Emergence of Quantum Phases in Novel Materials

VIII Edition ICMM School

Mott Physics

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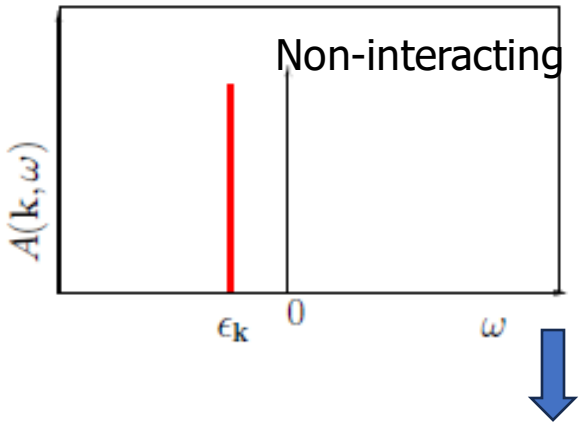
Mott physics: Some references

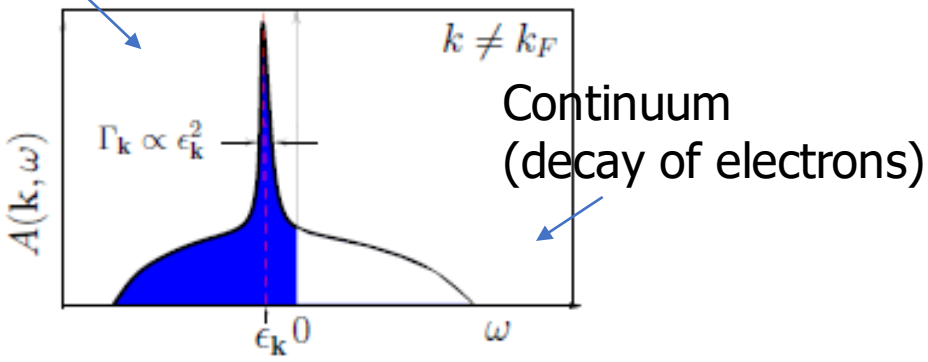
- Lecture notes on Electron Correlations and Magnetism, Patrik Fazekas, World Scientific Publishing Company
- A. Georges et al, Review Modern Physics 68, 13 (1996)
- A. Georges, arXiv:0403123

Fermi liquid description of electronic correlations in solids

$$c^{\dagger}_{\mathbf{k}\sigma} = \sqrt{Z_{\mathbf{k}}}\, a^{\dagger}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}_4+\mathbf{k}_3=\mathbf{k}_2+\mathbf{k}} A(\mathbf{k}_4\sigma_4, \mathbf{k}_3\sigma_3; \mathbf{k}_2\sigma_2, \mathbf{k}\sigma)\, a^{\dagger}_{\mathbf{k}_4\sigma_4} a^{\dagger}_{\mathbf{k}_3\sigma_3} a_{\mathbf{k}_2\sigma_2} + \ldots$$



Quasiparticle peak
(width decay of quasiparticle)



Continuum
(decay of electrons)

Fermi liquid behavior at low temperaturas
(renormalized parameters)

$C_v = \gamma^* T$ $\qquad$ $\chi_s = \mu_B^2 N^*(\varepsilon_F)$

$\rho = \rho_0 + AT^2$ $\qquad$ $A \propto (m^*)^2$

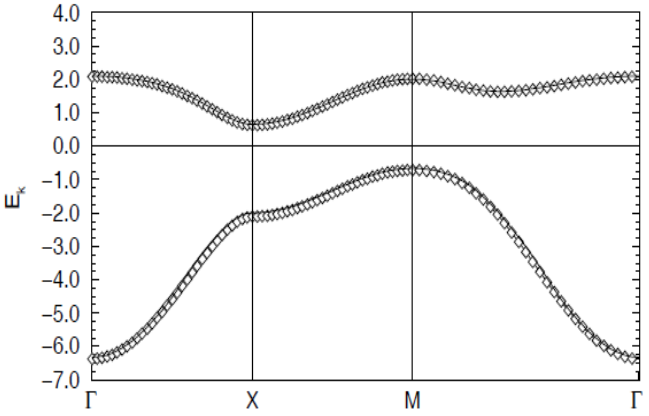
Quasiparticle bandstructure E*(k)

& more

Ref: Coleman's book

Metals and insulators

Assume a material with spin degeneracy:
Each band can hold 2 electrons per unit cell



Even number of electrons per unit cell → Insulating

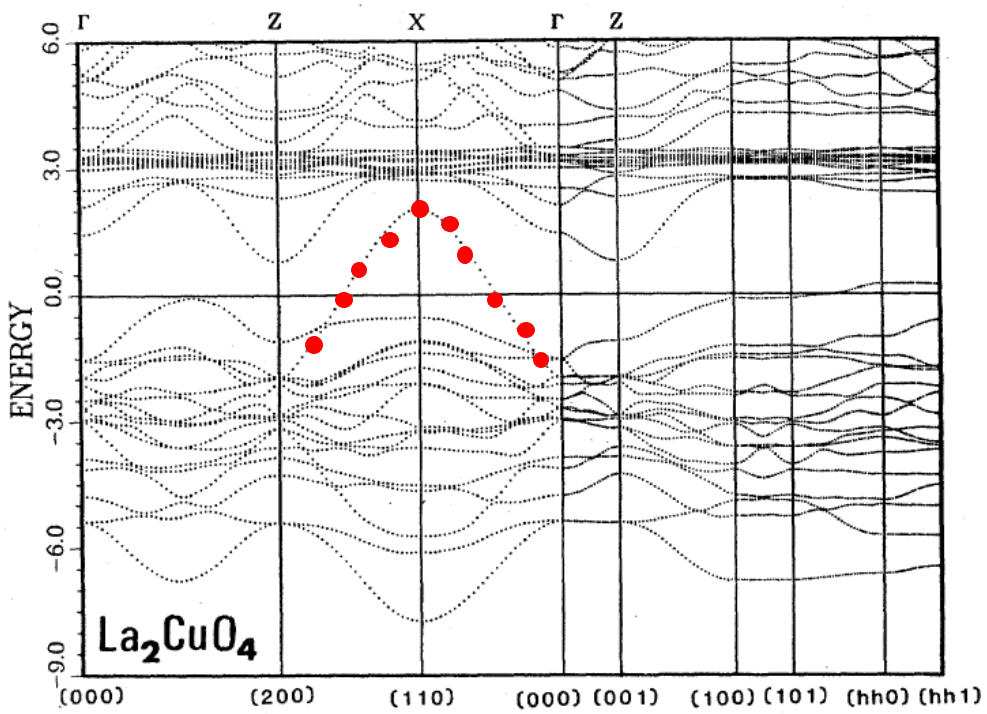
Even number of electrons per unit cell → Metallic (in case of band overlap)

The renormalization of the energies (mass enhancement) due to interactions could in principle modify the metallic or insulating character of a system with even number of electrons per unit cell

Odd number of electrons per unit cell → Metallic

Remains valid in Fermi liquid

Insulating state due to electronic correlations



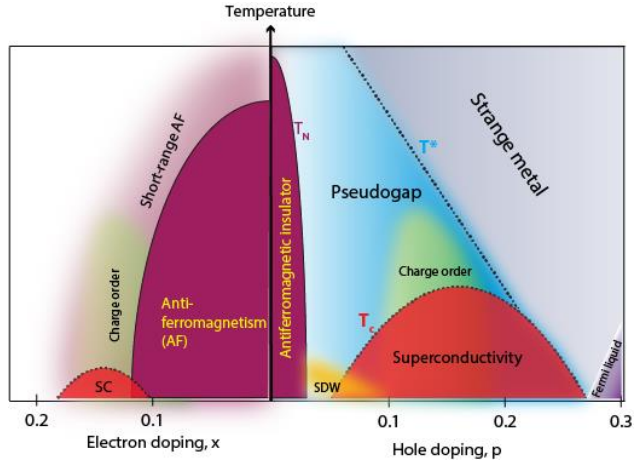
Metallic behavior expected

Fig: Pickett, RMP 61, 433 (1989)

Insulating behavior is found

Breakdown of independent electron picture

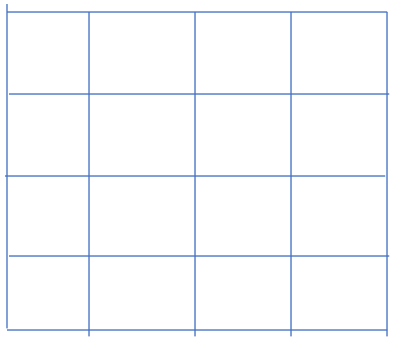
Cuprate

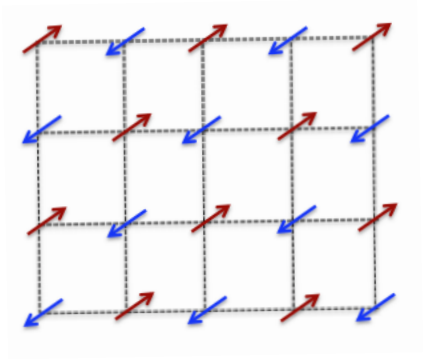


Slater insulators

Start from a spin degenerate metallic system with odd number of electrons per unit cell

Consider the case in which interactions induce an antiferromagnetic state and due to the antiferromagnetic order the system becomes insulating





(this may happen in 2D, 3D, …)

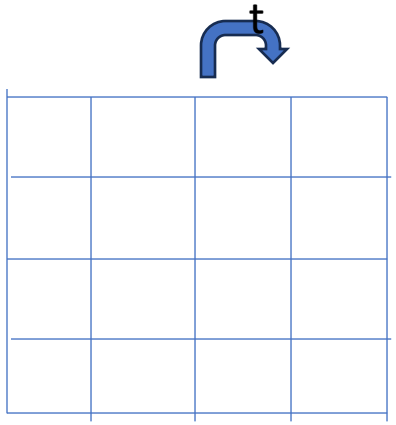
Symmetry Breaking

Satisfies the rule: insulating state due to even number of electrons in the unit cell (unit cell has been enlarged)

Slater insulator: Insulating state due to Antiferromagnetic Ordering

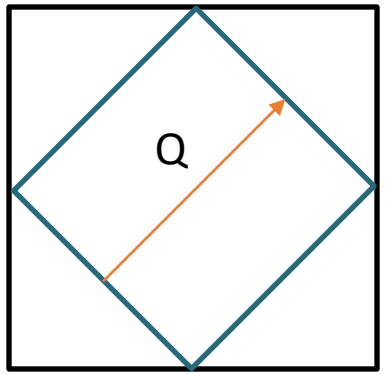
Slater insulators

Example:



Square lattice
with hopping
restricted to
1st nearest neighbors

Fermi surface
of the non-interacting
system at half-filling

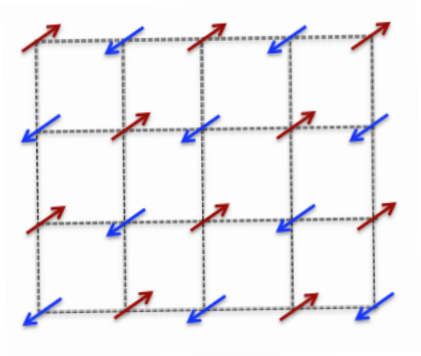


Perfect nesting

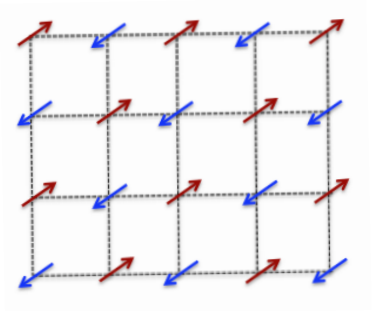
Ordering tendencies

Half-filling and hopping only to next nearest neighbors are required in this example to have this specific Fermi Surface (some deviations can be accepted)

Even at small U: AF ordering



Antiferromagnetic insulators: From Slater to Mott



Not all antiferromagnetic insulators are Slater insulators

Small U:

T

Metal

T_{Neel} Neel Temperature (Temperature at which the AF disppears)

Antiferromagnet & Insulating

Slater Insulator

Large U:

Insulating behavior not due to AF

T

Insulator (no broken symmetry) in spite of odd # of electrons/unit cell

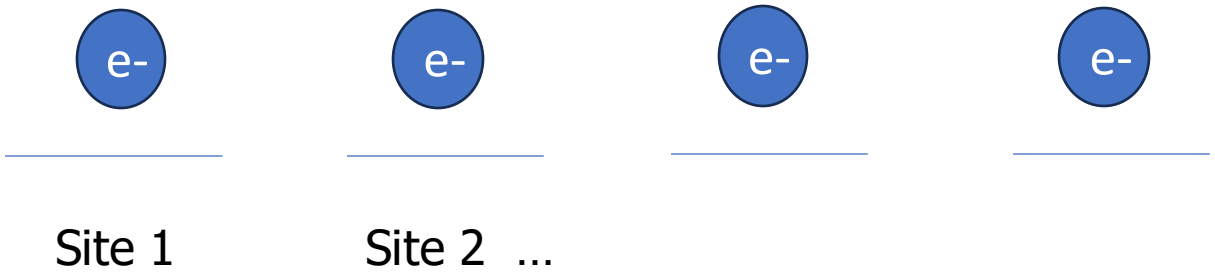
T_{Neel} Neel Temperature

Antiferromagnet & Insulating

Mott Insulator

Sometimes not so trivial (who is in the driver seat)

Mott insulators and local moments

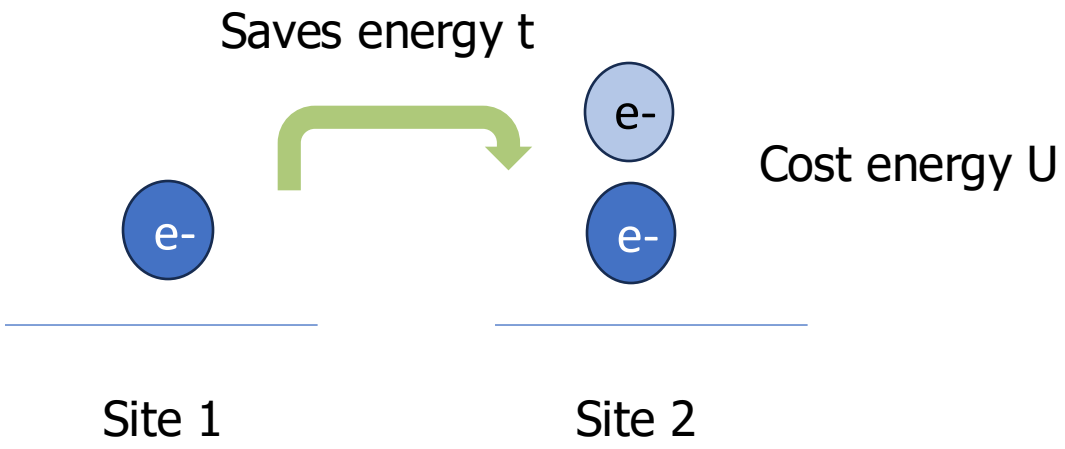


Hubbard model
(single orbital)

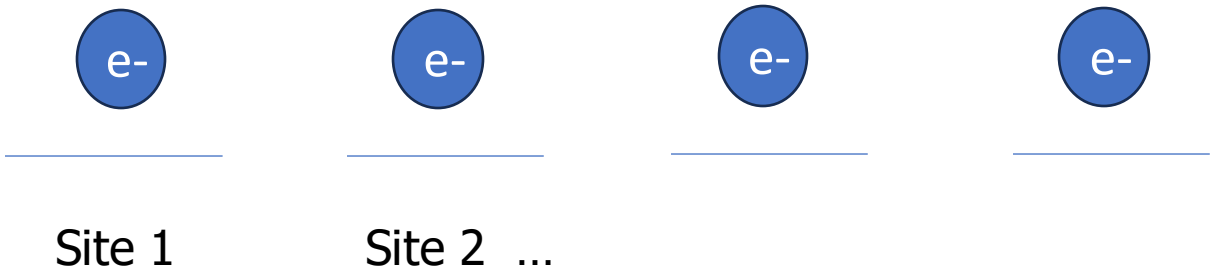
- Onsite repulsión U
- Hopping energy t

1 electron per site/atom

Hopping process:



Mott insulators and local moments



Hubbard model
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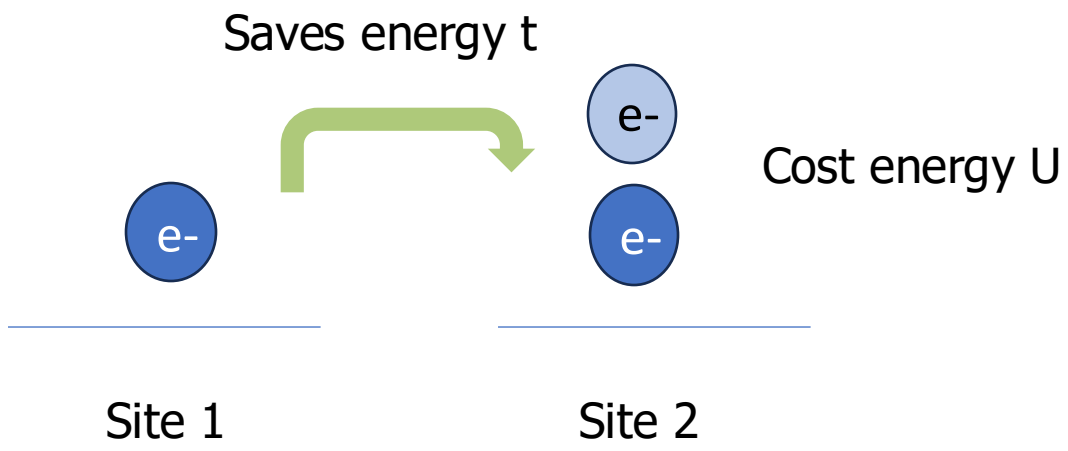
Hopping process:



U>>t Metal insulator transition due to localization of electrons

Mott transition @U_c

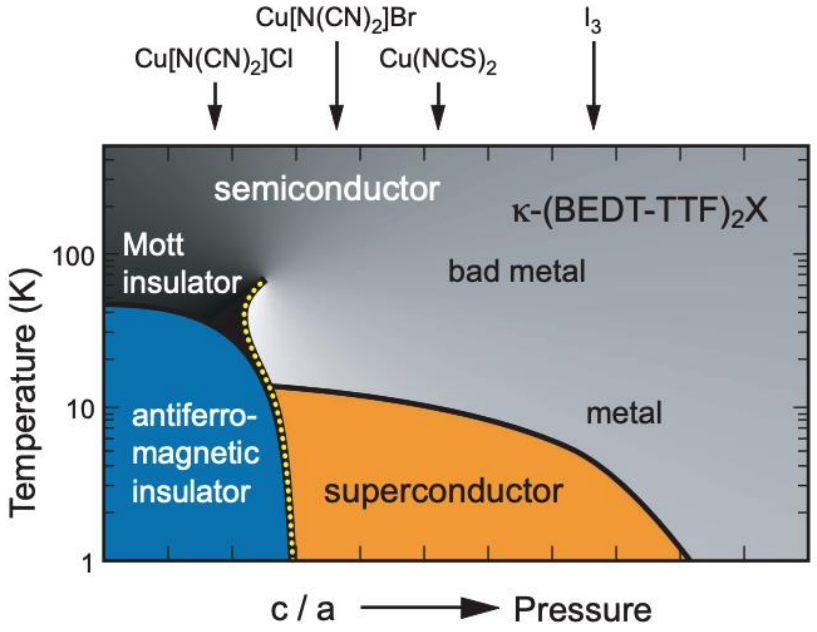
No symmetry breaking required for insulating behavior (including magnetic transition)

Suppression of charge fluctuations & Formation of local moments

Mott insulators and local moments

Hubbard model
- Onsite repulsión U
- Hopping energy t

1 electron per site/atom



U>>t Metal insulator transition due to localization of electrons

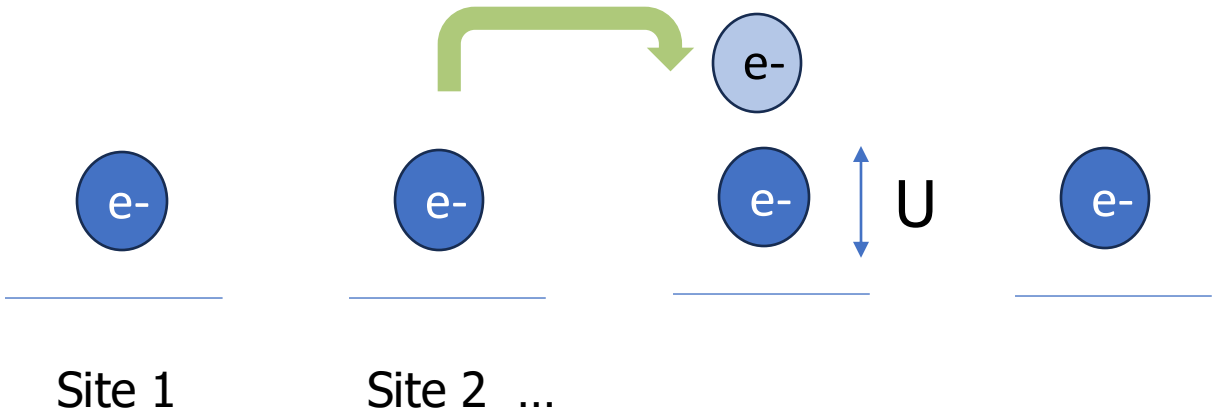
Mott transition @U_c

No symmetry breaking required for insulating behavior (including magnetic transition)

Suppression of charge fluctuations & Formation of local moments

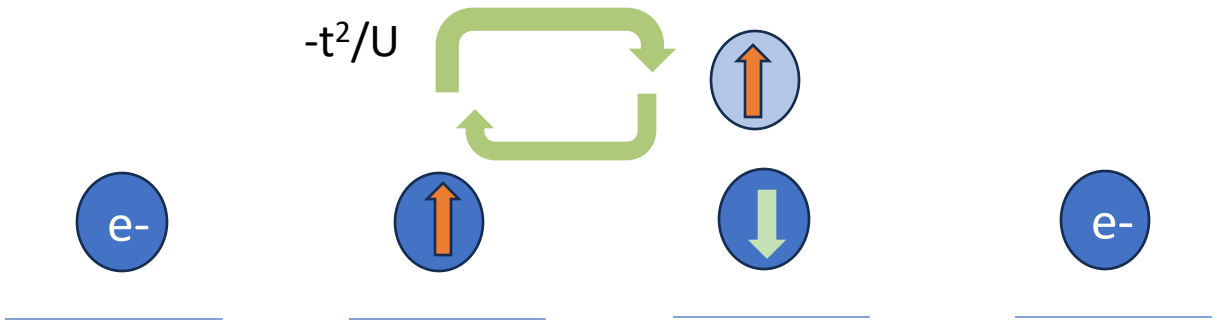
Antiferromagnetic tendencies of some Mott insulators

Hubbard U Single Orbital
Hopping to 1st nearest neighbors
Half-filling



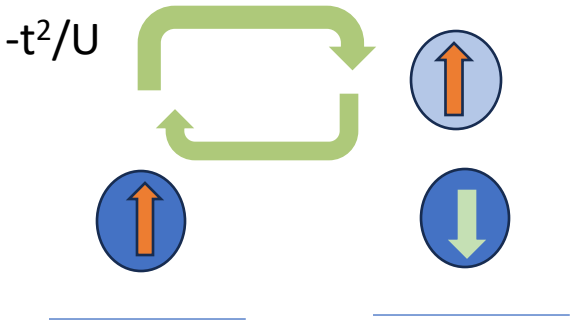
Mott insulator

Real hopping processes cost interaction energy U and are forbidden



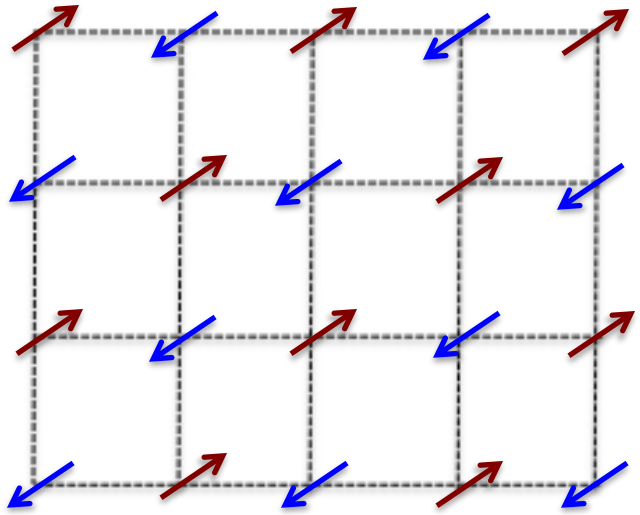
Virtual hopping processes save kinetic energy $-t^2/U$ but they are only allowed if nearest neighbors have antiparallel spins

