] \)

in \( \psi_0^{\text{off}} \phi \) have \( k \) as good g.m.

\( H_{\text{eff}}^{\text{off}} \text{ has Transl. symm.} \)

\( H_{\text{eff}} \psi_0^{\text{off}} = E_1 \psi_0^{\text{off}} \)
The terms \( \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \) will always have matrix elements scattering

\[ h^\prime \rightarrow h'' \]  

i.e. from below to above \( k^\prime \)

e.g. \( \Phi_h = \frac{1}{\sqrt{N}} \sum \Phi_{\mathbf{r}}(\mathbf{r} - \mathbf{R}_i) e^{i \mathbf{k} \cdot \mathbf{R}_i} \) [Ligth binding]

For \( R \ll \langle d \rangle < \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \) will dominate for two electrons on one site.

\( \langle \Phi_1 | \Phi_2 \rangle = U \)

Interaction between two Bloch wave electrons = \( U/N \sim 0 \)
So is correlation negligible?
\[
\langle \Phi \mid \hat{H}_{int} \mid \Phi'_{k_1 k_2} \rangle = \frac{1}{N} U S(k_1, k_2, k_1', k_2')
\] 
\rightarrow 0 \quad \text{for} \quad N \rightarrow \infty

Small if \( U << W \) so only few electrons are involved.

For \( U >> W \) must sum over all other electrons \( \frac{nU}{N} \) or \( n = N \rightarrow U \) and diagonal matrix elements are large \( \Phi^0 \) is not an eigenfunct.

For \( R << d \) \( \frac{1}{2} \) filled s band if we neglect \( W \) (Evansl. symm.)

\[
\Phi_k = \frac{1}{\sqrt{|N|}} \Phi_1 \Phi_2 \ldots \Phi_N
\]

one electron/atom
Surely a lattice of H atoms separated by say 1 cm would not behave like a metal.

What have we forgotten?
The electron electron repulsive interaction.
Experimental evidence for atomic like behaviour in transition metal compounds and rare earths. Photoemission/inverse photoemission and Auger spectroscopy.
PES (Photo electron Spectroscopy) involves low $\hbar \omega \rightarrow$ valence electrons. Consider a metal.

\[ E_{\text{kin}} = \hbar \omega - E_b \]

\[ \hbar \omega \rightarrow \text{photon in} \rightarrow E_{\text{kin}} \]

Occupied $e(\varepsilon)$

$\rightarrow$ Intensity of emitted electrons as a function of $E_k$

Measure density of states for electron removal $\times$ Matrix element.
Inverse PES / PES / BIS (Bremsstrahlung isochromat spectra) involves conduction band states

Measure $I(h\nu)$ as a function of $E_R$

$E_h$ → electron in (relative to $E_F$)

Intensity of photons at constant photon energy as a function of $E_R$

→ new two photon out

For BIS $h\nu$ = const incident electron energy is changed

Measures $\rho(E)$ for electron addition
High resolution angular resolved photoelectron spectroscopy

\[ \mathbf{K} = \frac{\mathbf{p}}{\hbar} = \sqrt{2mE_{\text{kin}}}/\hbar \]

\[ K_x = \frac{1}{\hbar} \sqrt{2mE_{\text{kin}}} \sin \vartheta \cos \varphi \]
\[ K_y = \frac{1}{\hbar} \sqrt{2mE_{\text{kin}}} \sin \vartheta \sin \varphi \]
\[ K_z = \frac{1}{\hbar} \sqrt{2mE_{\text{kin}}} \cos \vartheta \]

Vacuum

\[ E_{\text{kin}} \]
\[ \mathbf{K} \]

Conservation laws

\[ E_f - E_i = h\nu \]
\[ \mathbf{k}_f - \mathbf{k}_i = \mathbf{k}_{\text{hv}} \]

Solid

\[ E_B \]
\[ \mathbf{k} \]
Example of a simple metal in one electron theory

**ARPES: Energetics and Kinematics**

Energy Conservation

\[ E_{\text{kin}} = h\nu - \phi - |E_B| \]

Momentum Conservation

\[ \hbar k \parallel = \hbar K \parallel = \sqrt{2mE_{\text{kin}}} \cdot \sin \vartheta \]
Example of a metal in which electrons are dressed