Antiferromagnetic tendencies and lattice

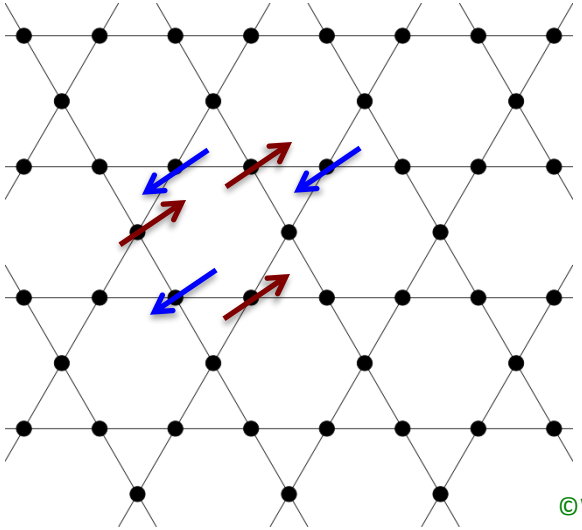


Even when the Mott insulator presents antiferomagnetic tendencies, whether it orders or not depends on the specific system

Bipartite lattice



Frustrated lattice



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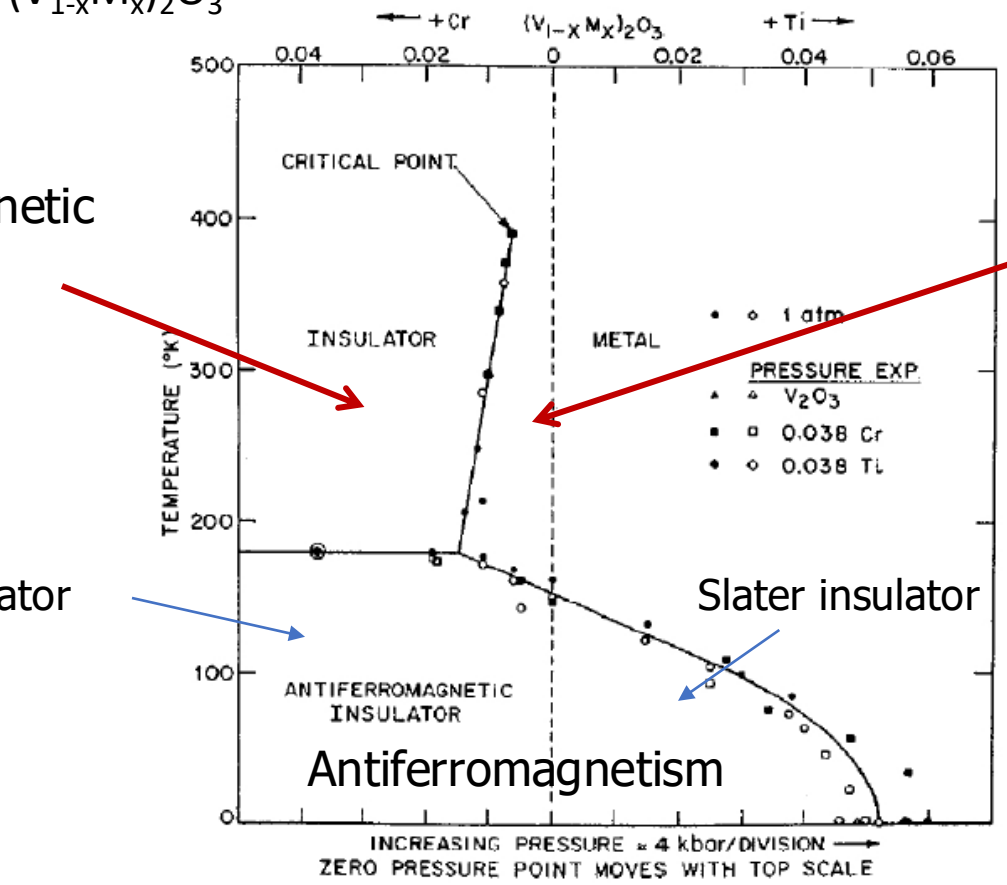
Mott insulators and local moments

Vanadium Oxide
(chemical pressure)

$(V_{1-x}M_x)_2O_3$



Paramagnetic
Mott
Insulator

Metal-Insulator
transition with
decreasing pressure

Mott insulator

Slater insulator

Antiferromagnetism

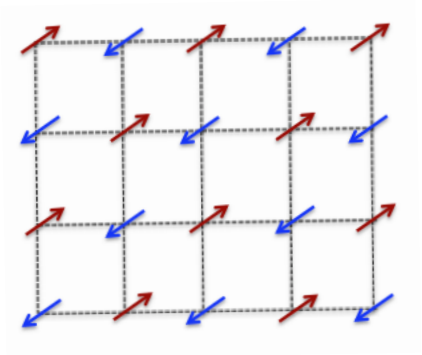
Increasing Pressure: decreasing U/W

From Slater to Mott

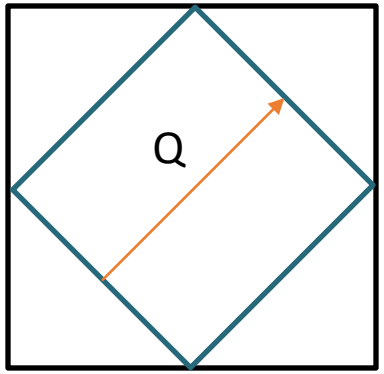
McWhan et al, PRB 7, 1920 (1973)

Antiferromagnetic tendencies

Hubbard U Single Orbital
Hopping to 1st nearest neighbors
Half-filling



Small U



Perfect nesting

↓

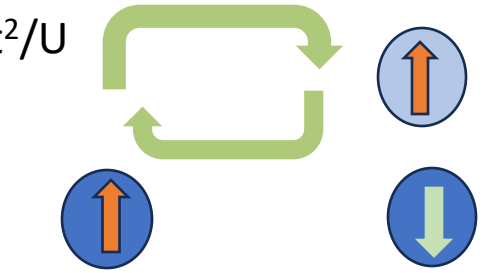
Ordering tendencies increase with incresing interaction

Antiferromagnetism (interaction driven)

T_{Neel}, ↑ U ↑

Large U

$-t^2/U$



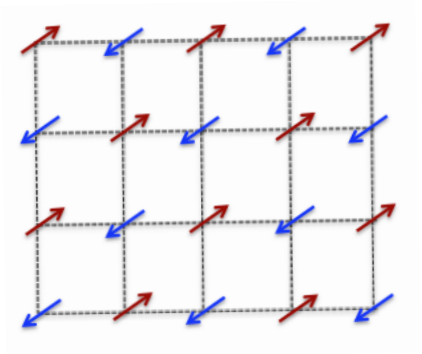
Antiferromagnetism (kinetically driven)

Ordering tendencias decrease with incresing interaction

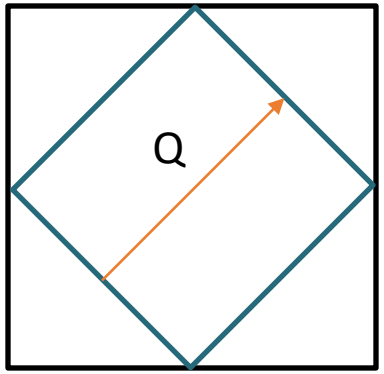
T_{Neel} ↓ U ↑

Antiferromagnetic tendencies

Hubbard U Single Orbital
Hopping to 1st nearest neighbors
Half-filling



Small U

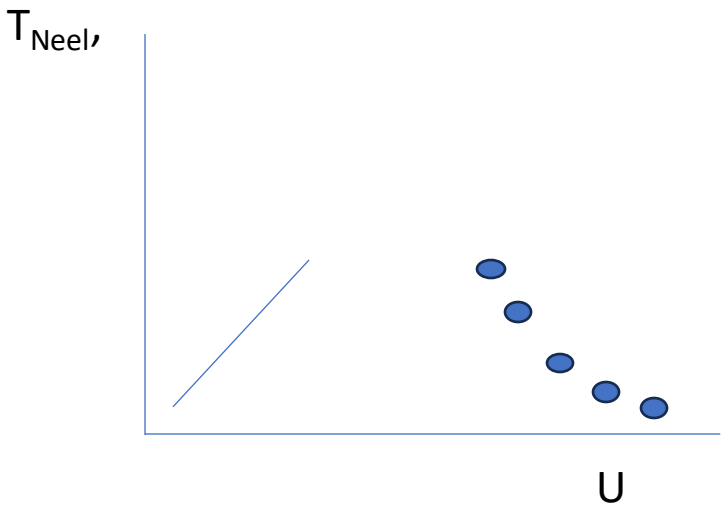


Antiferromagnetism
(interaction driven)

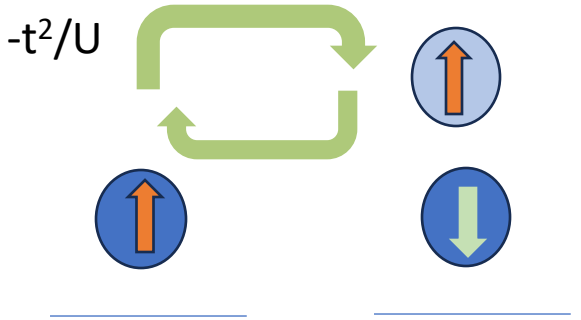
Perfect nesting

Ordering tendencies
increase with incresing
interaction

T_{Neel}, ↑ U ↑



Large U



Antiferromagnetism (kinetically driven)

Ordering tendencias decrease with
incresing interaction

T_{Neel} ↓ U ↑

Antiferromagnetic tendencies

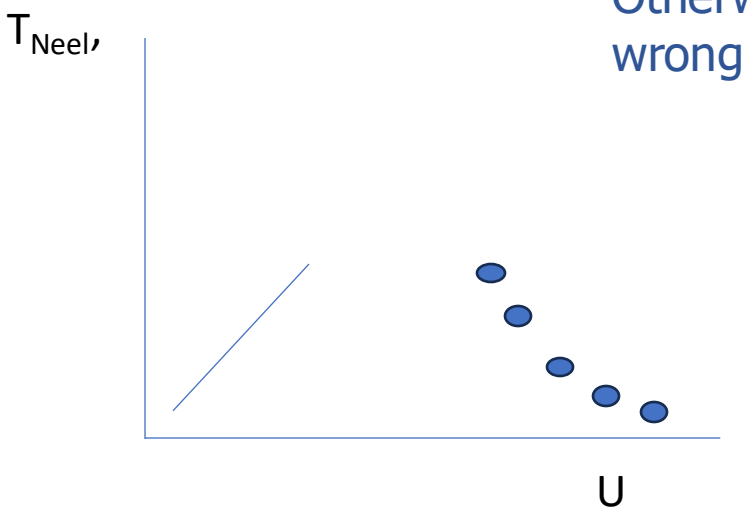
Small U

Antiferromagnetism
(interaction driven)

Large U

Antiferromagnetism (kinetic driven)

Importance of which type of approximation we do (starting from itinerant or localized electrons)
Otherwise we may get the dependences wrong



Slater insulators, Mott insulators and Antiferromagnetic tendencies

- Slater Insulator: Insulating state due to antiferromagnetic ordering. Break symmetry

- Mott Insulator:

  Insulating state due to localization of the charge (local interaction). No broken symmetry required (for Mott-Hubbard)

  Frequently (not always) it promotes (kinetically driven) antiferromagnetic tendencies t^2/U .
  It may order or not

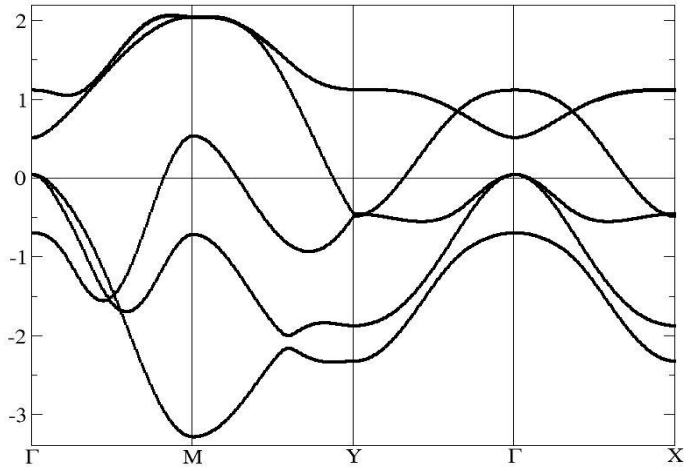
  When the Mott insulator orders at low temperatures, the insulating behavior remains even if the ordering disappears with increasing temperature

Itinerant versus localized electrons

Small U

Metal:

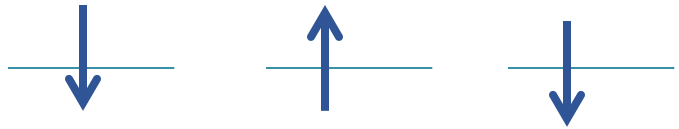
Electrons delocalized in real space, localized in k-space.
Description in terms of electronic bands



Large U/W

Mott Insulator

Description as localized spins is meaningful . Electrons localized in real space, delocalized in k-space. Spin models.



Hubbard U
Single Orbital
Half-filling

The correlated metal

Small U/W

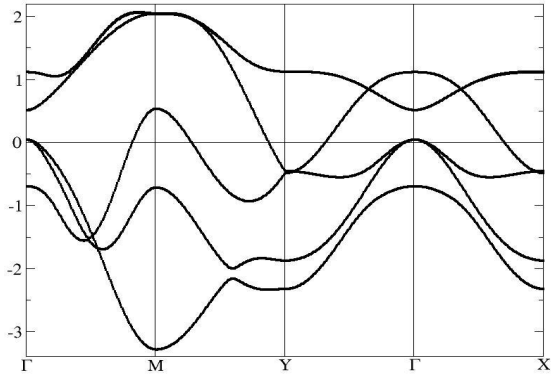
Metal

Increasing U/W
Mott transition

Large U/W

Mott Insulator

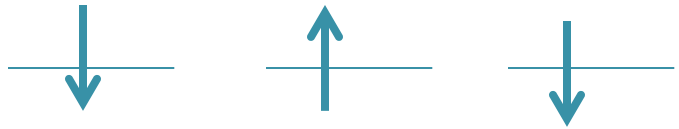
Description in terms of electronic bands.
Electrons delocalized in real space, localized in k-space.



Fermi surface physics

?

Description as localized spins is meaningful . Electrons localized in real space, delocalized in k-space. Spin models.



How do we describe the metal at $U < U_{Mott}$?
How do we describe its instabilities?

Correlated metal

Hubbard U
Single Orbital
Half-filling

The correlated metal and the Mott transition

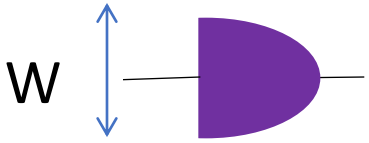
Small U/W

Metal

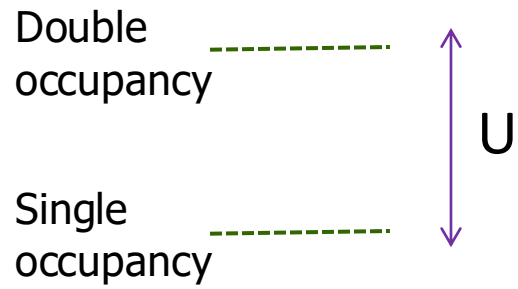
Large U/W

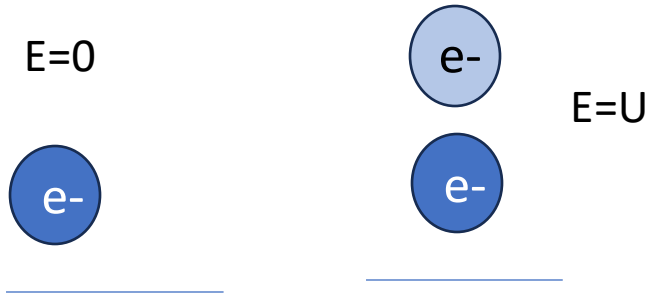
Atomic limit

Density of states
electronic bands



How does it happen the Mott transition between these two limits?





Hubbard U
Single Orbital
Half-filling

The correlated metal and the Mott transition

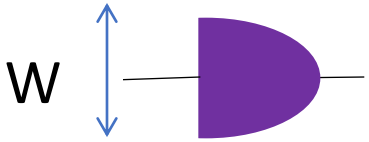
Small U/W

Metal

Large U/W

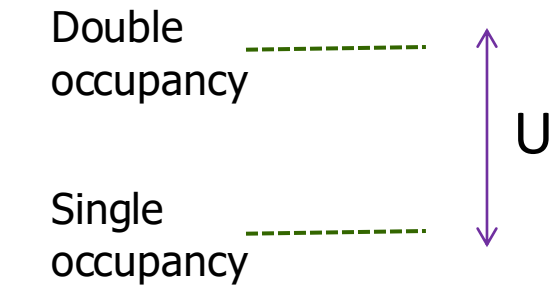
Atomic limit

Density of states
electronic bands

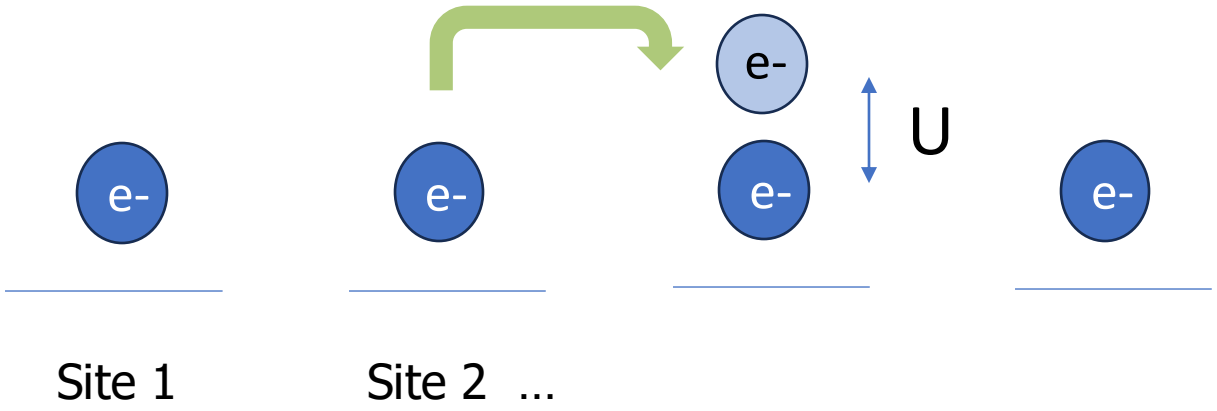


How does it happen the Mott transition between these two limits?

Approaching the Mott transition
from both sides (metallic and insulating)



Electronic correlations in the metallic state



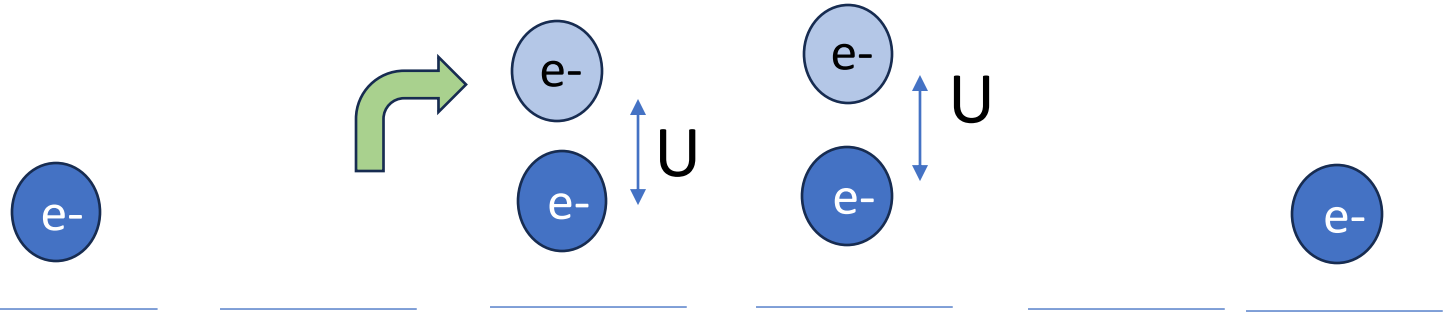
Hubbard model
- Onsite repulsión U
- Hopping energy t

Single orbital & 1 electron per site

with $U < U_{Mott}$

Hopping to an occupied site costs energy U but if $U < U_{Mott}$ it is not completely forbidden

Electronic correlations in the metallic state



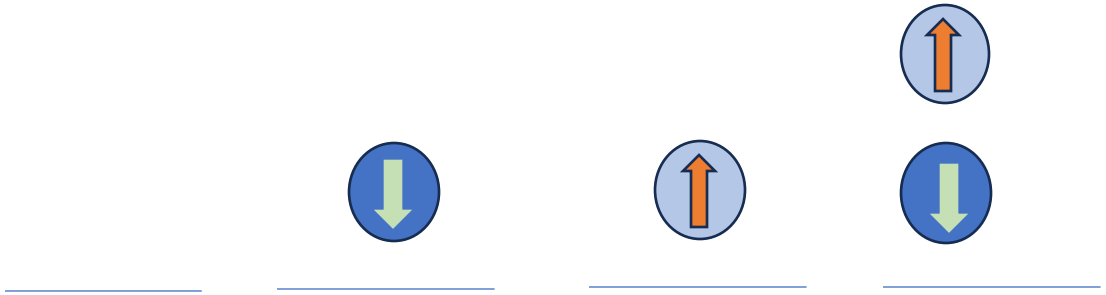
Hubbard model
- Onsite repulsión U
- Hopping energy t

Single orbital & 1 electron per site

with $U < U_{Mott}$

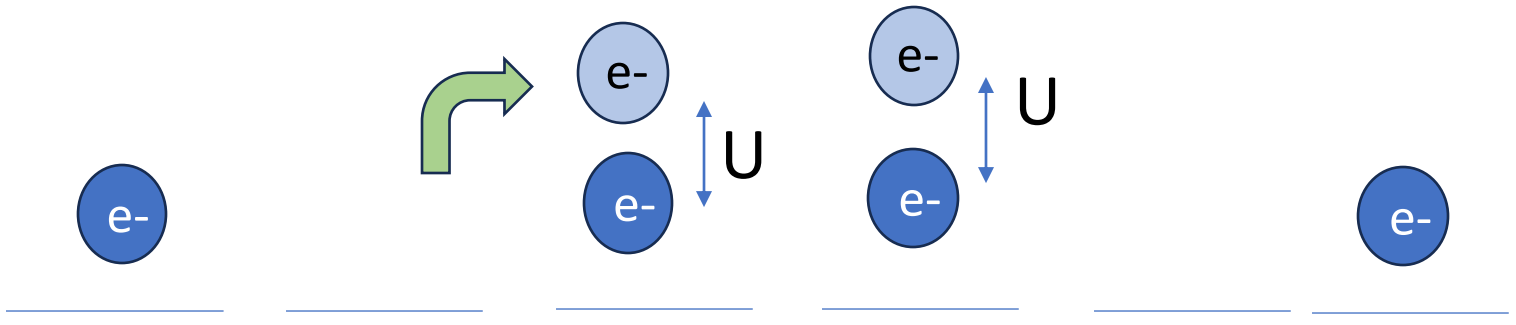
Free movement & occupancies: Many double occupancies
Gain kinetic energy but cost in interaction energy

The uncorrelated metallic state: The Fermi sea |FS>



The four states with
equal probability 1/4

Electronic correlations in the metallic state



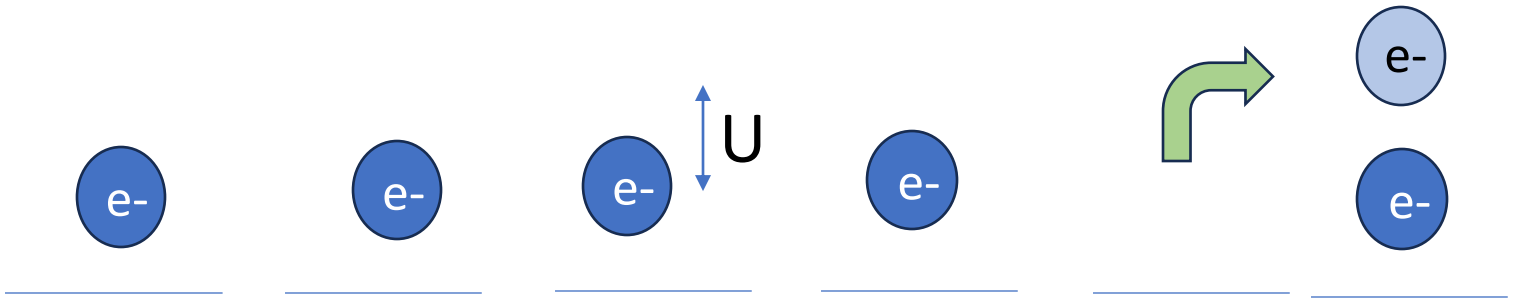
Hubbard model
- Onsite repulsión U
- Hopping energy t

Single orbital & 1 electron per site

with $U < U_{Mott}$

Free movement & occupancies: Many double occupancies
Gain kinetic energy but cost in interaction energy

Few double occupancies but still allowing transport
the cost in interaction energy is reduced but still some gain kinetic energy



Metal at $U < U_{Mott}$

Correlated metal

Reduced number of double occupancies

Electronic correlations in the metallic state

The uncorrelated metallic state: The Fermi sea $|FS\rangle$

Energy states are filled according to their kinetic energy. States are well defined in k-space

(Doubly occupied sites are not suppressed)

A metallic correlated state: The Fermi sea $|FS\rangle$

$$|\Psi\rangle=\Pi_j[1-(1-\eta)n_{j\uparrow}n_{j\downarrow}]|FS\rangle$$

Gutzwiller wave function

Suppression of double occupancy

η variational parameter

See Fazekas' book

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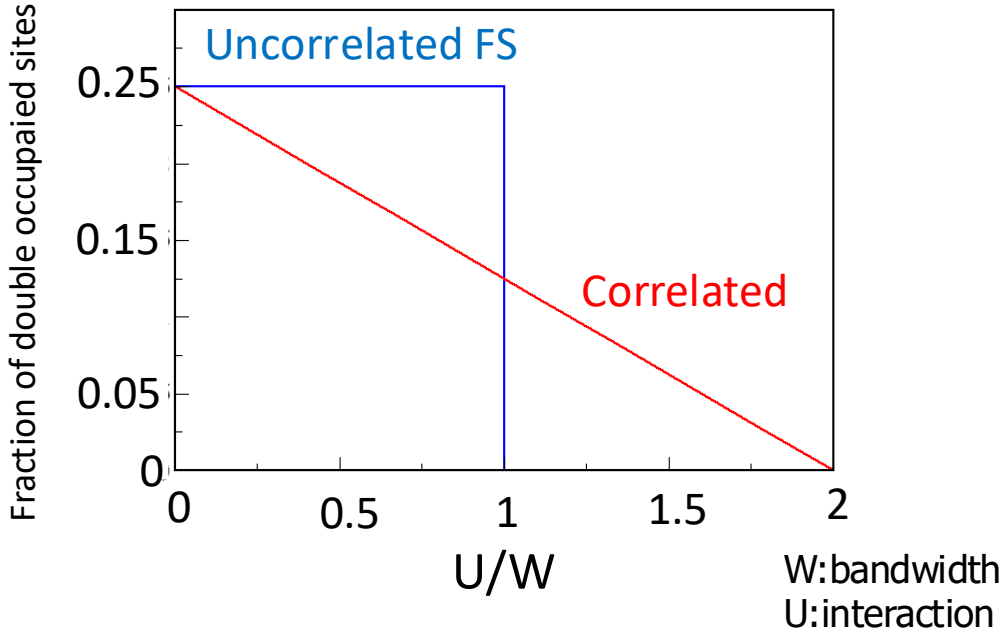

η Static Mean Field. Gutzwiller Approximation.

(calculation for Hubbard model, half-filling constant DOS)

See Fazekas' book

Correlated metal: Gutzwiller approximation

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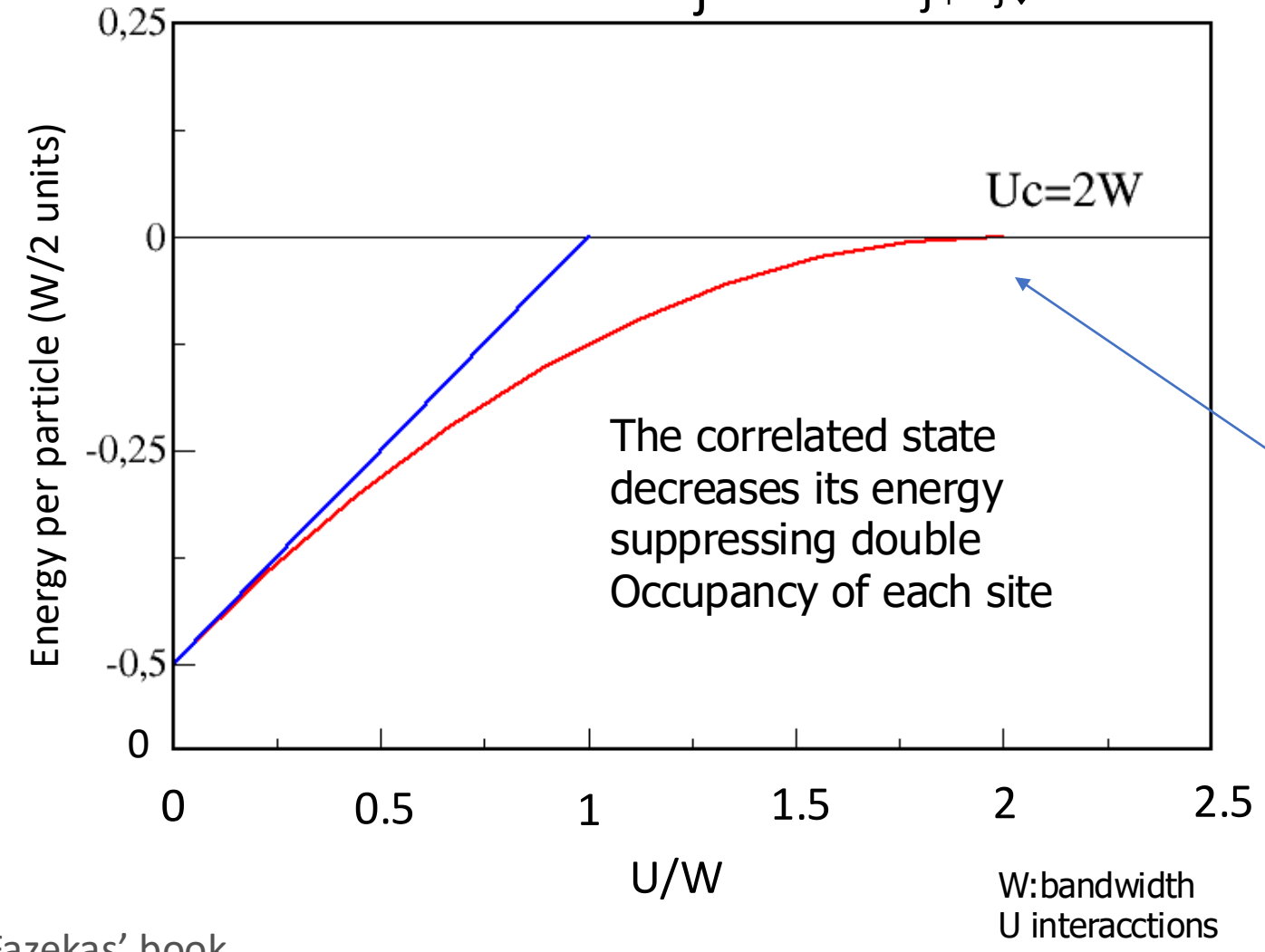
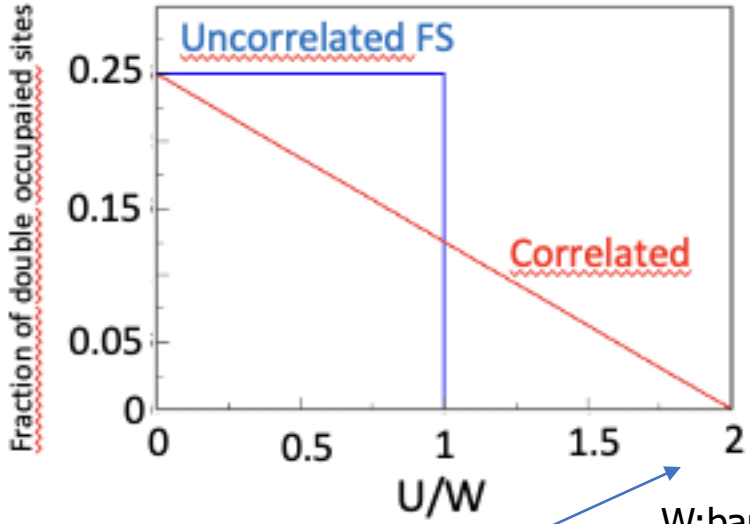


W:bandwidth
U interacctions



W:bandwidth
U:interactions

Mott transition

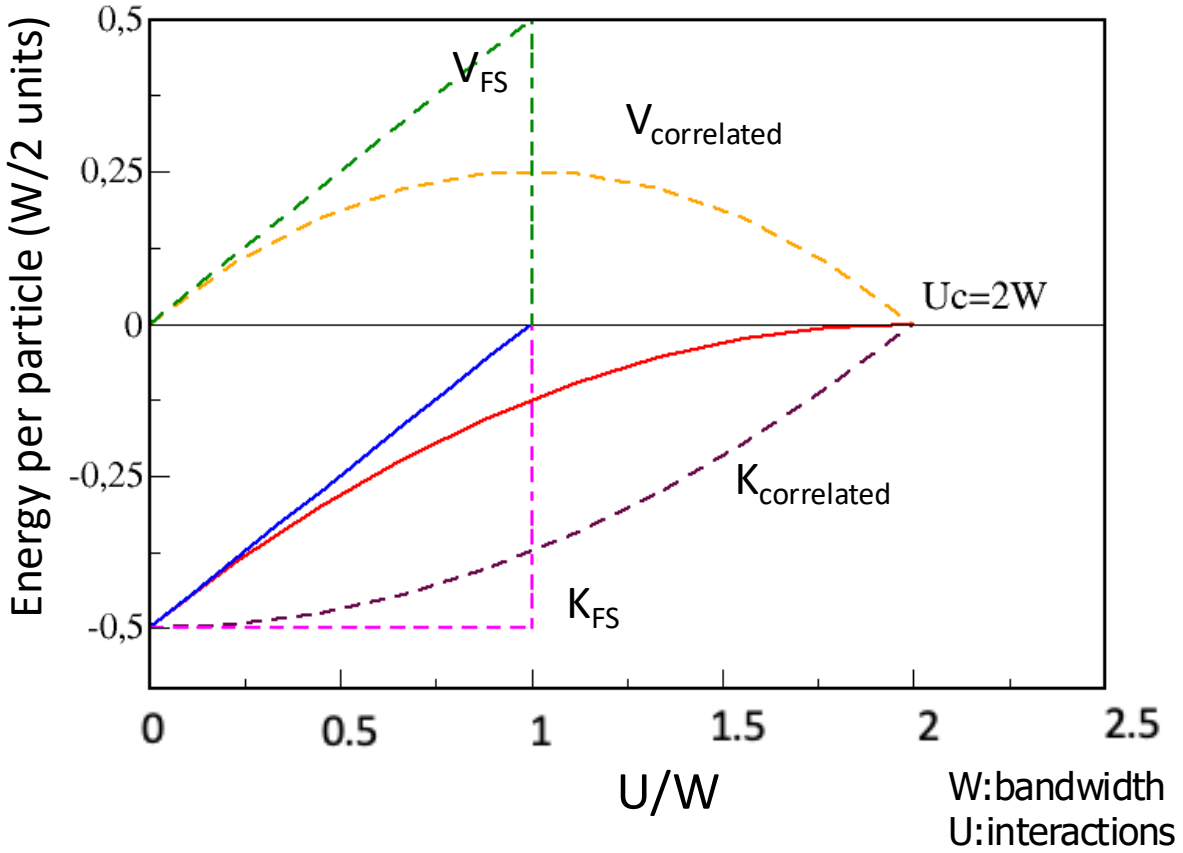
Reducing the number of double occupied sites moves the Mott transition to larger U

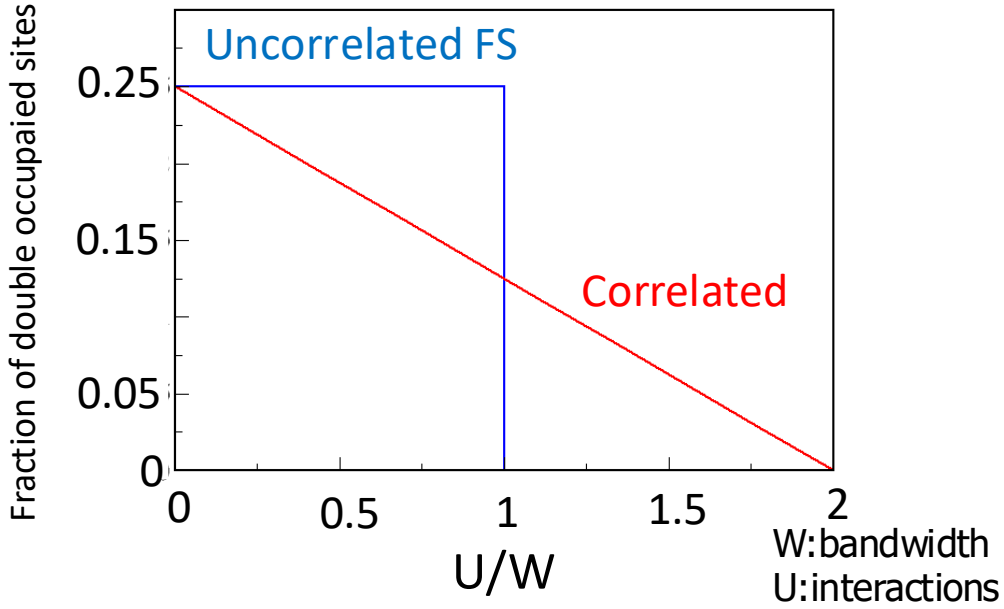
See Fazekas' book

η Static Mean Field. Gutzwiller Approximation.
(calculation for Hubbard model, half-filling constant DOS)

Correlated metal: Gutzwiller approximation

$$|\Psi\rangle = \Pi_j [1-(1-\eta) n_{j\uparrow} n_{j\downarrow}] |FS\rangle$$

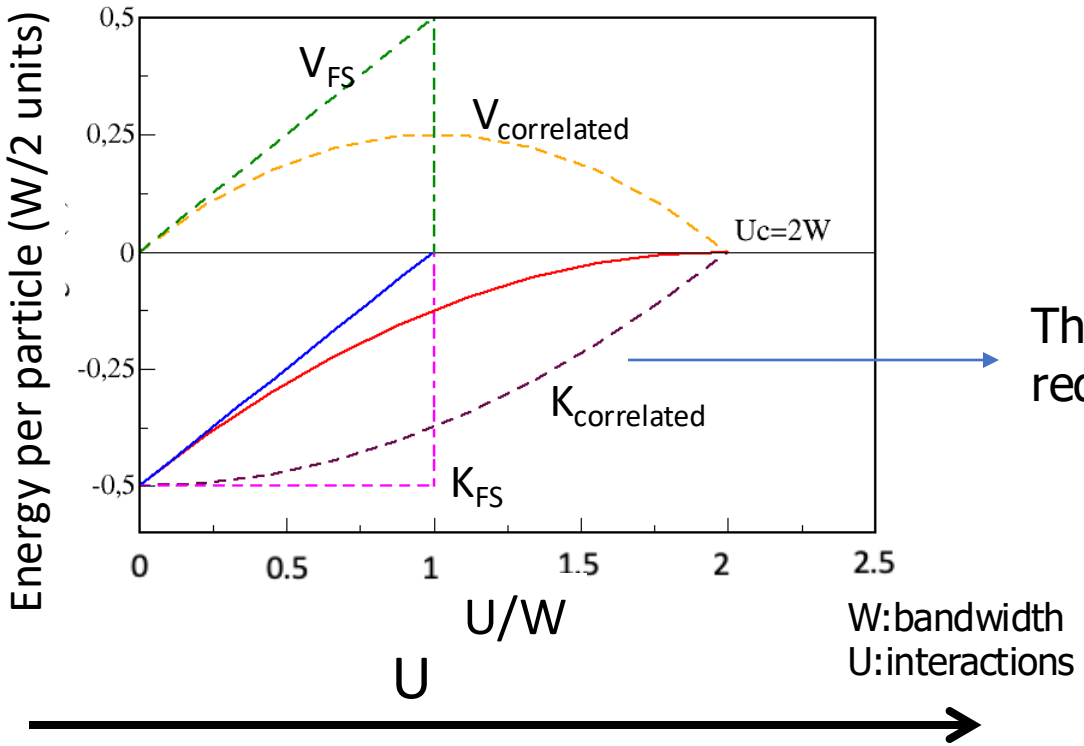




See Fazekas' book

η Static Mean Field. Gutzwiller Approximation.
(calculation for Hubbard model, half-filling constant DOS)

Correlated metal and the Brinkman-Rice transition



W:bandwidth
U:interactions

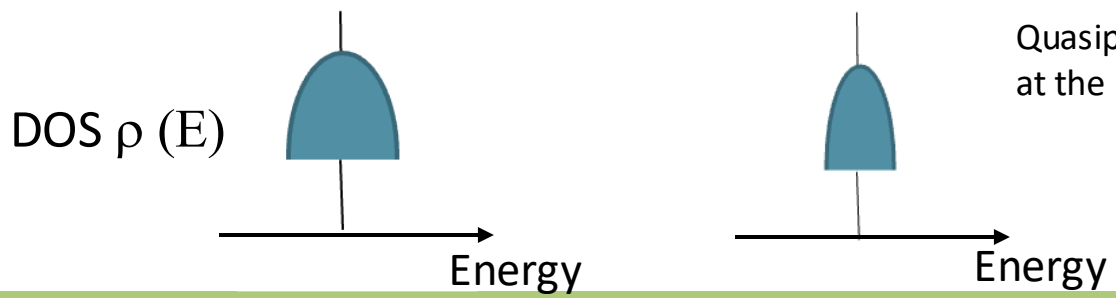
The presence of correlations reduces the kinetic energy

Correlations produce band narrowing

$W^*/W < 1$

W

Narrower quasiparticle band
W* (reduced Kinetic Energy)



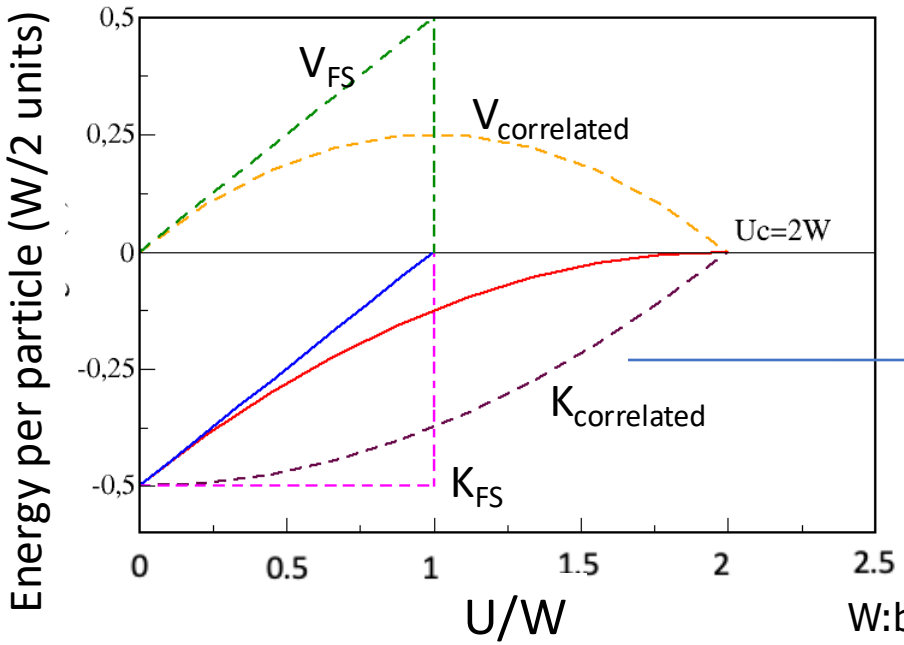
Quasiparticle peak at the Fermi level

Enhanced mass of the quasiparticle
(smaller quasiparticle weight)

$$m^* = \frac{m}{Z}$$

Quasiparticle weight

Correlated metal and the Brinkman-Rice transition



The presence of correlations reduces the kinetic energy

Correlations produce band narrowing

$W^*/W < 1$

W:bandwidth
U:interactions

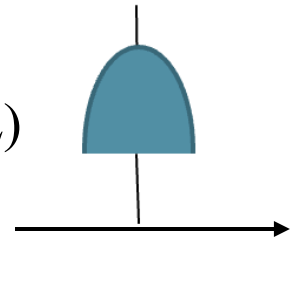
U

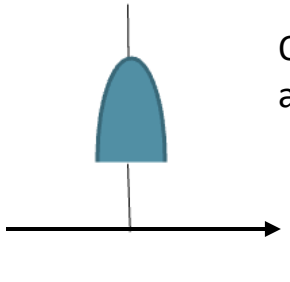
W

Narrower quasiparticle band
W* (reduced Kinetic Energy)

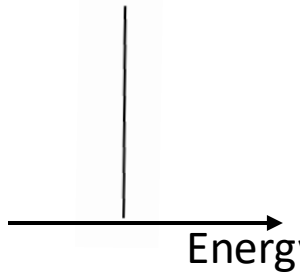
Quasiparticle disappears at the Mott transition with a zero v_F (infinite mass)

DOS ρ (E)





Quasiparticle peak at the Fermi level



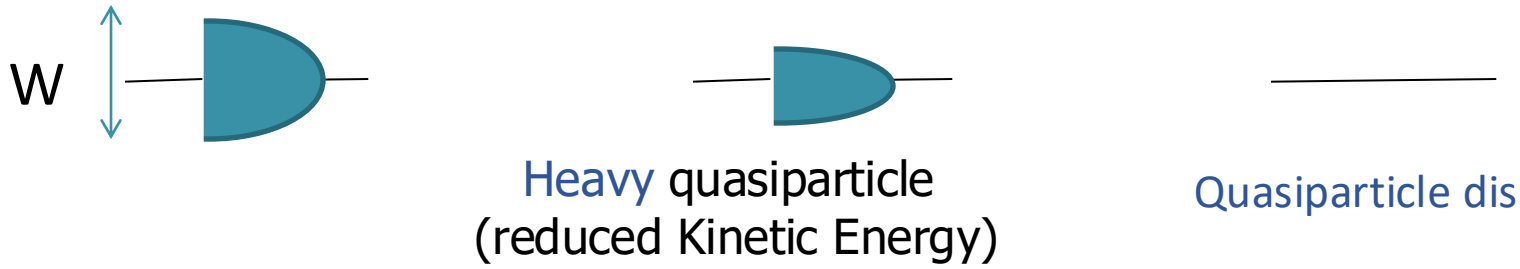
Brinkman-Rice description of the Mott transition (Fermi liquid approach)

Correlated metal and the Brinkman-Rice transition

Increasing U

W: Bandwdith

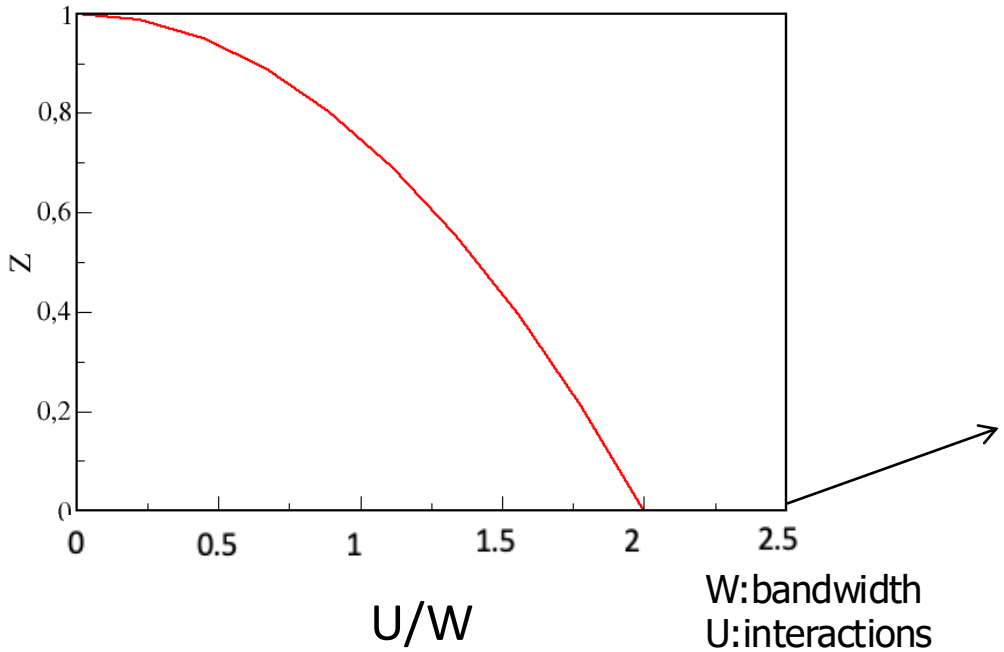
DOS ρ (E)