**ARPES: The One-Particle Spectral Function**


Photoemission geometry

Non-interacting electron system

Fermi liquid system

**Photoemission intensity:** \( I(k, \omega) = I_0 |M(k, \omega)|^2 f(\omega) A(k, \omega) \)

**Single-particle spectral function**

\[
A(k, \omega) = -\frac{1}{\pi} \frac{\Sigma''(k, \omega)}{[\omega - \epsilon_k - \Sigma'(k, \omega)]^2 + [\Sigma''(k, \omega)]^2}
\]

\( \Sigma(k, \omega) \): the "self-energy" captures the effects of interactions
Angular resolved photoelectron spectroscopy (ARPES) of Cu metal
Thiry et al 1979

ARPES Cu

Cu is d10 so one d hole
Has no other d holes to
Correlate with so 1 part.
Theory works if the only
Important interaction is
The d-d interaction.
Great agreement with
DFT

Points – exp.
Lines - DFT

3d bands
4s, 4p, band
We note that for Cu metal with a full 3d band in the ground state one particle theory works well to describe the one electron removal spectrum as in photoelectron spectroscopy this is because a single d hole has no other d holes to correlated with. So even if the on site d-d coulomb repulsion is very large there is no phase space for correlation.

The strength of the d-d coulomb interaction is evident if we look at the Auger spectrum which probes the states of the system if two electrons are removed from the same atom.

If the d band had not been full as in Ni metal we would have noticed the effect of d-d coulomb interaction already in the photoemission spectrum as we will see.
What if we remove 2- d electrons?
Two hole state with Auger spectroscopy

Example is for Cu with a fully occupied 3d band

\[ E(\text{photon}) - E(\text{photoelectr}) = E(2p) \]
\[ E(2-\text{d holes}) = E(2p) - E(3d) - E(\text{Auger}) \]
\[ U = E(2-\text{d holes}) - 2xE(1-\text{d hole}) \]
Auger spectroscopy of Cu metal

Atomic multiplets
Looks like gas phase
U > W
Two hole bound states

Hund’s rule
Triplet F is Lowest

The L3M45M45 Auger spectrum of Cu metal i.e final state has 2 -3d holes on the Atom that started with a 2p hole. Solid line is the experiment. Dashed line is one Electron DFT theory, vertical bars and lables are the free atom multiplets for 8- 3d electrons on a Cu atom . Ef designates the postion of the Fermi level in the DFT .

Antonides et al 1977

Sawatzky theory 1977
Two particles in Hubbard
(5 band)

\[ H = \sum_{R,S,\sigma} c_{R \sigma}^+ c_{S \sigma} + U \sum_R c_{R+}^+ c_{R+} c_{R-} c_{R-} \]

\[ = \sum_R \epsilon_R c_{R+}^+ c_{R+} + \frac{U}{N} \sum_{\sigma} c_{R+}^+ c_{R+} c_{R-} c_{R-} \]

Momentum + Spin conservation

\[ L_H, K_I = 0 \quad L_H, S_I = 0 \]

\[ K = \text{Total momentum} \quad S = 0 \text{ or } 1 \]

For \( G^{\alpha \beta}_{q+q' - q} = \langle 0 | c_{q+\alpha}^+ c_{q+\beta} G(q) c_{q'\beta}^+ c_{q'\alpha} | 0 \rangle \)

contains both singlet or triplet

Triplet - soln. - self convolution of 1 part.

\[ G = \left( S_{q} - S_{q+q' - q} \right) \frac{1}{2 - \epsilon_R - \epsilon_{R+} - \epsilon_{R-}} \]
Dyson \[ G = G_0 + G_0 \mathcal{H}_V G ; \quad G_0 = \frac{1}{z - \mathcal{H}_0} \]

\[ G_{\alpha \beta k k'} = S_{kk'} \frac{1}{z - E_k - E_{k'} k'} = S_{kk'} G_0(k, k'; z) \]

\[ G_{\alpha k k'}^{\text{H}} = \delta_{k k'} G_0(k, k') + G_0(k, k') \frac{U}{N} \sum_{\beta} G_{\beta k k'}^{\text{H}} \]

\[ \xi_k = G_0(k, k) + \frac{1}{N} \sum_{\beta} G_0(k, k') \frac{U}{N} \]

\[ \sum_{\beta} G_{\beta k k'}^{\text{H}} = \frac{G_0(k, k')}{1 - \frac{1}{N} \sum_{\beta} G_0(k, k')} \]