Heavy quasiparticle
(reduced Kinetic Energy)

Quasiparticle disappears

Quasiparticle weight



W:bandwidth
U:interactions

Reduced quasiparticle weight

$Z^{-1}=m^*/m$

Quasiparticle disappears
at the Mott transition
(mass diverges)

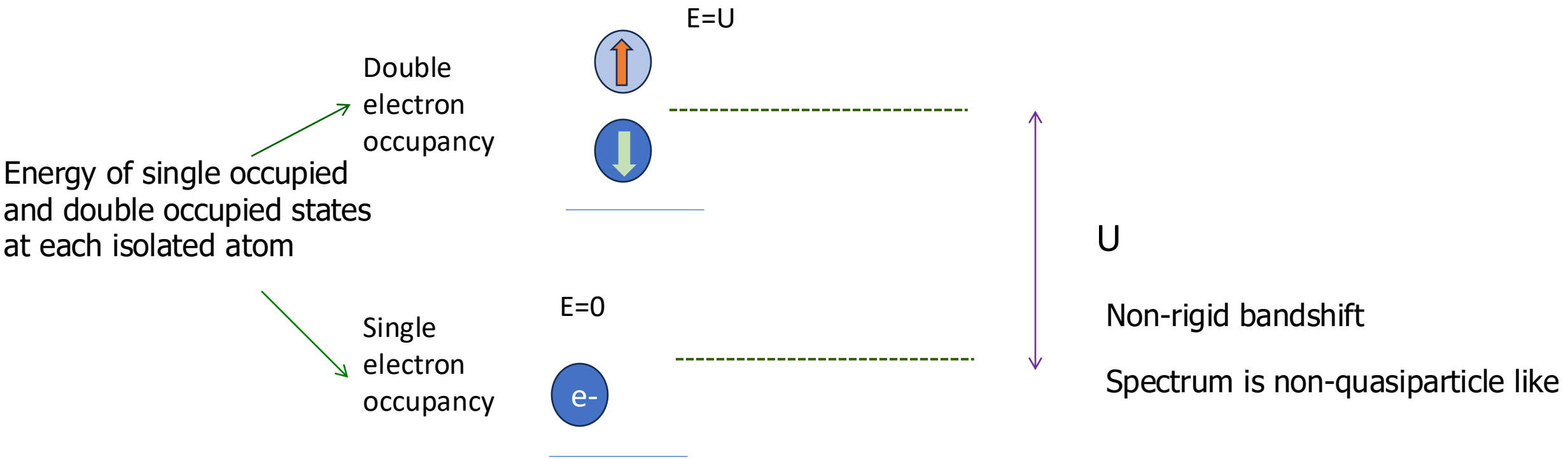
Atomic limit (no kinetic energy)

Single orbital Hubbard model
- Onsite repulsión U
- Hopping energy t

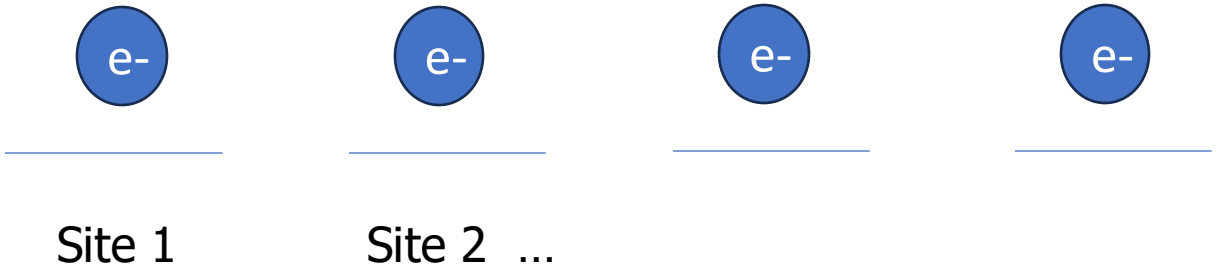
1 electron per site/atom

U>>t Start from t=0

Site 1 Site 2 …



Atomic limit (no kinetic energy)



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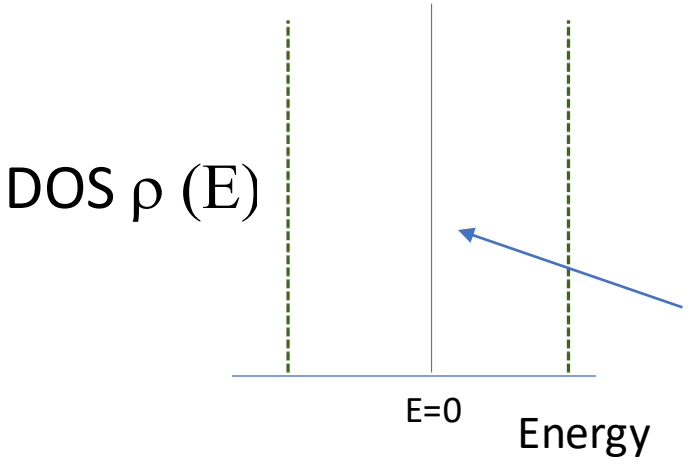
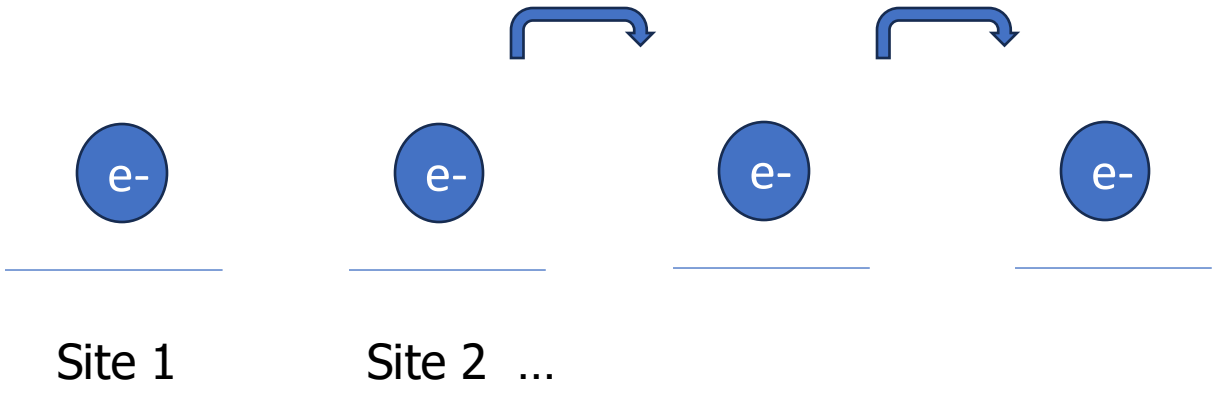


Chemical potential at E=0

Half-filling

Spectrum splitted in two peaks (Hubbard bands)

Mott insulator but with dispersion (finite t)



Single orbital Hubbard model
- Onsite repulsión U
- Hopping energy t

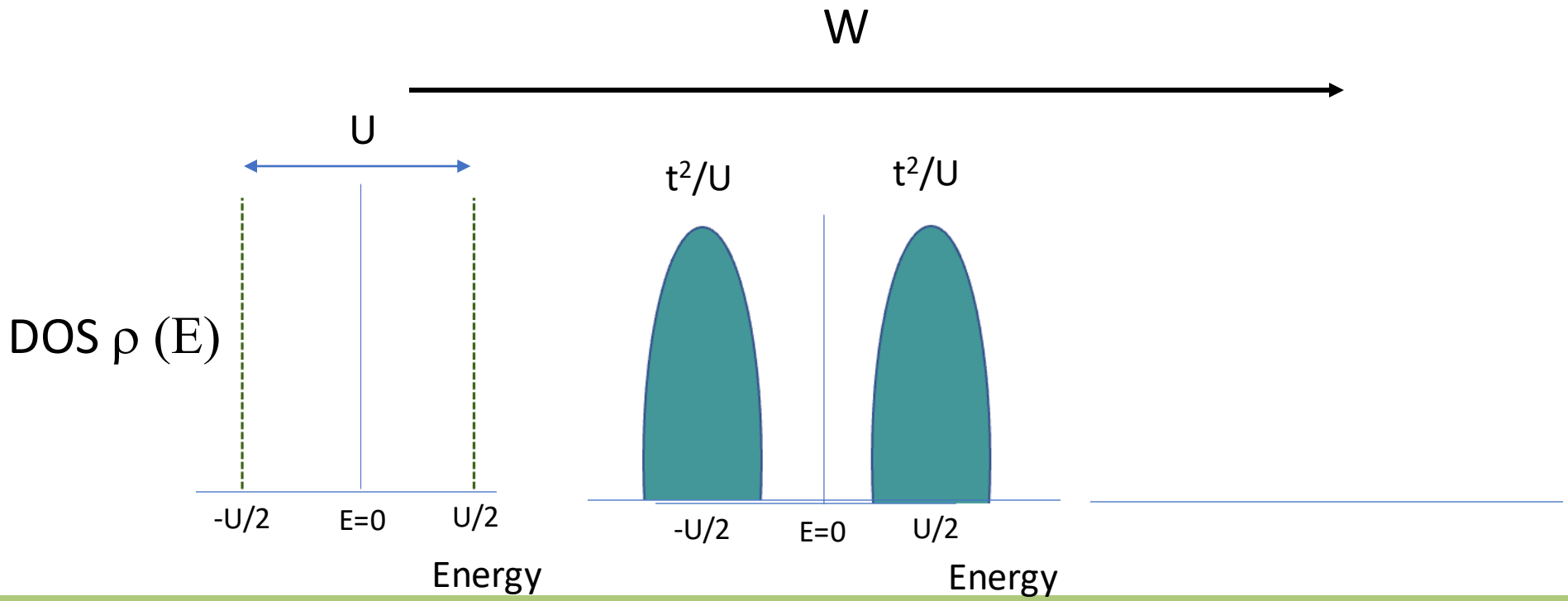
1 electron per site/atom

U>>t Start from t=0

Increasing the kinetic energy

↓

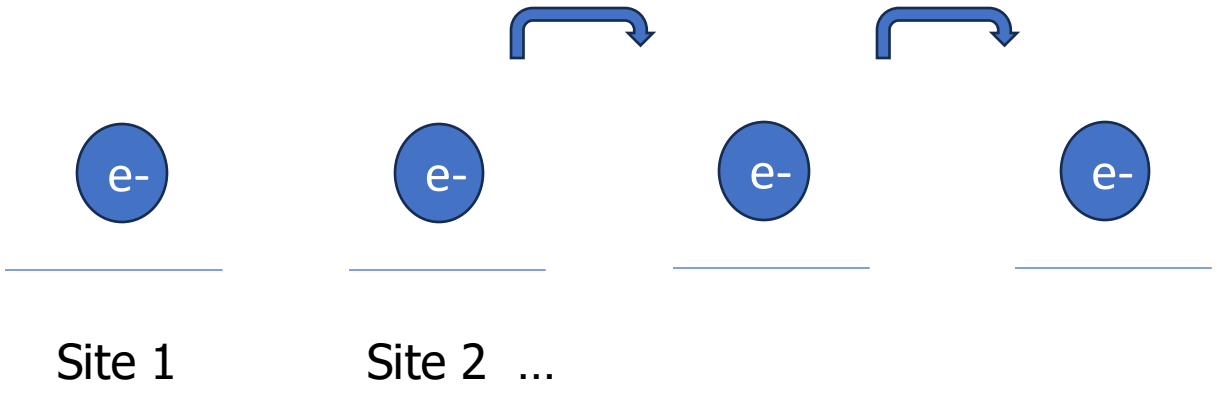
Peaks with larger width



Half-filling

Spectrum splitted in two peaks (Hubbard bands)

Approaching the Mott transition from the insulator (larger t)



Single orbital Hubbard model
- Onsite repulsión U
- Hopping energy t

1 electron per site/atom

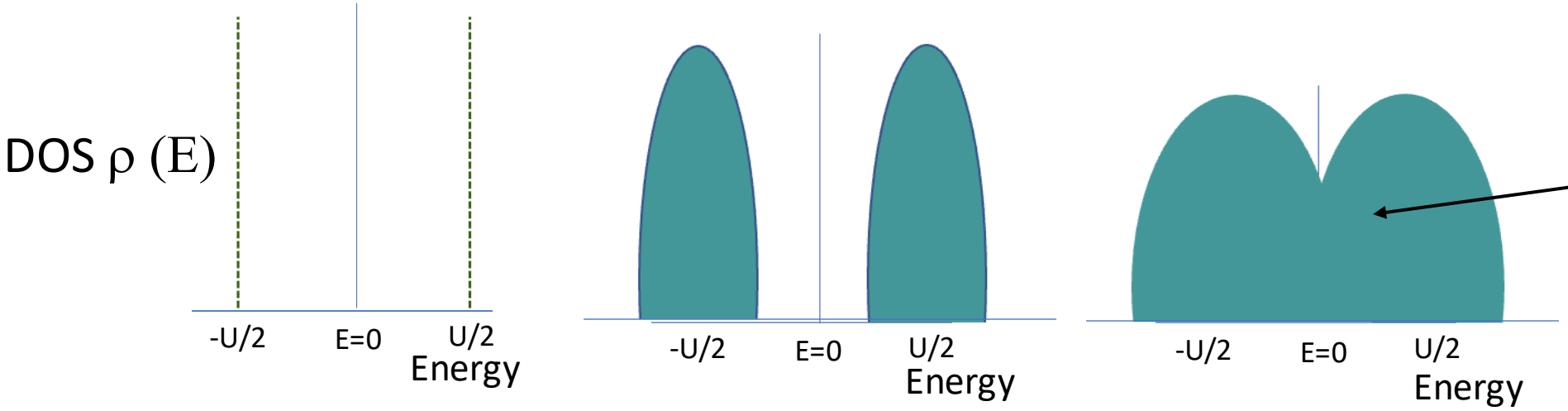
U>>t Start from t=0

Increasing the kinetic energy

↓

Peaks with larger width

W

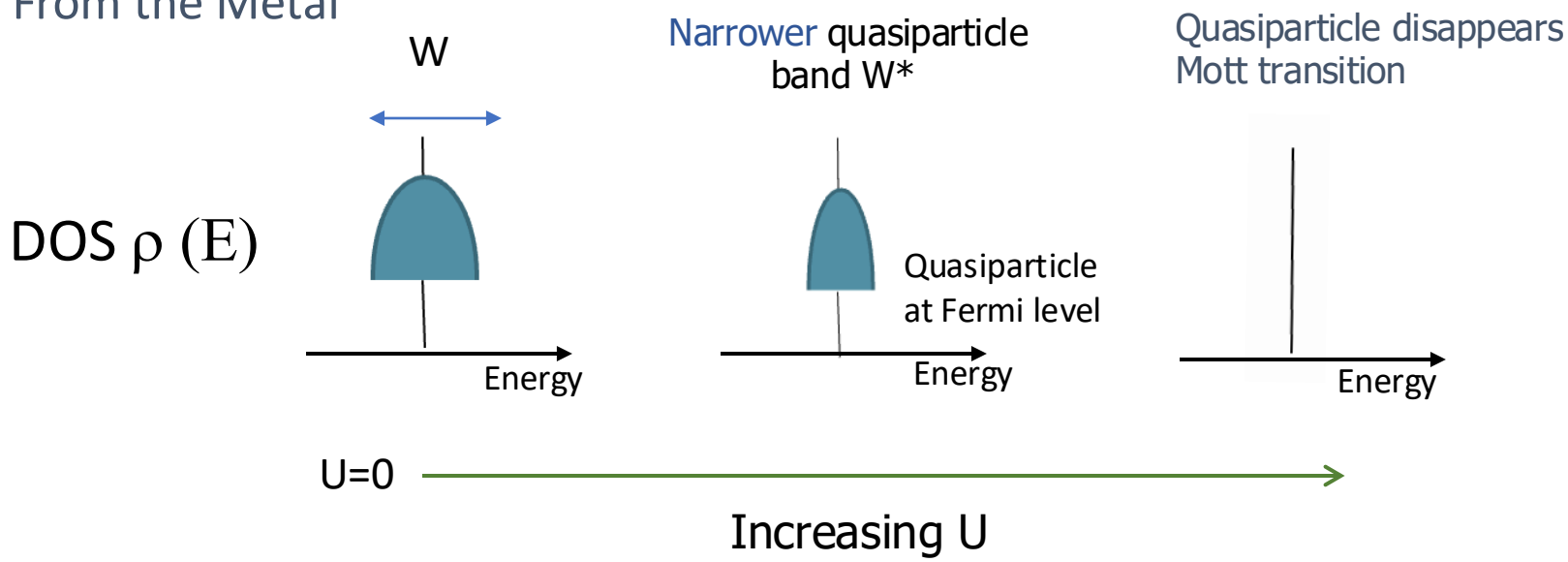


Closing of the gap
(insulator-metal transition)

But no quasiparticle peak

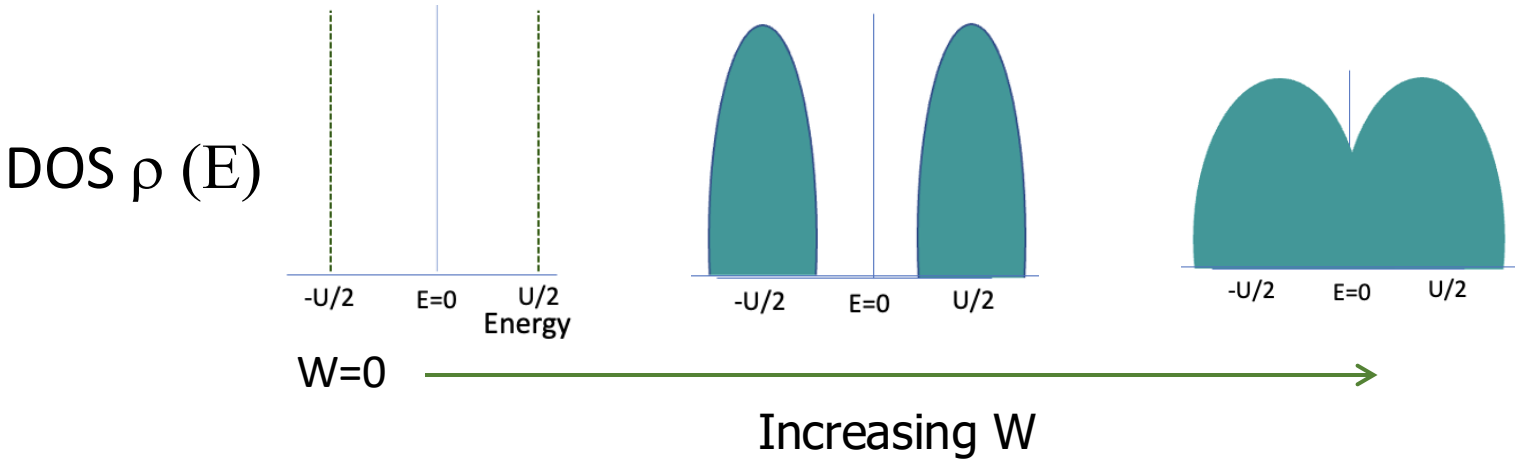
Approaching the Mott transition from the metal and the insulator

From the Metal



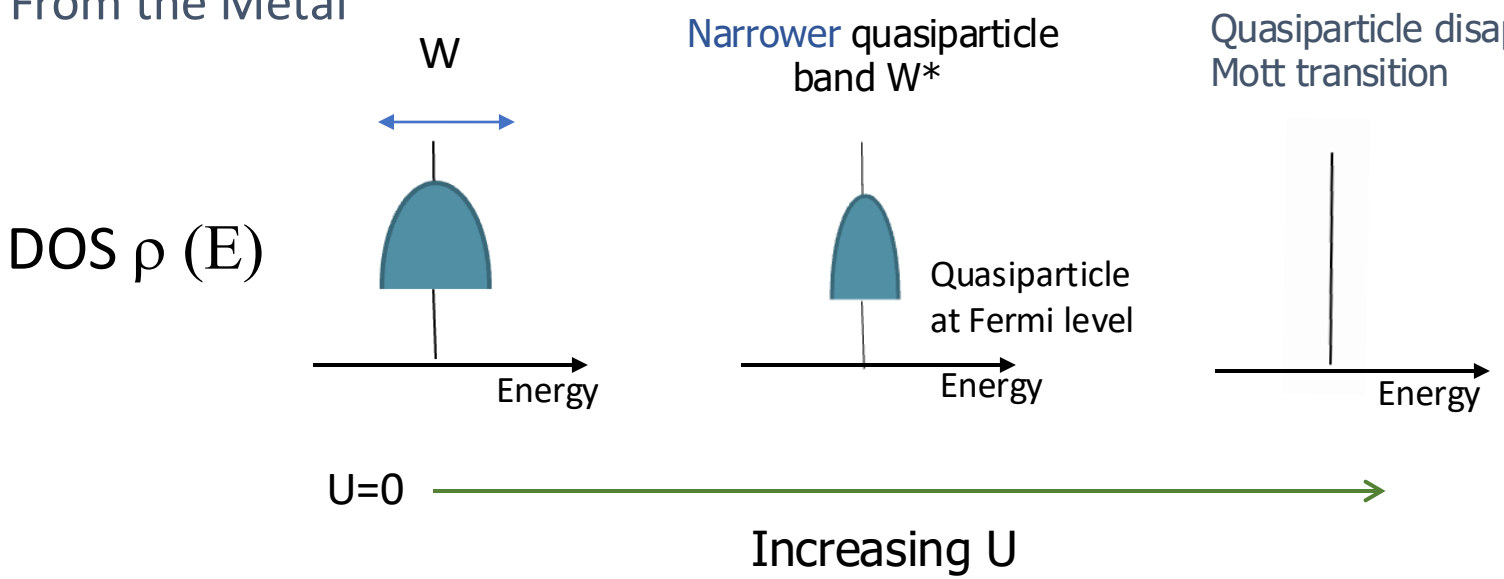
Very different descriptions of the Mott transition