Ladder approximation is exact for only two particles

Zero's on real axis provide single energy

\[ \text{Re} \left[ \xi_k G_0(k, k' k'; x_k) \right] = \frac{N}{U} \]

For \( U \gg W \) (band width)

Two sets of poles
- Centered around self convolution of one particle energy is new set of states
- Centered close to \( z = \text{tree} \) with little dispersion
for $W \gg U$ one electron theory
for $W \ll U$ strong correlation

For strong correlation energy levels depend on the number of electrons
For 1 electron $N_e = 0$

For 2 spin parallel electrons same as for 1 electron
For 2 spin antiparallel electrons

and $U \gg W$
D shells are complicated by multiplet structure

- Atomic physics – d orbital is 5 fold degenerate not including the spin and neglecting the spin orbit coupling.
- Two d electrons or holes with orbital angular momentum =2 and spin of ½ can couple into total angular momentum states L with total spin 1 or 0 as follows; singlet S, singlet G, singlet D and triplet P and triplet F
- The energy separations in the Cu Auger spectrum are from atomic coulomb integrals with triplet F as the lowest energy state for 8 d electrons as given by Hunds’ rule
For $U \gg W$ and in the presence of unfilled bands the one particle removal spectrum will be very different from that of a filled band.

Compare the PES of Cu metal with a full d band to that of Ni with an average 0.6 holes in the 3d band.
The image shows a graph with the y-axis labeled as "Intensity (arb. units)" and the x-axis labeled as "Binding Energy (eV)". The graph compares the intensity for different elements: Cu, CuPd, and CuPt. The peak for CuPt is labeled with an arrow pointing to Cu 3d.
The relative weights of the d9 and d8 (satellite) configurations depend on initial d occupation and i.e. mixing i.e. band width. Both in the initial and final states.

For a LDA/DMFT try see Lichtenstein et al PRL 067205 (2001)
In one electron theory

\[ P(n) = \frac{m!}{(m-n)! n!} (1-c)^{m-n} c^n \]

= Probability that a site has \( n \) electrons
\( m = \) degeneracy difficulty
\( C = \) concentration of electrons = \( \frac{<n^2>}{m} \)

So for Ni: \( C = 0.94 \) all conf.

d\(^9\) \( \rightarrow \) d\(^{10}\) occur without energetic considerations

In atom starting point

Ni fluctuates between d\(^9\) and d\(^{10}\)

\[ d^9 d d d d d d d d d d \]

\( d^{10} \) costs \( U \)

Atomic theory minimizes polarity fluctuations
Note the atomic like multiplet structure as for the rare earths.
We will come back to the Photoemission and Zhang Rice singlets later.
Transition metal d-d interactions

• The satellite position gives an estimate of the F0 Slater integral or U. More details below.

• Important is that the multiplet spread is given by only slightly decreased gas phase atomic values i.e. F2 and F4 Slater integrals or J\text{hund} = (1/14)(F2 + F4) is reduced by at most 20% from the atomic values.

• F0 on the other hand is reduced from the atomic >20eV to about 7 eV!!!!!
• Photoemission and inverse photoemission of all the rare earth metals
• Demonstrates the atomic multiplets of the 4f electron removal and addition states
• Intensities given by atomic coefficients of fractional parentage starting from the Hunds’ rule ground state
$U = 12\, \text{eV}$

$\frac{4f^7}{S = \frac{7}{2}}$
MORE ON RARE EARTHS

• The Hubbard U; as clearly demonstrated, its definition depends on which multiplets you take and depends strongly on the element. Convention is to either take the multiplet average or the Slater F0 integral.

• The multiplet splitting is very close to the atomic value little SCREENING OF THE HUNDS RULES INTERACTIONS I.E. SLATER F2,F4,F6 INTERACTIONS
Note the atomic physics needed to describe the rare earth 4f electron removal and addition spectrum.