From the Insulator

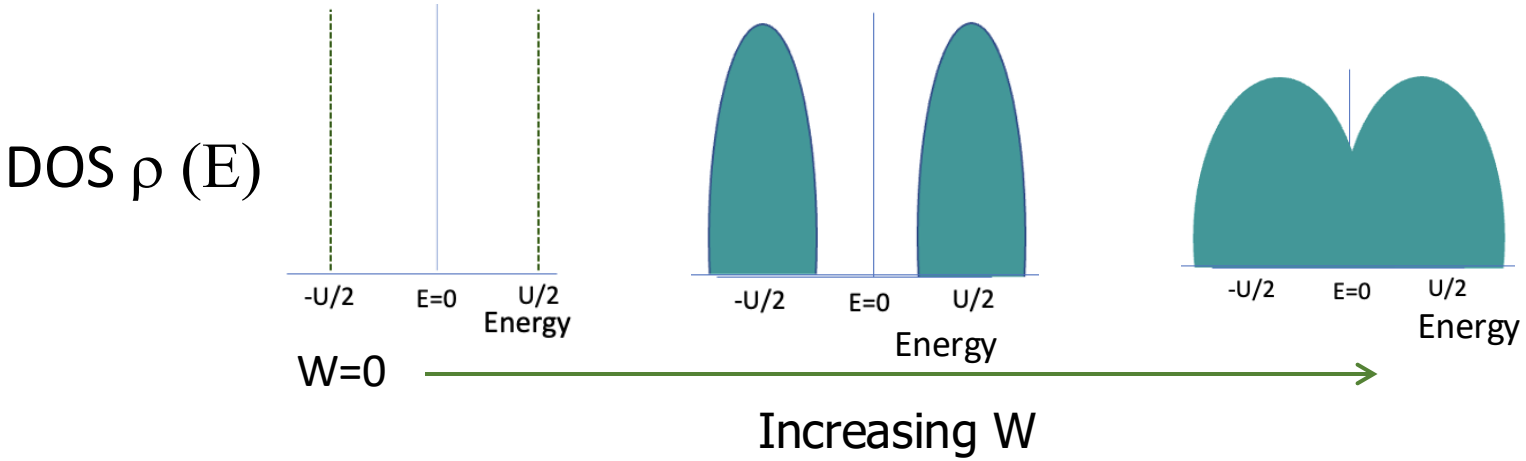


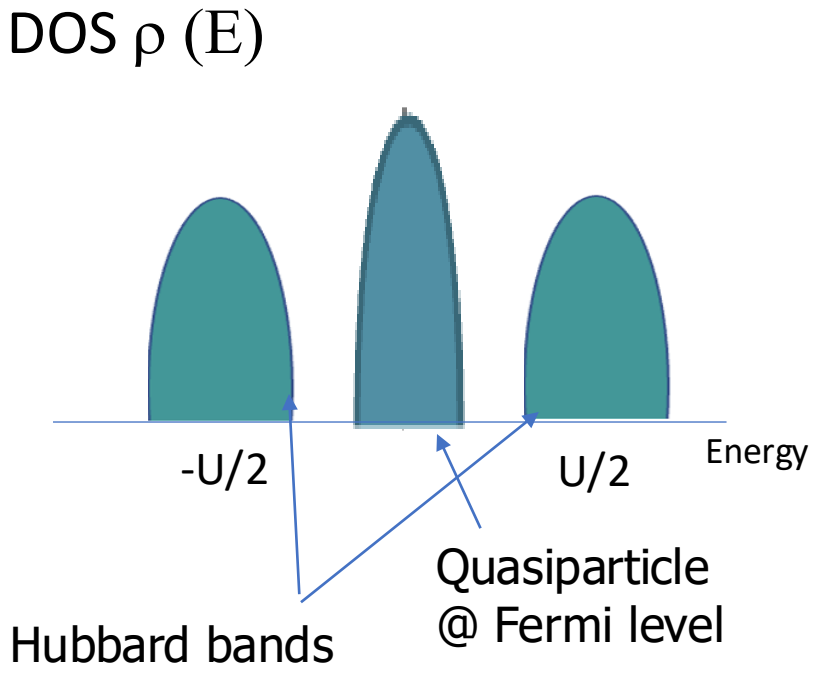
Approaching the Mott transition from the metal and the insulator

From the Metal



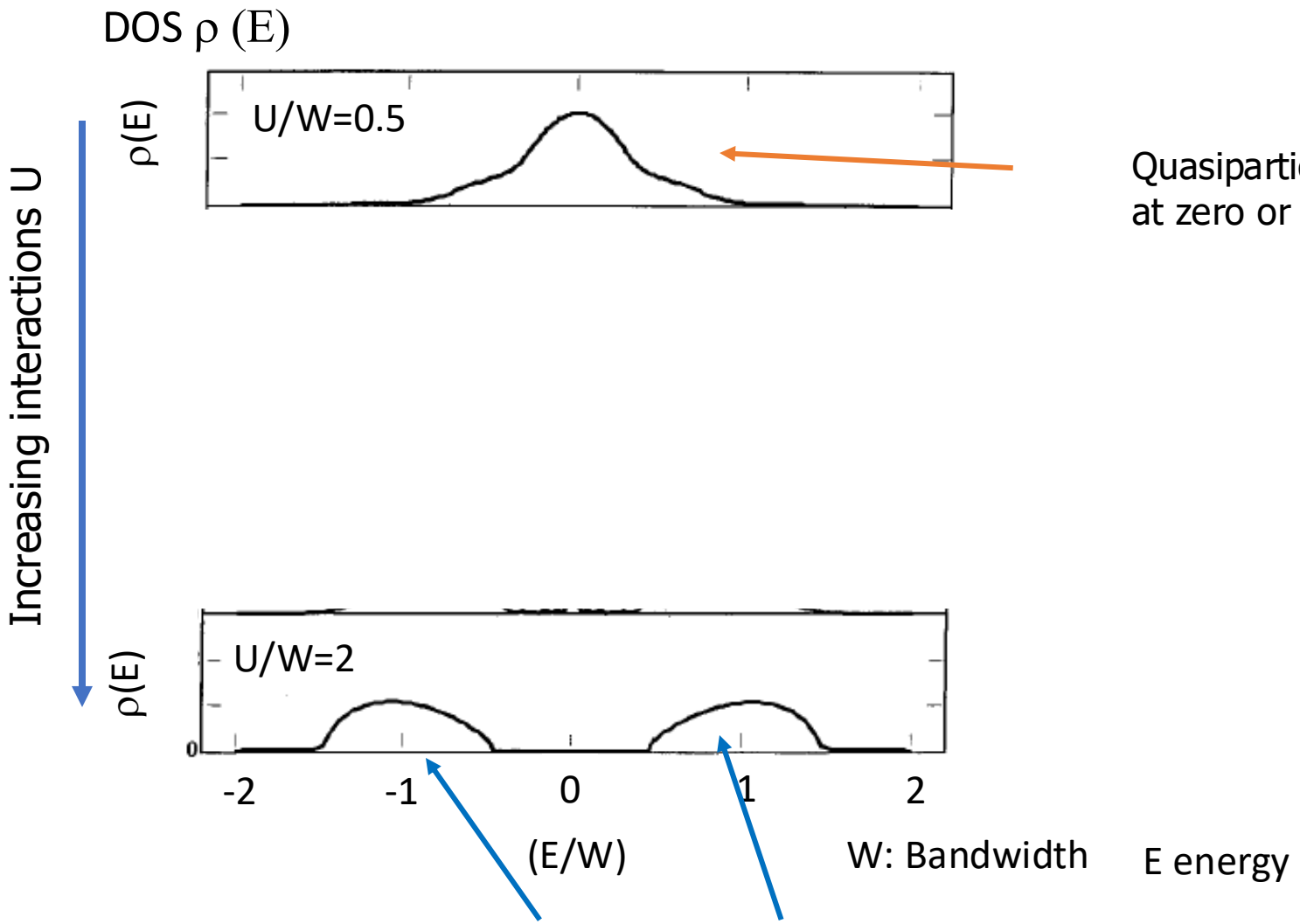
From the Insulator





From non-interacting electrons to local moments. DMFT

Half-filling.
Single-orbital Hubbard model.



Quasiparticle band (Band structure)
at zero or weak interactions

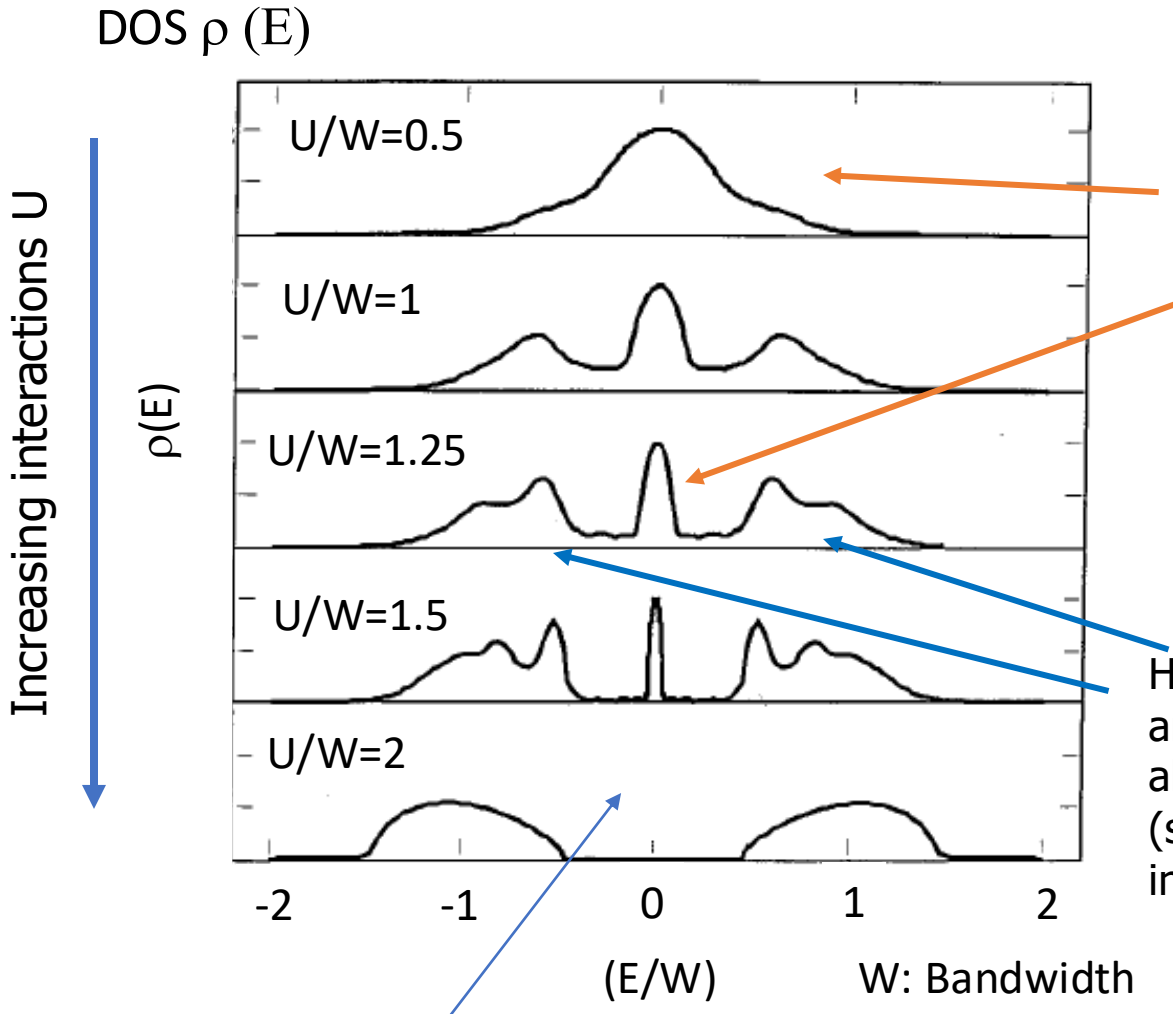
Hubbard bands centered at $\omega = \pm U/2$
at large interactions (local moments)
resembles atomic limit (insulating @integer filling)

Dynamical Mean Field Theory (DMFT)
Bethe lattice. Infinite dimensions

Georges et al , RMP 68, 13 (1996)

From non-interacting electrons to local moments

Half-filling.
Single-orbital Hubbard model.



Quasiparticle band (Band structure) becomes narrower with increasing interactions

Hubbard bands well developed and even well separated already in the metal (signatures of magnetic moments in the metal)

The metal insulator Mott transition happens when the quasiparticle Peak disappears

Strong modification of the spectrum
& not always a binary choice:

Dynamical Mean Field Theory (DMFT)
Bethe lattice. Infinite dimensions

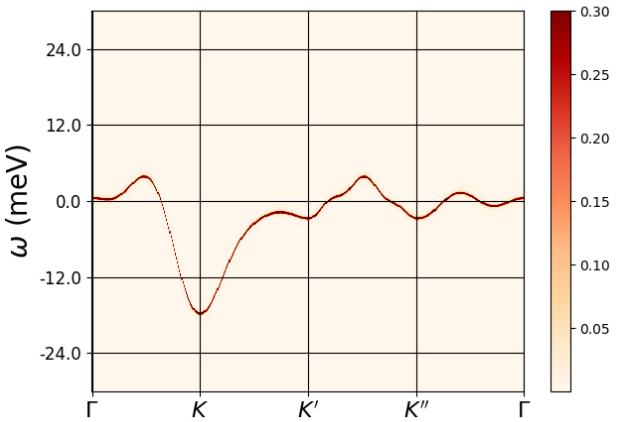
Georges et al , RMP 68, 13 (1996)

Two-orbital Hubbard model at half-filling for trilayer ABC/hBN

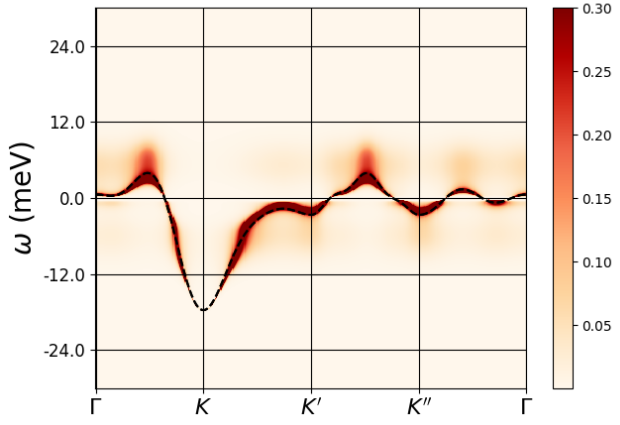
From non-interacting electrons to local moments

Uc: Interaction at which the Mott transition takes place

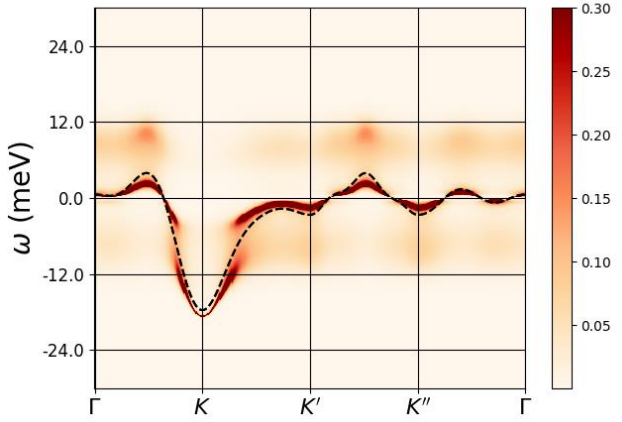
Non-interacting band n=2



U= 0.18 Uc

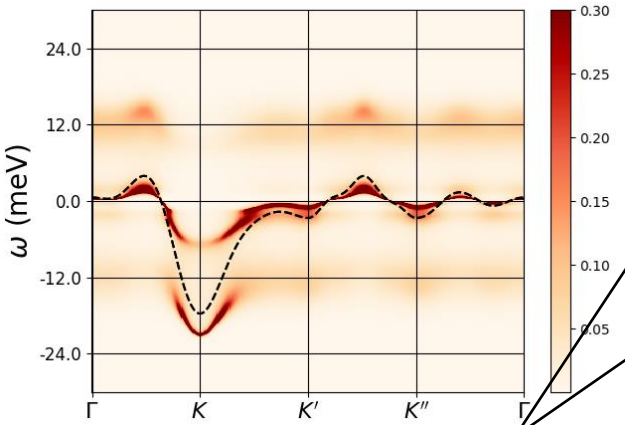


U= 0.36 Uc

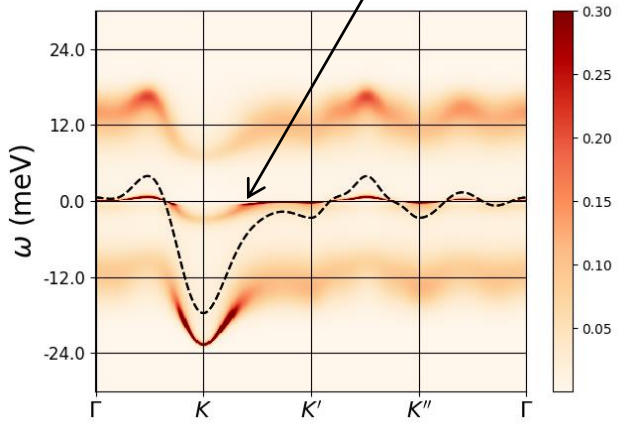


Strongly renormalized quasiparticle band

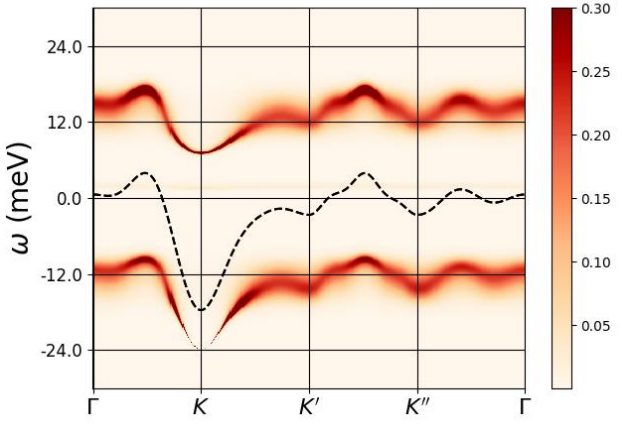
U= $U_c/2$



U= 0.82 Uc



U=1.07 Uc



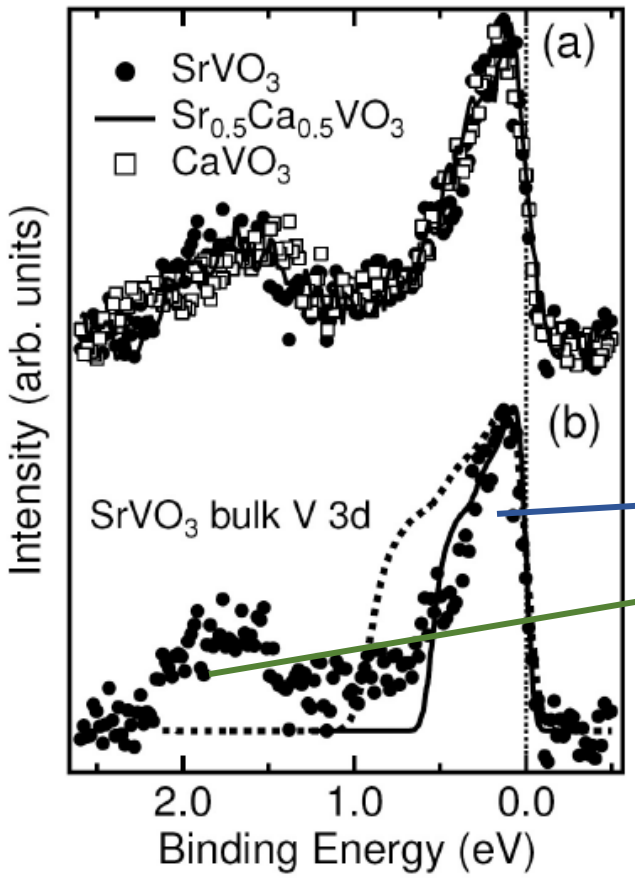
Hubbard bands (incoherent)

U_{Mott}

This is not just a simple gap opening

Calderón, Camjayi & EBascones, PRB 106, L081123 (2022)

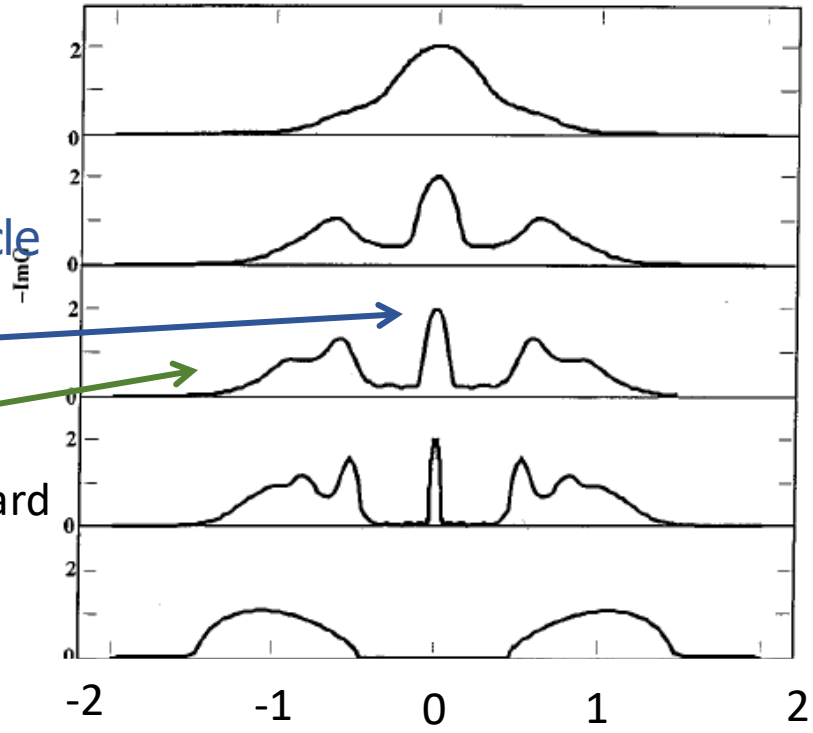
The spectral function



Photoemission

Quasiparticle peak

Hubbard band



Increasing interactions U

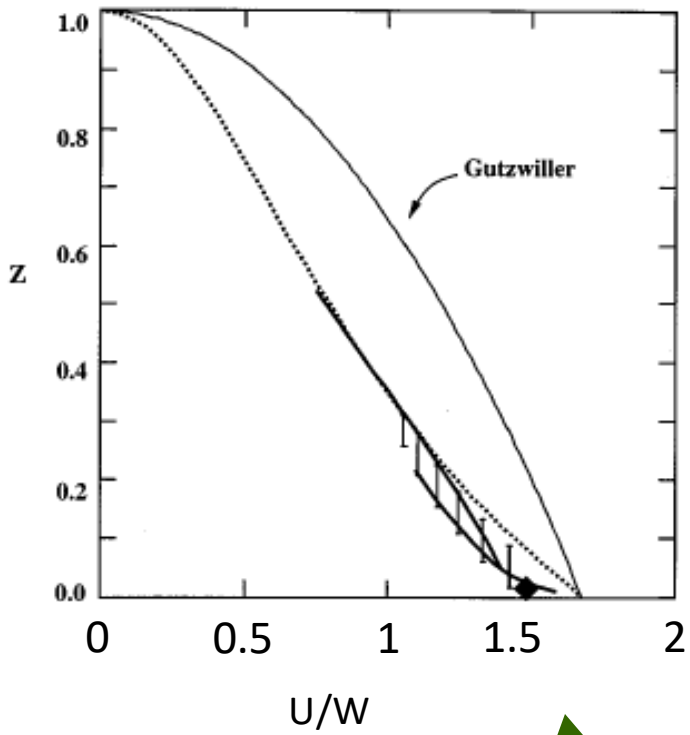
(E/W)

E: Energy
W: Bandwidth

Sekiyama et al, arXiv:0206471; Georges, arXiv:0403123

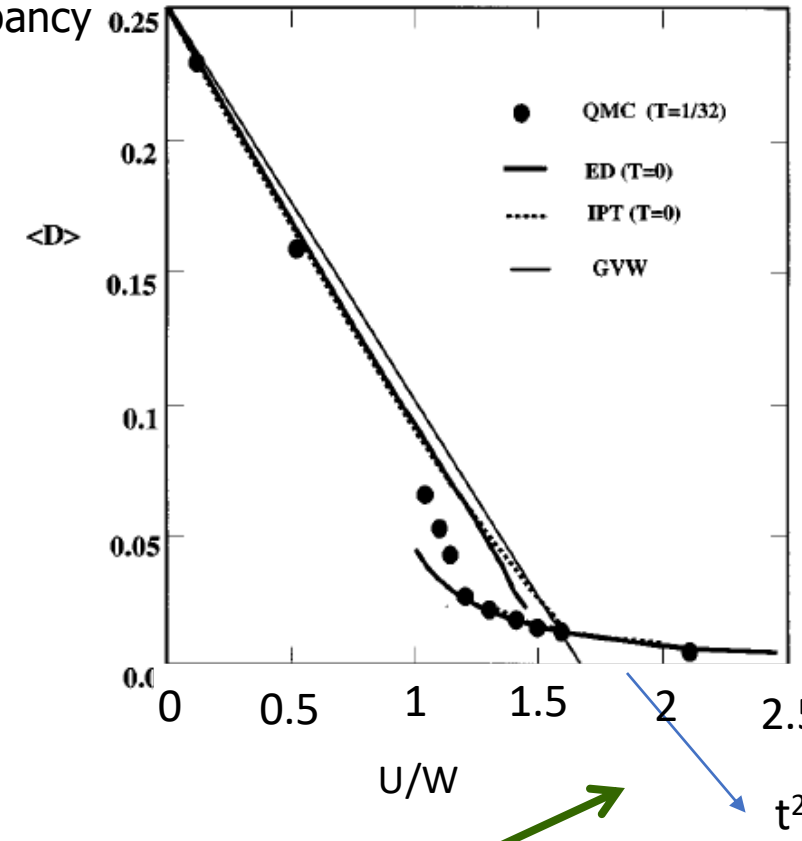
The Mott transition. DMFT picture

Quasiparticle weight



U: Interaction
W: Bandwidth

Double occupancy



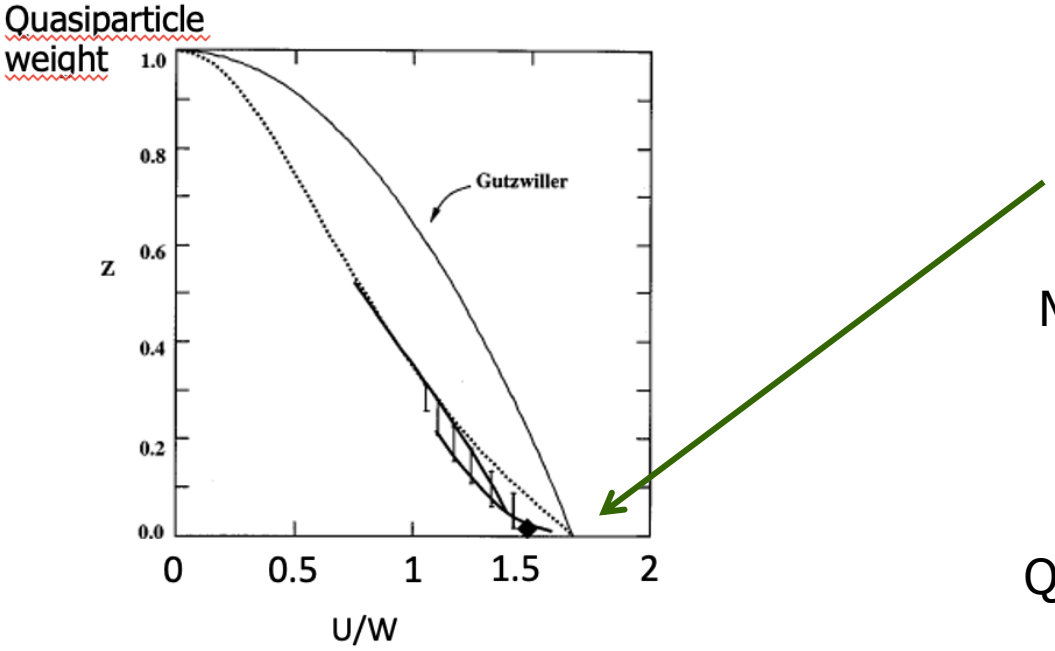
U: Interaction
W: Bandwidth

Quasiparticle weight vanishes at the Mott transition
but double occupancy does not (it is nevertheless very strongly suppressed)

Georges et al , RMP 68, 13 (1996)

DMFT numerical results can depend on the approximation used to solve the impurity problem

The Mott transition. DMFT picture



Georges et al , RMP 68, 13 (1996)

Quasiparticle weight vanishes
at the Mott transition

Maybe the best "order parameter" for the transition

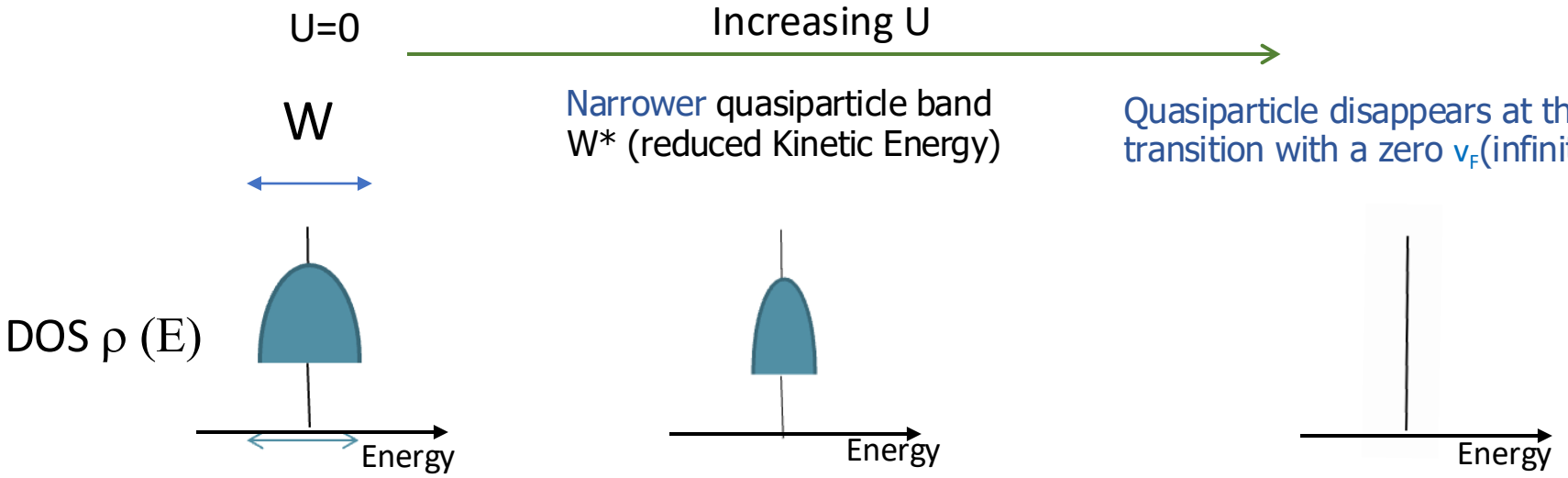
Quasiparticle weight : Step at Fermi surface

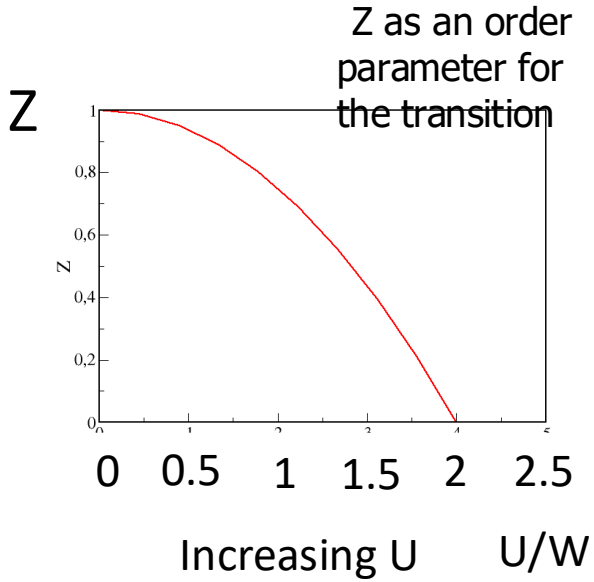
At the Mott transition
the Fermi surface disappears
(this is not just a simple gap opening)

Localization
In real space → Delocalization
in momentum space

Summary: The Mott transition

- Brinkmann-Rice approach: Metal as starting point. Fermi liquid description In the correlated metal double occupancy is reduced (Gutzwiller). Quasiparticles with larger mass, renormalized Fermi energy, reduced quasiparticle weight Z. Transition U ~ 2 W (constant DOS) with Z=0





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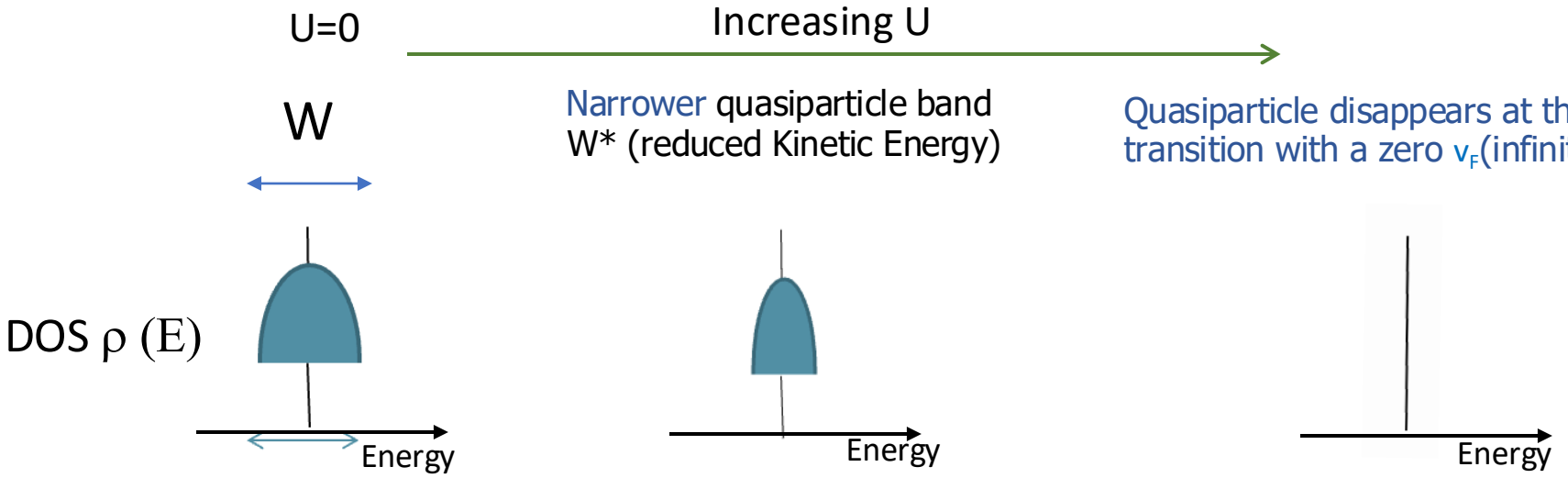
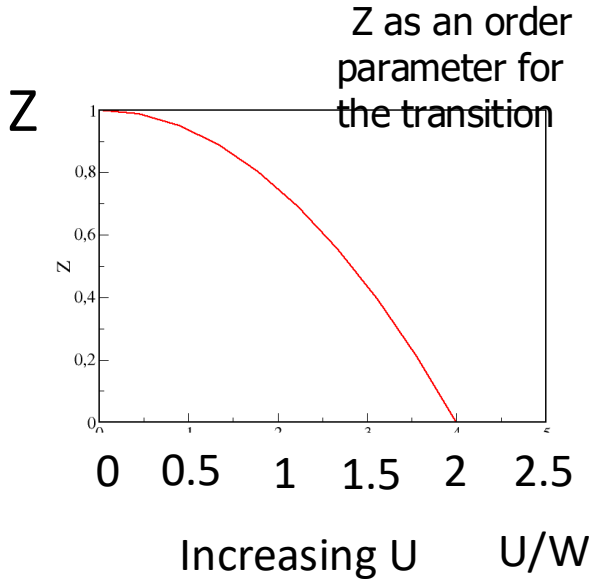
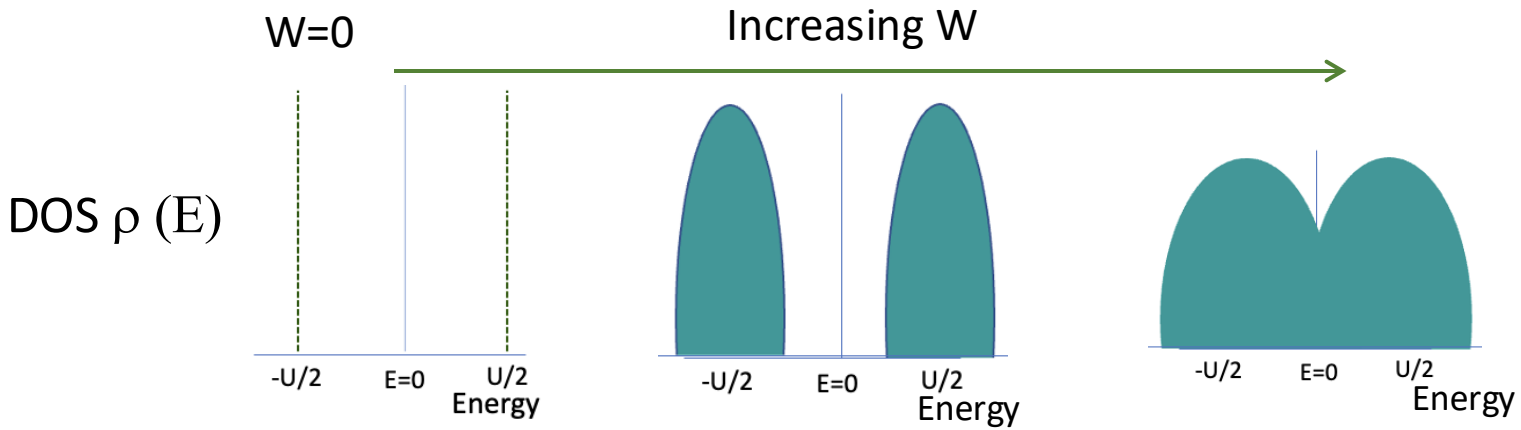




- Insulator as starting point

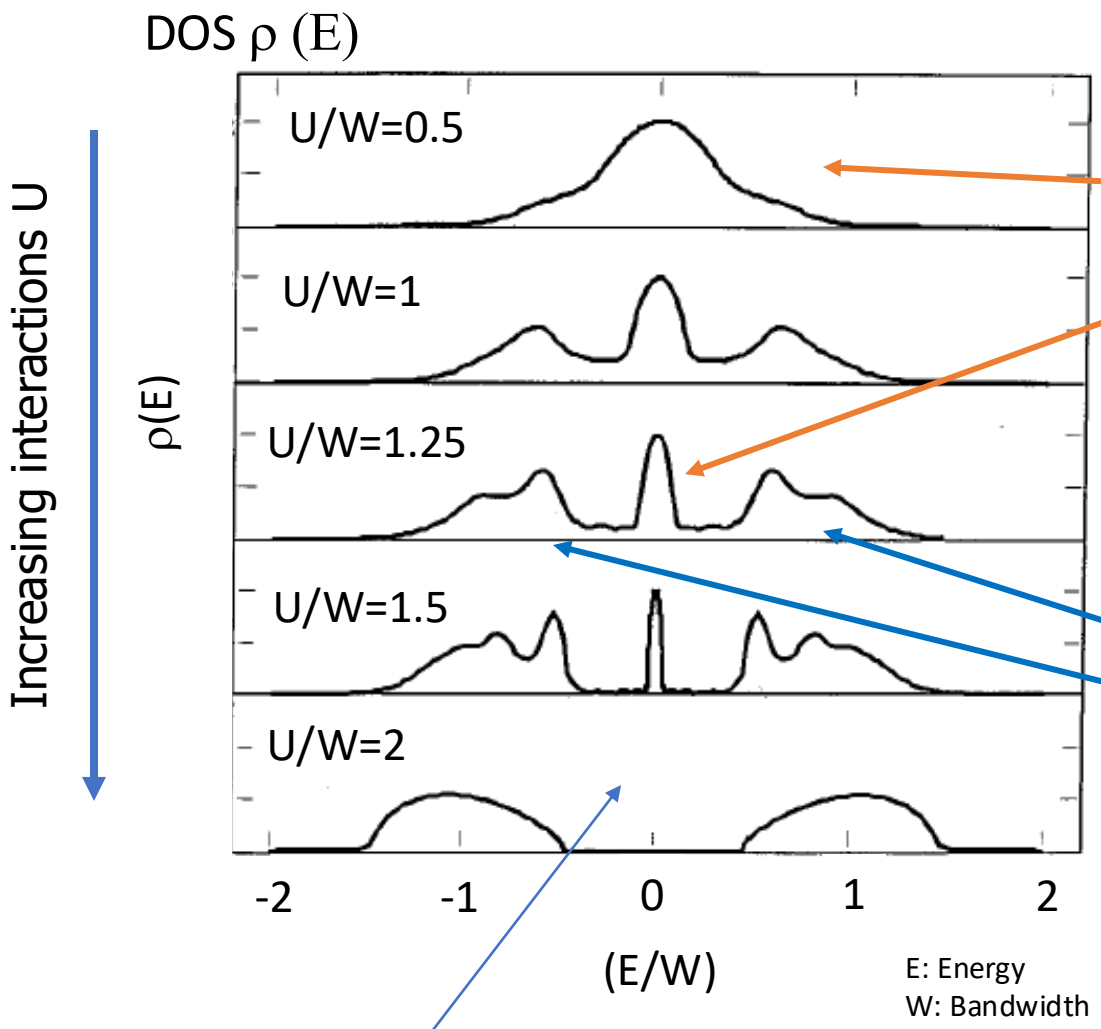


U: Interaction
W: Bandwidth

- Hubbard bands
- No quasiparticle peak

Summary: The Mott transition. The DMFT Description. Three peak structure

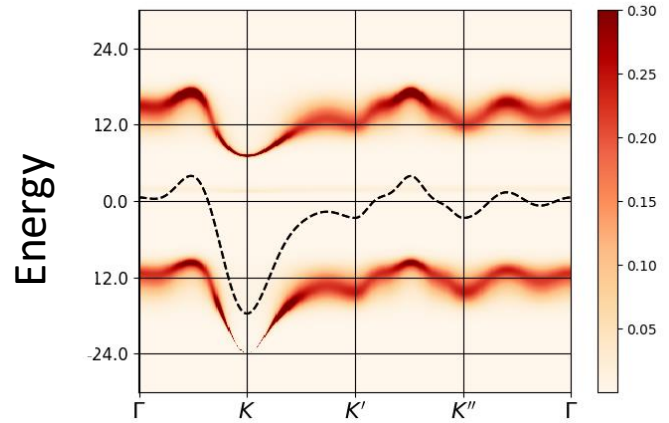
Half-filling.
Single-orbital Hubbard model.



E: Energy
W: Bandwidth

Quasiparticle band (Band structure) becomes narrower with increasing interactions

Hubbard bands well developed and even well separated already in the metal (signatures of magnetic moments in the metal)



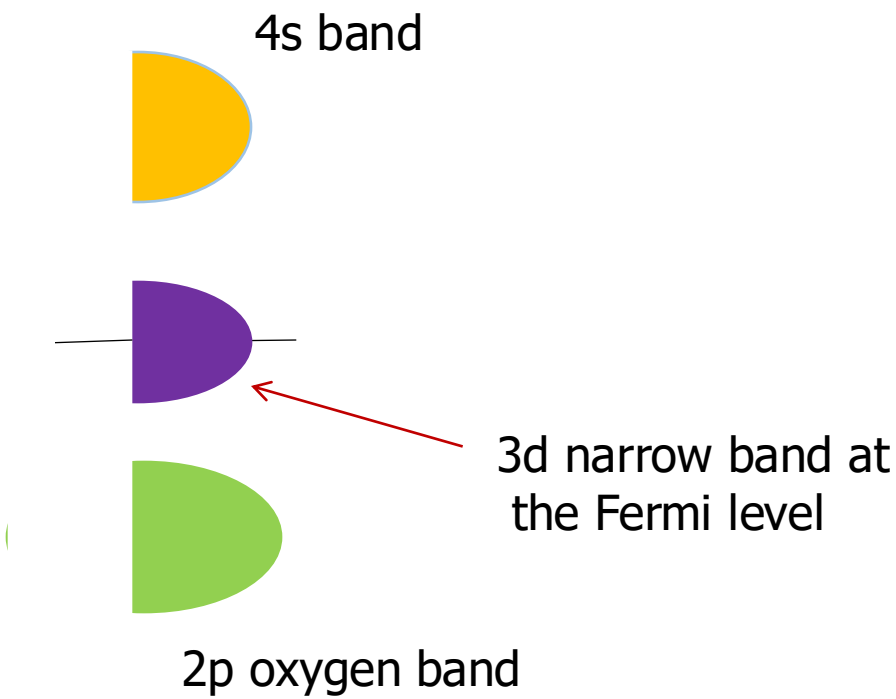
The metal insulator Mott transition happens when the quasiparticle Peak disappears

Georges et al , RMP 68, 13 (1996)

Mott versus Charge Transfer Insulators

3d oxides

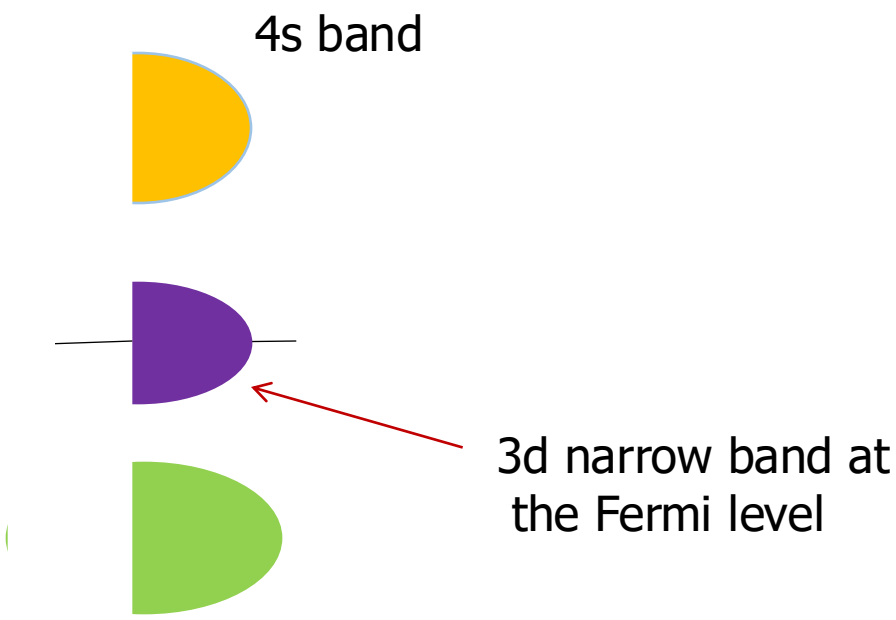
U=0



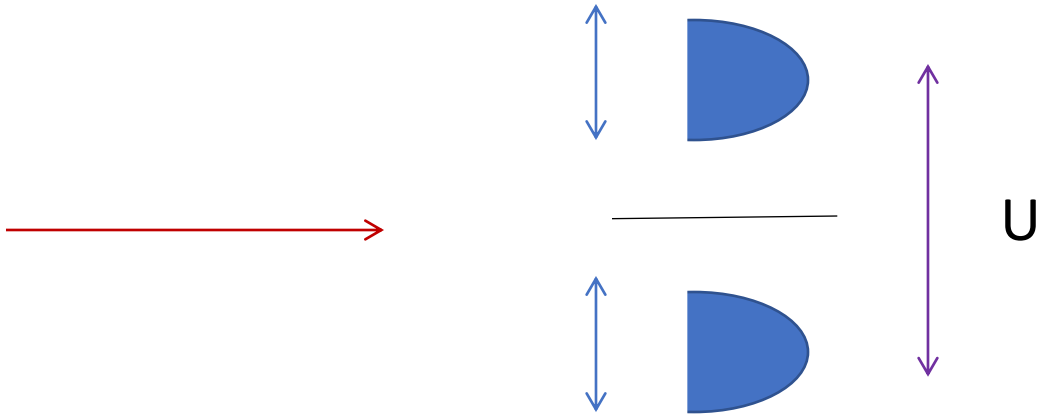
Mott versus Charge Transfer Insulators

3d oxides

U=0



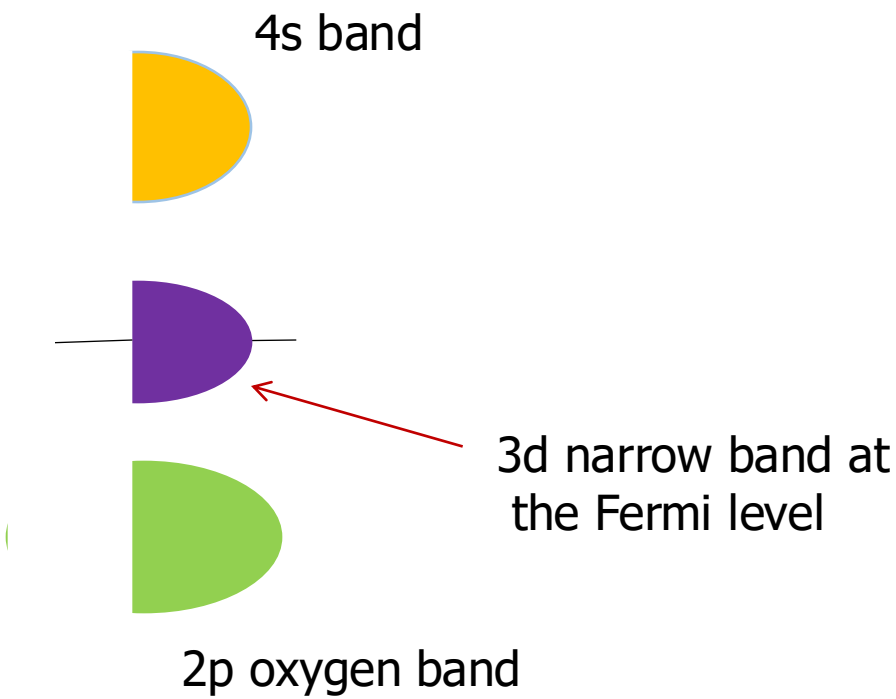
The Mott gap opens in the 3d narrow band