For the 3d transition metal compounds things are a lot more subtle. In some cases we need the atomic approaches and in others one particle theory seems to work very well.
Simplest model single band Hubbard

Row of H atoms
1s orbitals only

The hole can freely Propagate leading to a width

E gap = 12.9eV-W

Largest coulomb Interaction is on site U

The electron can freely Propagate leading to a width

The actual motion of the Particles will turn out to be more complicated
For large $U \gg W$ and 1 electron per site

- --- Insulator
- Low energy scale physics contains no charge fluctuations
- Spin fluctuations determine the low energy scale properties
- Can we project out the high energy scale?

$$H = \sum_{i,j} J S_i S_j \quad J = 4t^2 / U$$

Heisenberg Spin Hamiltonian
We should be a bit careful about decoupling spin and charge degrees of freedom even in this case.
The charge distribution for the antiparallel and parallel nn spin states are different! For the singlet there is admixture of doubly occupied sites. For triplets there is not!

Has strong consequences!

Temperature dependent Optical conductivity

Tsvetkov et al. PRB 69, 075110 (2004)
Spin order dependent Optical transitions

A 13

A 13
Before we go on let's look at a specific property of the Hubbard model which is measurable for a "doped" MH system.

Seamus Davis the STS asymmetry CT Shen X ray absorption in doped Cuprates.
Spectral weight transfer

The real signature of strong correlation effects

Meinders et al, PRB 48, 3916 (1993)
Doping a Mott – Hubbard system

Meinders et al, PRB 48, 3916 (1993)
These states would be visible in a two particle addition spectral function.
These particles block 2 or more states

Bosons – block 0 states
Fermions – block 1 state

These – block 2 states
The low energy scale

Note the even larger slope for finite hopping integrals
Dynamic spectral weight transfer

Phillip Phillips uses this to define “Mottiness”
Eskes et al. PRL 67, (1991) 1035
Meinders et al. PRB 48, (1993) 3916
What would a mean field theory give you?

SC Hydrogen

\[ a = 2.7 \text{ Å} \]
\[ U = 12\text{eV} \]

Note that there is no spectral weight transfer and a gap closing with doping From half filled . Both opposite to the real situation.
We come back to spectral weight transfer later for the transition metal compounds
Hubbard model is not exactly solvable except in 1 D but even then the spectral functions are difficult to extract

Lieb and Wu  PRL 20, 1445, (1968)
A bit more about simple models and some peculiar properties in 1 and 2 dimensions of the simple models
Don’t know of a rigorous Proof of Hubb---t,J (U>>w)

less than 1/2 filled Hubbard
First U>>t

\[ H = \sum_{ij} \left\{ v_{ij} \hat{c}^+_i \hat{c}_j + \begin{cases} J & \text{if } i \neq j \\ 0 & \text{otherwise} \end{cases} \right\} + H_0 \]

avoids double occ.

goes to Heisenberg for 1/2 filled.
Also this is not solvable
Spin charge separation in 1D

Antiphase Domain wall

Now the charge is free to move
Magnons and spinons in 1D

Spinons propagate via $J S_i^+ S_{-1}^{-1}$

Magnon $S=1$

Two spinons
Inelastic Neutron scattering

Figure 2.14: Neut continuum in 1D.
Quantum Spin Excitations in the Spin-Peierls System CuGeO₃

M. Aral, M. Fujita, M. Motokawa, J. Akimitsu, and S. M. Bennington

Fig. (color). A color contour map of the dynamical structure factor at 10 K (b) and 50 K (b).

Fig. (color). The dynamical structure factor at 300 K. The spin excitations persist, but with the minima reduced from 11 to 7 eV. The lower boundary has changed completely.

T = 300 K

T = 10 K

T = 50 K
in 2D things are much less clear!!

fig. 5

Self Confinement?
Similar is some sense to the 1D case it is proposed that one has 2D rivers of charge separating anti-phase domain walls. Charges can now fluctuate from left to right without costing $J$. 

Anisimov, Zaanen, Andersen, Kivelson, Emery-----
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