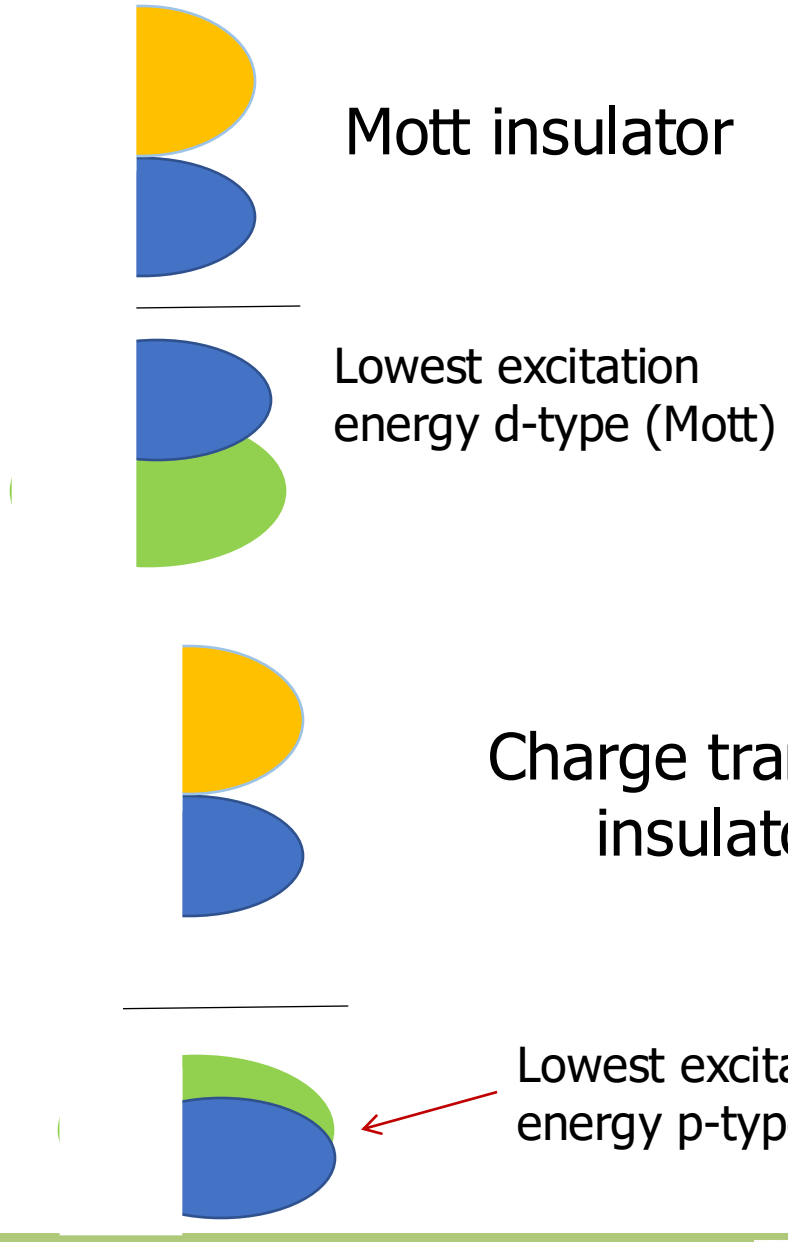


Mott versus Charge Transfer Insulators

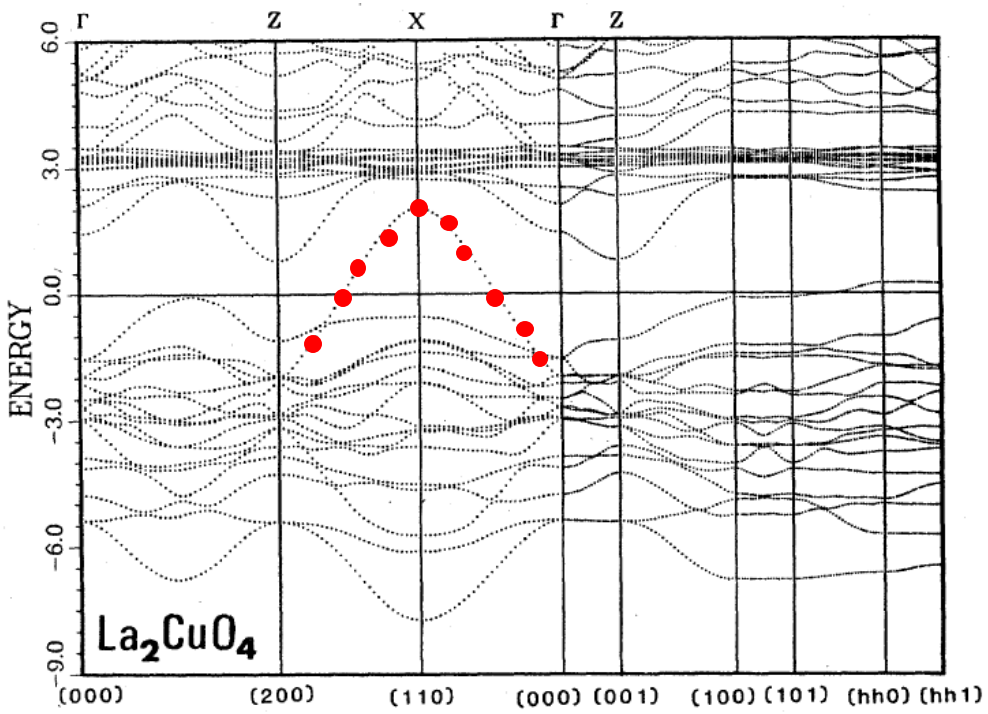
3d oxides

U=0

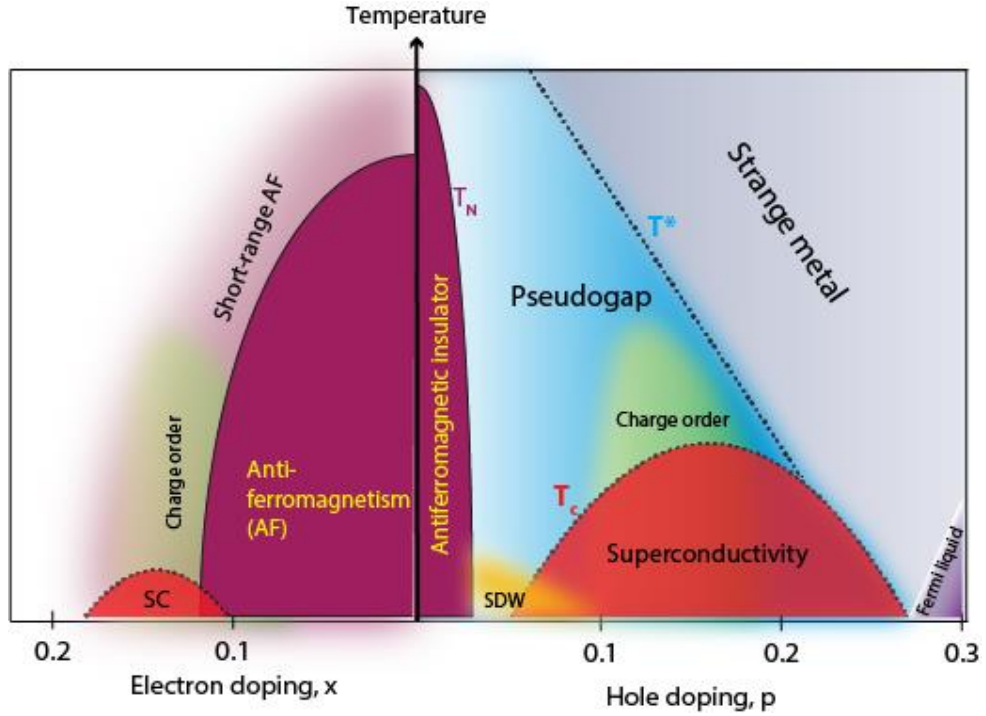




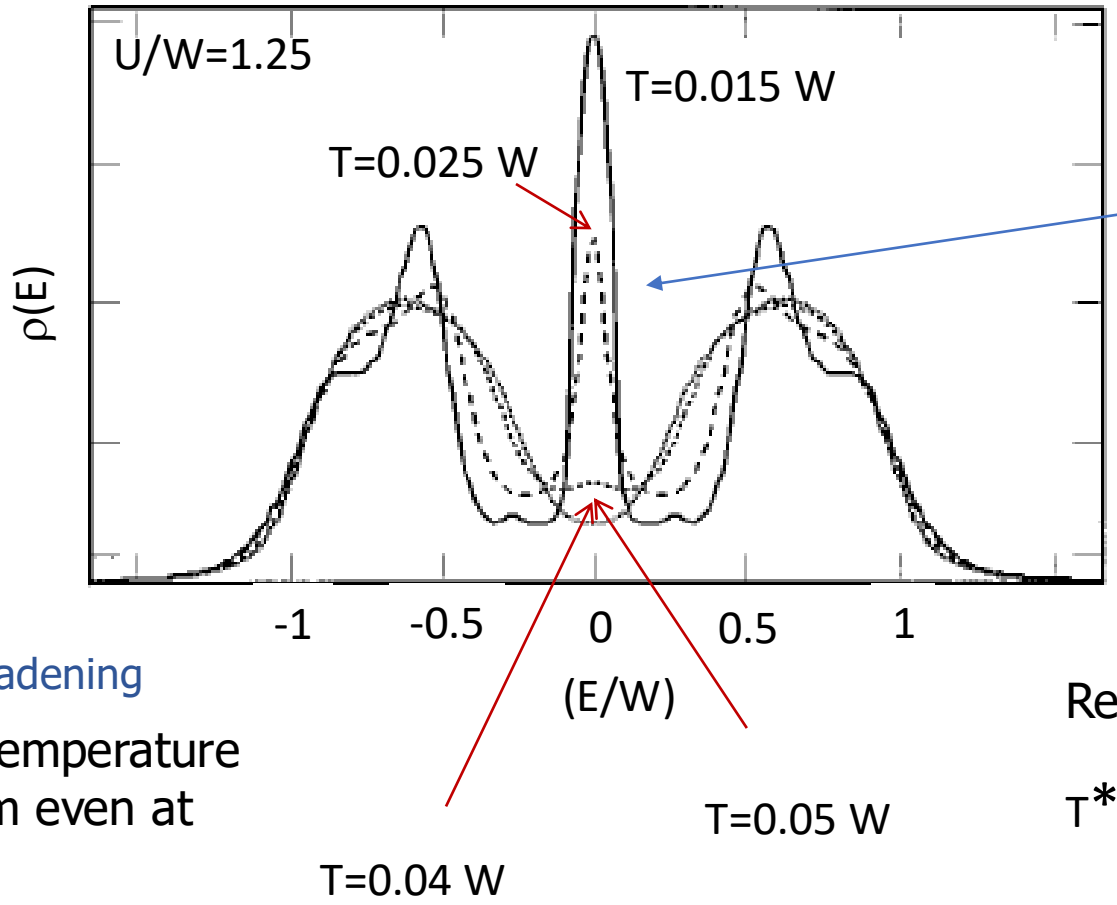
Mott versus Charge Transfer Insulators



Cuprates are
charge transfer insulators



Temperature effects on the spectral weight



The quasiparticle peak melts with increasing temperature

At high temperature the spectral weight resembles the one corresponding to local moments

Not just thermal broadening

Small changes in temperature affect the spectrum even at large energies

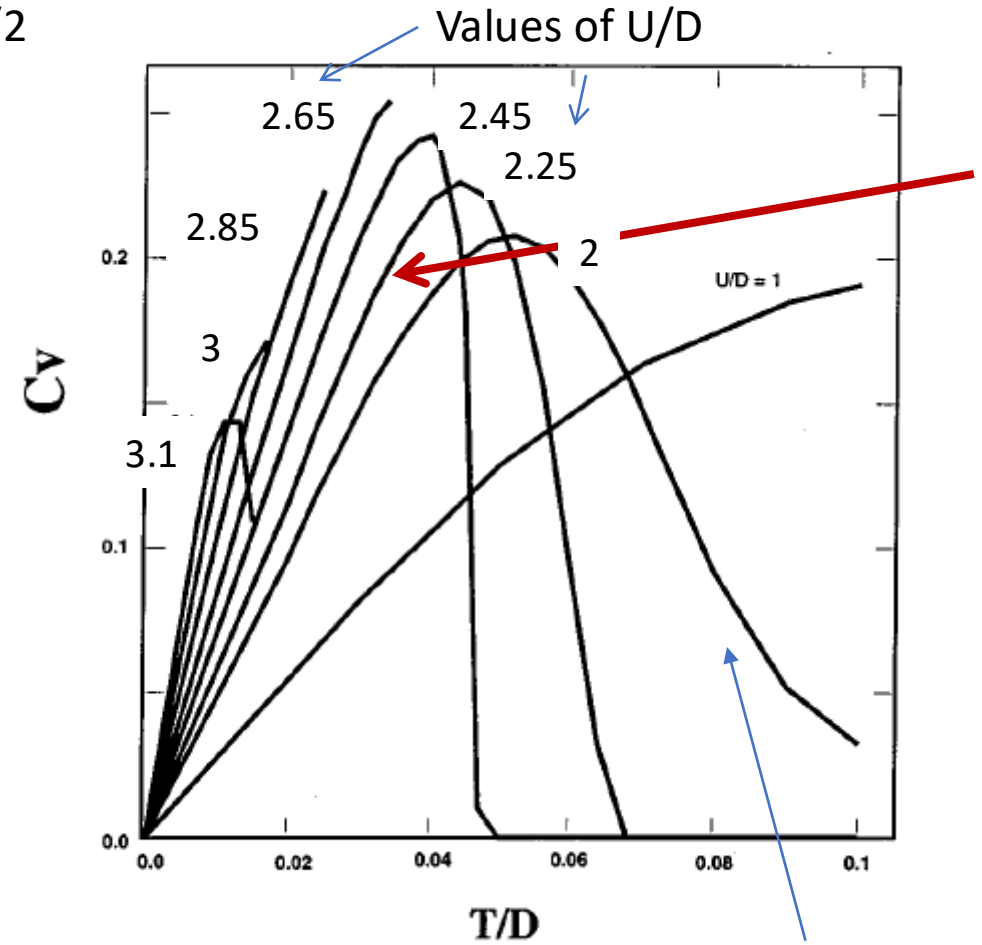
Renormalized Fermi energy: temperature scale

$T^* \sim E_F^* \sim Z\, E_F$

Georges et al , RMP 68, 13 (1996)

Specific heat: Mass enhancement and Temperature effects

D=W/2



The slope of the linear T dependence increases with interactions

Fermi liquid: Specific heat linear with temperature

$C \sim \gamma T \qquad \gamma \sim m^*$

Mass enhanced with interactions

DMFT calculations for the single orbital Hubbard model at half-filling

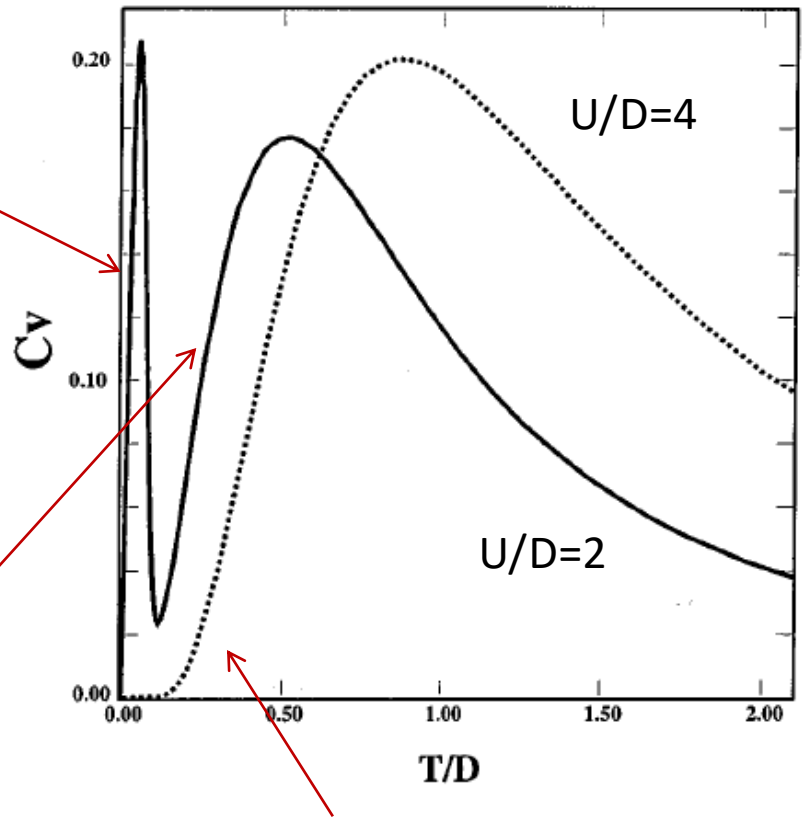
Non monotonous behavior (promoted by interactions)

Georges et al , RMP 68, 13 (1996)

Specific heat: Mass enhancement and Temperature effects

D=W/2

T-linear dependence at low temperatures (Metallic)



Fermi liquid behavior observed only at low temperatures

Change to insulating like behavior at high temperatures

Activated behavior at low temperatures (Insulating)

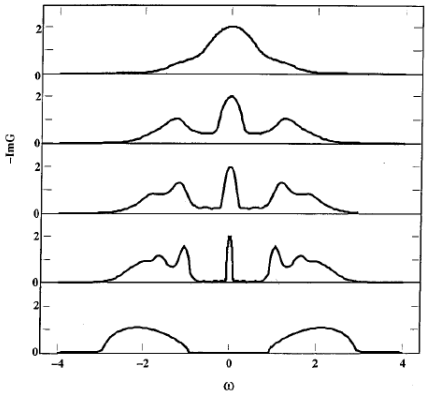
DMFT

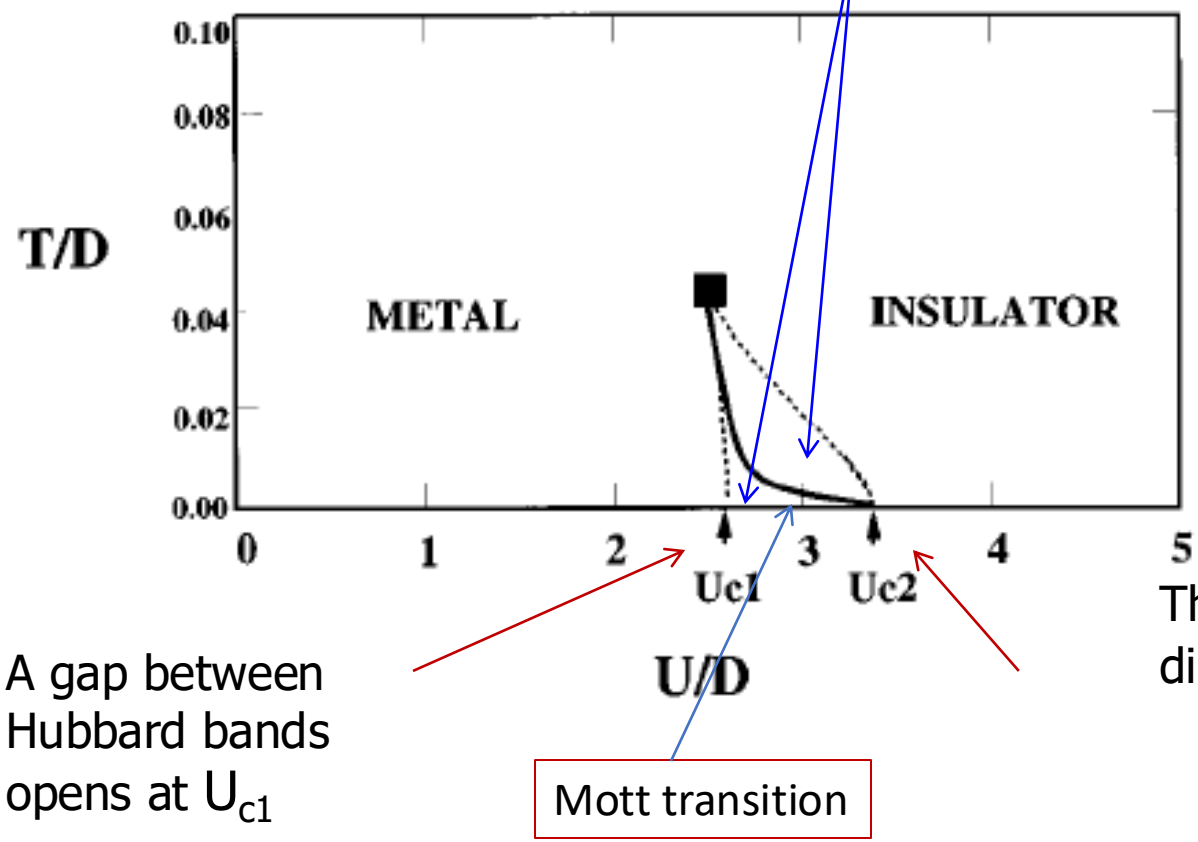
Georges et al , RMP 68, 13 (1996)

The Mott transition at Finite Temperature

Georges et al ,
RMP 68, 13 (1996)

In the region between the dotted lines both a metallic and an insulator solution exist





D=W/2

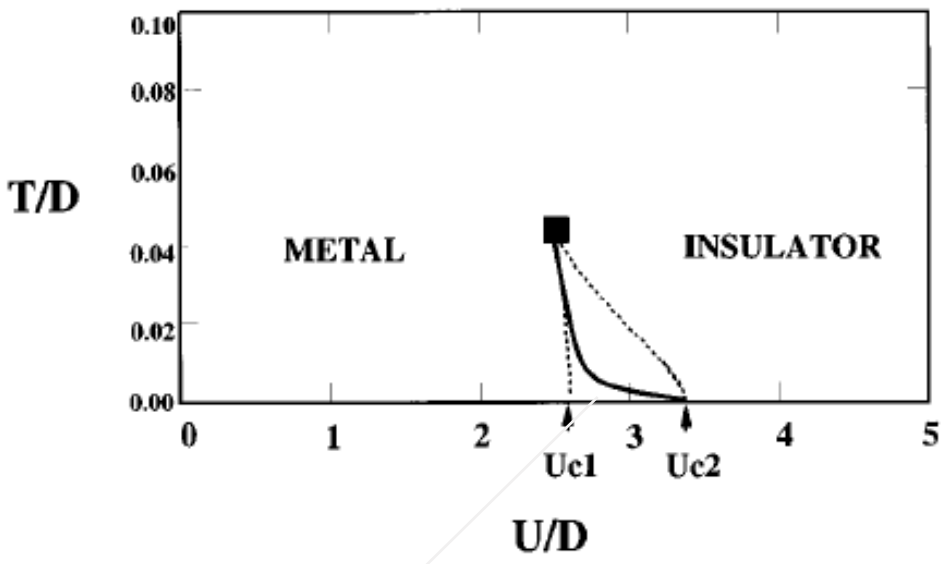
A gap between Hubbard bands opens at U_{c1}

The quasiparticle peak disappears at U_{c2}

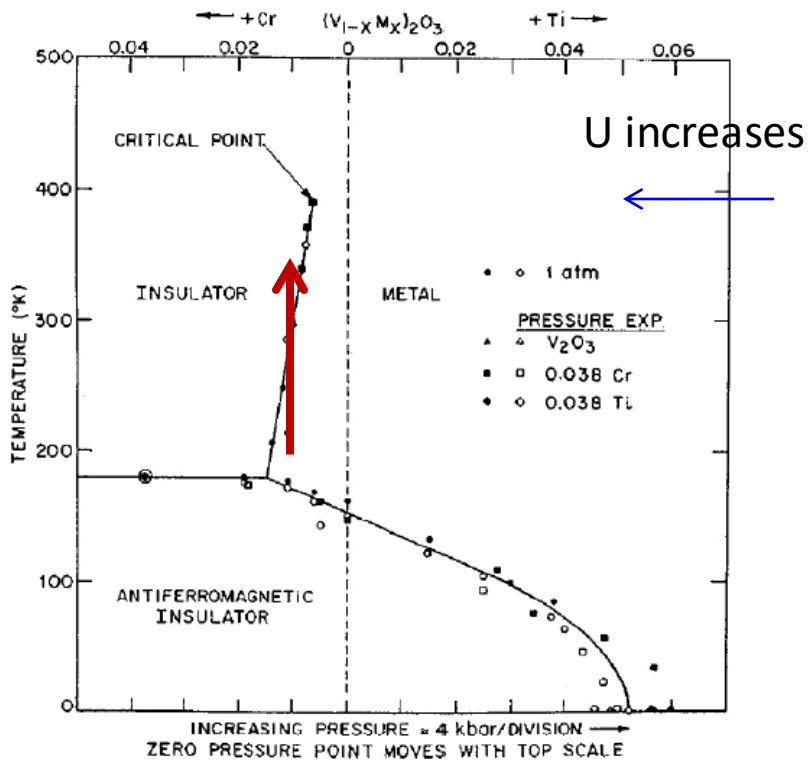
Mott transition

At zero temperature the Mott transition happens at U_{c2} when the quasiparticle peak disappears

The Mott transition at Finite Temperature

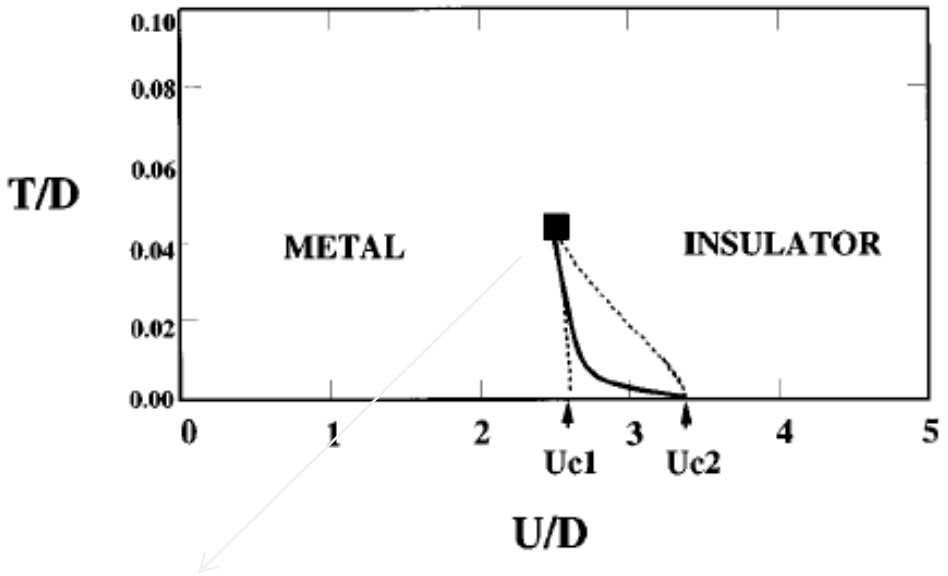


The system becomes insulating with increasing temperature



Georges et al ,
RMP 68, 13 (1996)

The Mott transition at Finite Temperature



Insulator: Resistivity decreases with temperature

Metal: Resistivity increases with temperature

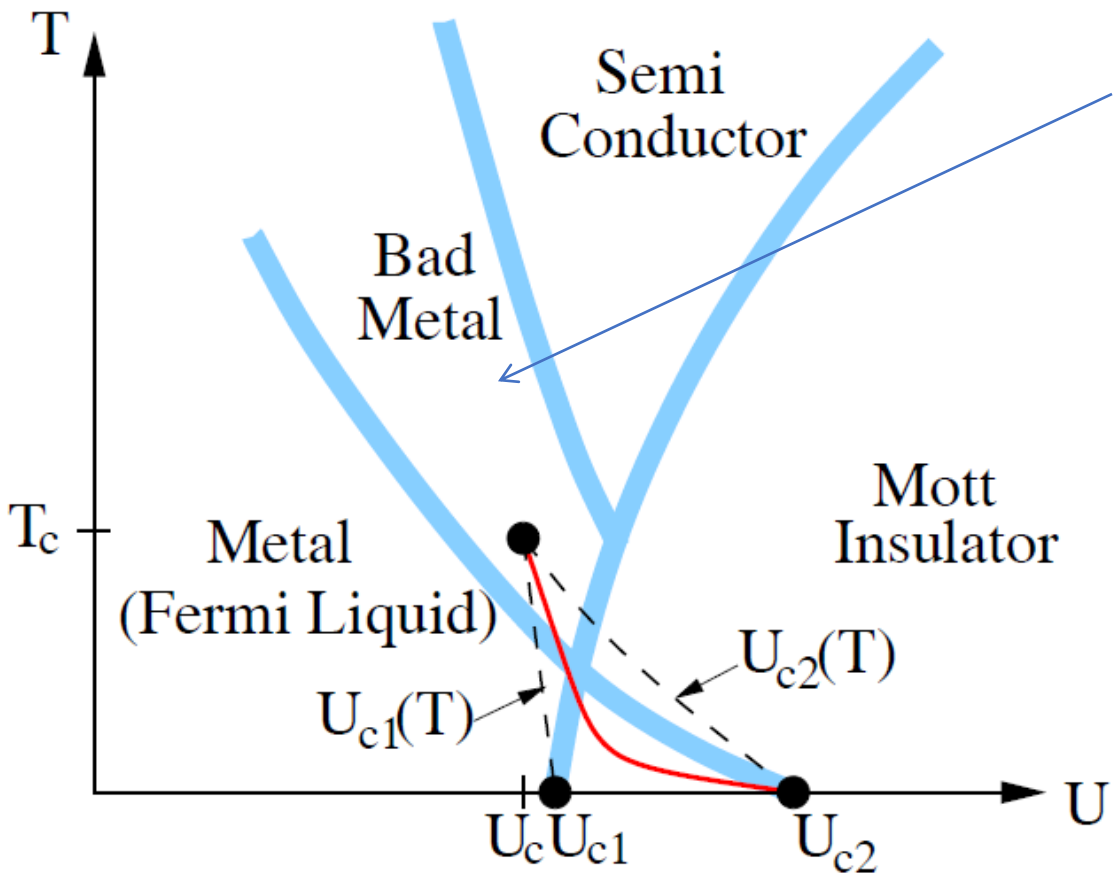
Critical point:

No distinction of what it is a metal and what an insulator at higher temperatures

Georges et al ,
RMP 68, 13 (1996)

The Mott transition at Finite Temperature

Not so clear distinction between a metal and an insulator at finite temperatures



Bad metal: the electronic scattering mean free path is smaller than the lattice constant

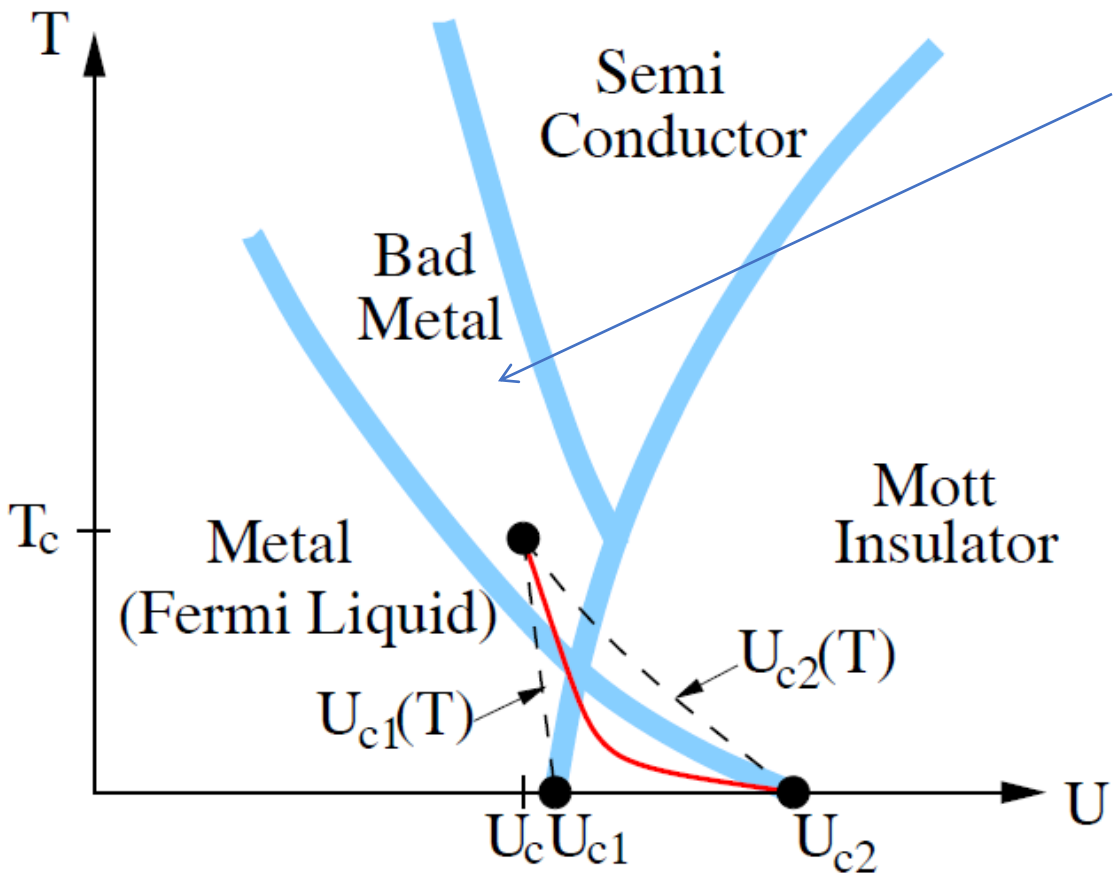
Mott-Ioffe-Regel limit $\rho > \rho_{MIR}$

At high temperature the system is more conducting but it does not becomes metallic (ρ increases with T)

Georges et al, J. de Physique IV 114, 165 (2004), arXiv:0311520

The Mott transition at Finite Temperature

Not so clear distinction between a metal and an insulator at finite temperatures



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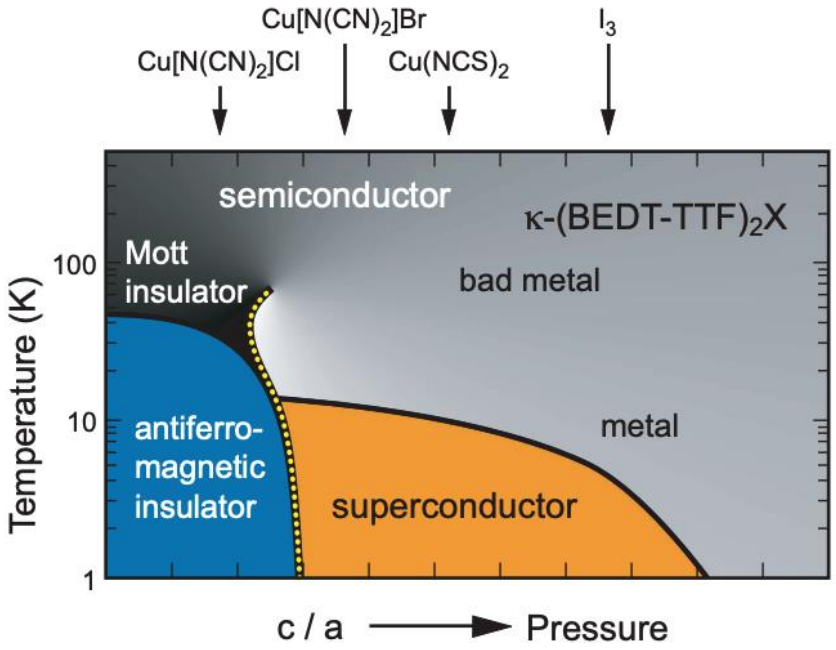


organic salt

Georges et al, J. de Physique IV 114, 165 (2004), arXiv:0311520

The Mott transition at Finite Temperature

Analogy between Mott transition & liquid-gas transition

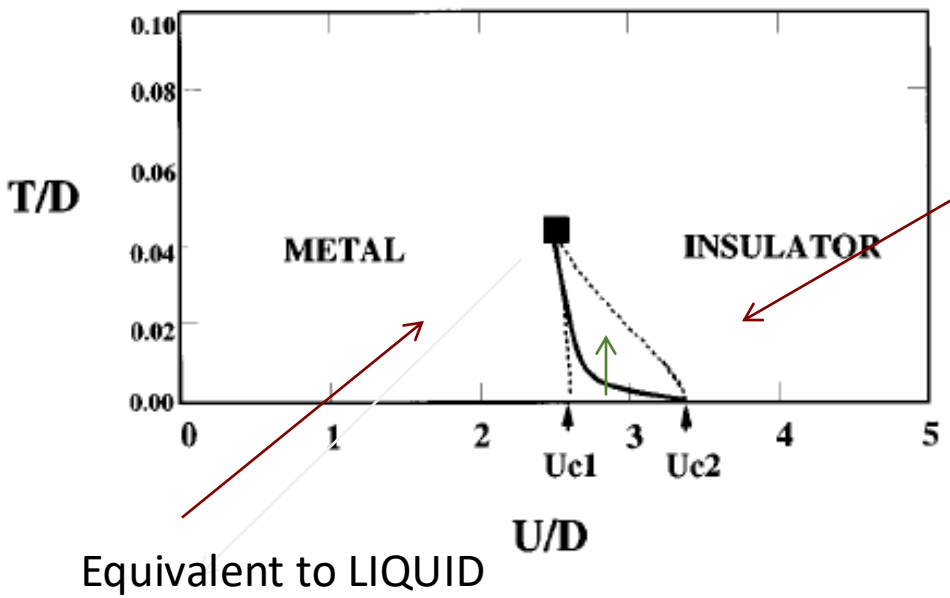
Metal: liquid

Insulator: gas
(larger entropy)

The particles in the gas are the doubly occupied sites. Density is smaller in the insulator (gas)

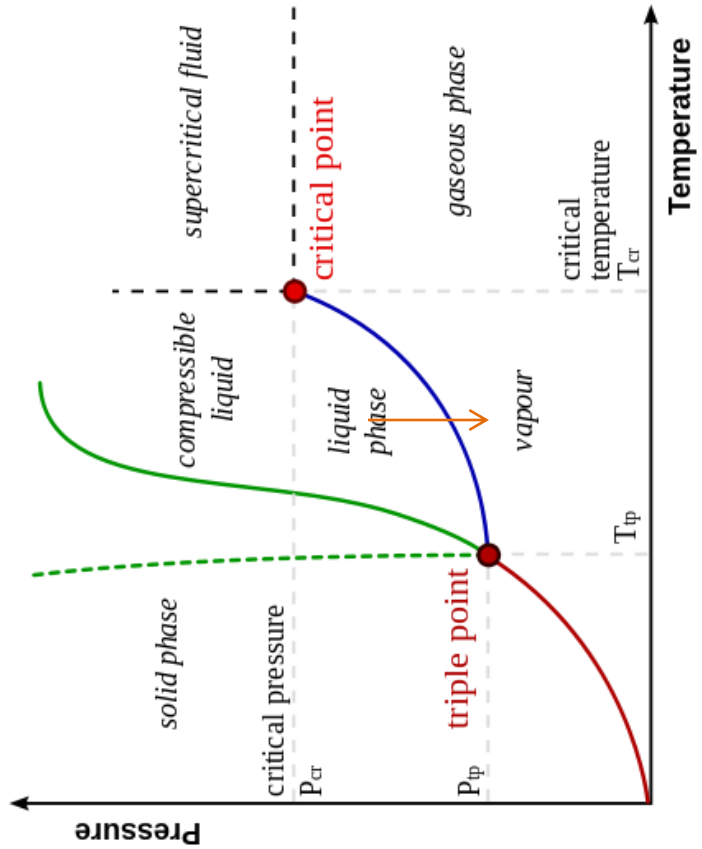
At the transition there is a jump in the density
(particles in water and double occupied in the Mott insulator)

The Mott transition at Finite Temperature



Equivalent to GAS

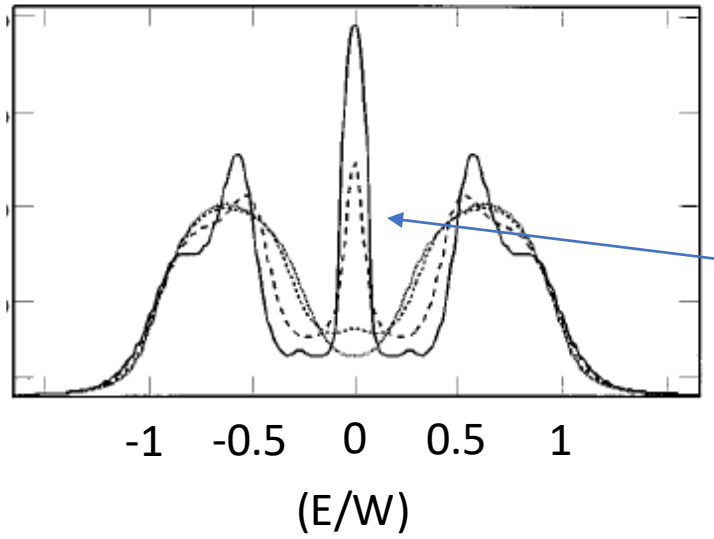
Equivalent to LIQUID



Liquid Gas Transition

Summary: Mott physics. Temperature Dependence

Density of states

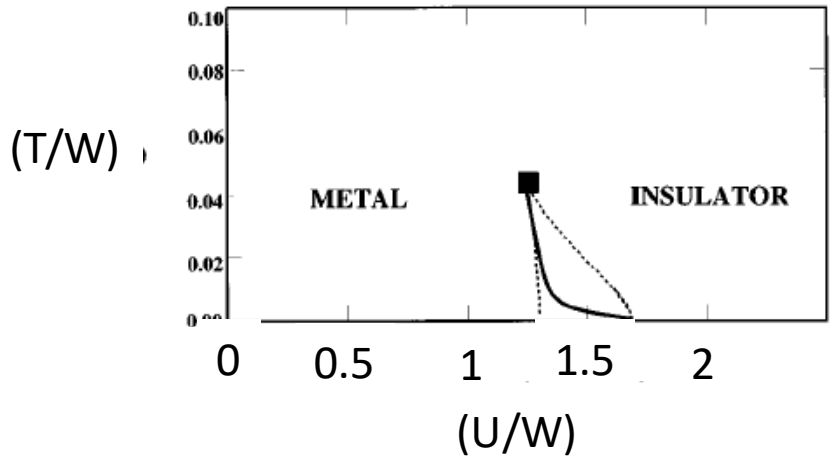


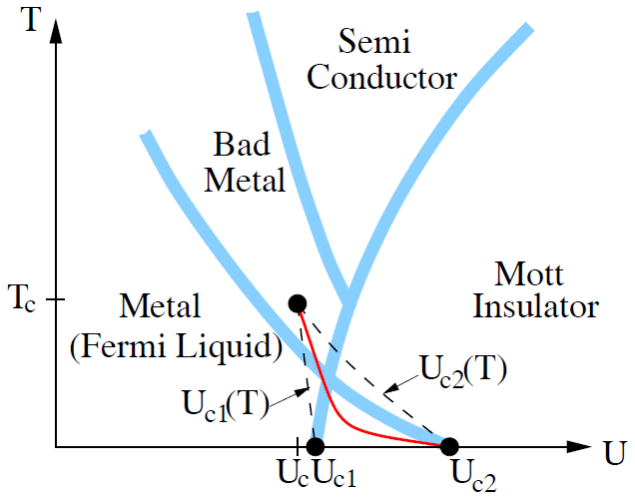
E: Energy
W: Bandwidth
T: Temperature

When Mott correlations are strong, small changes in the temperature produce important changes in the spectrum in a large energy range

Close to the Mott transition the quasiparticle peak melts with increasing temperature

Not just thermal broadening





Large resistivity even in the metallic state with increasing temperature

Bad metal: the electronic scattering mean free path is smaller than the lattice constant

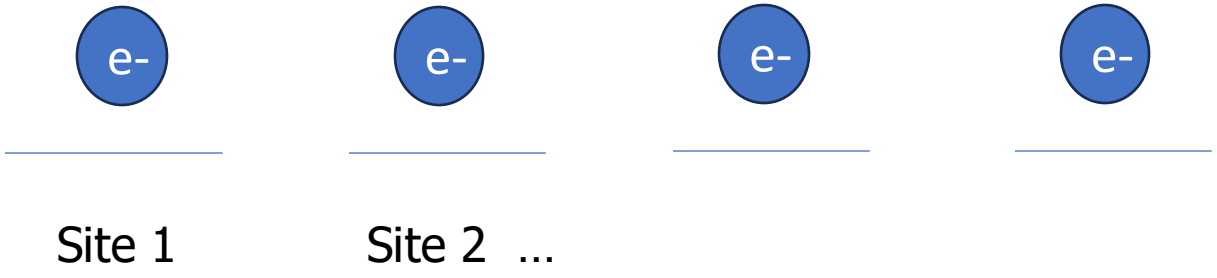
$\rho > \rho_{MIR}$ Mott-Ioffe-Regel limit

The entropy of the Mott insulator larger than the one of the metallic state. Analogy liquid-gas transition

Mott transition and electronic filling

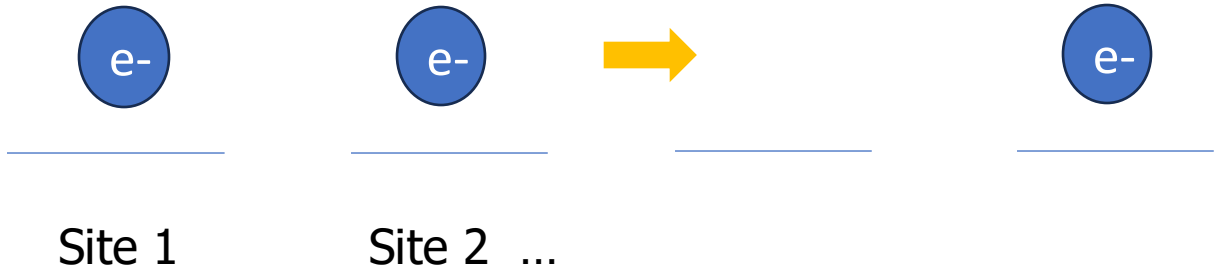
Onsite repulsión U

Hopping energy t



1 electron per site/atom

U>>t Metal insulator transition due to localization of electrons



Partial electronic filling per site/atom

Metallic (if no symmetry breaking)

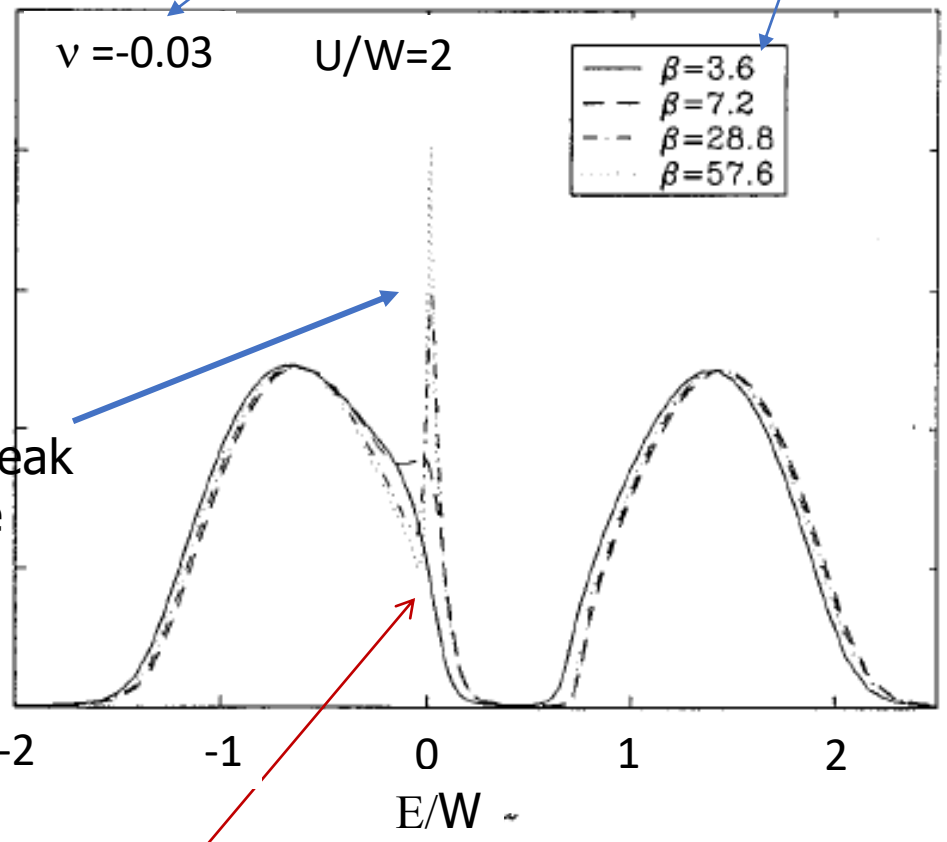
In multiorbital Hubbard models: Mott transition at integer electron filling per site

Doping dependent Density of States

Single-orbital
Hubbard model
hole-doped band

Doping with
respect to half-filling

Different Temperatures



Quasiparticle peak
emerges at the
Hubbard band

Hubbard band
shifts towards
the Fermi level

The metallic state which emerges when the Mott insulator is doped is a correlated metal

Finite density of states at the Fermi level
but correlation features remain

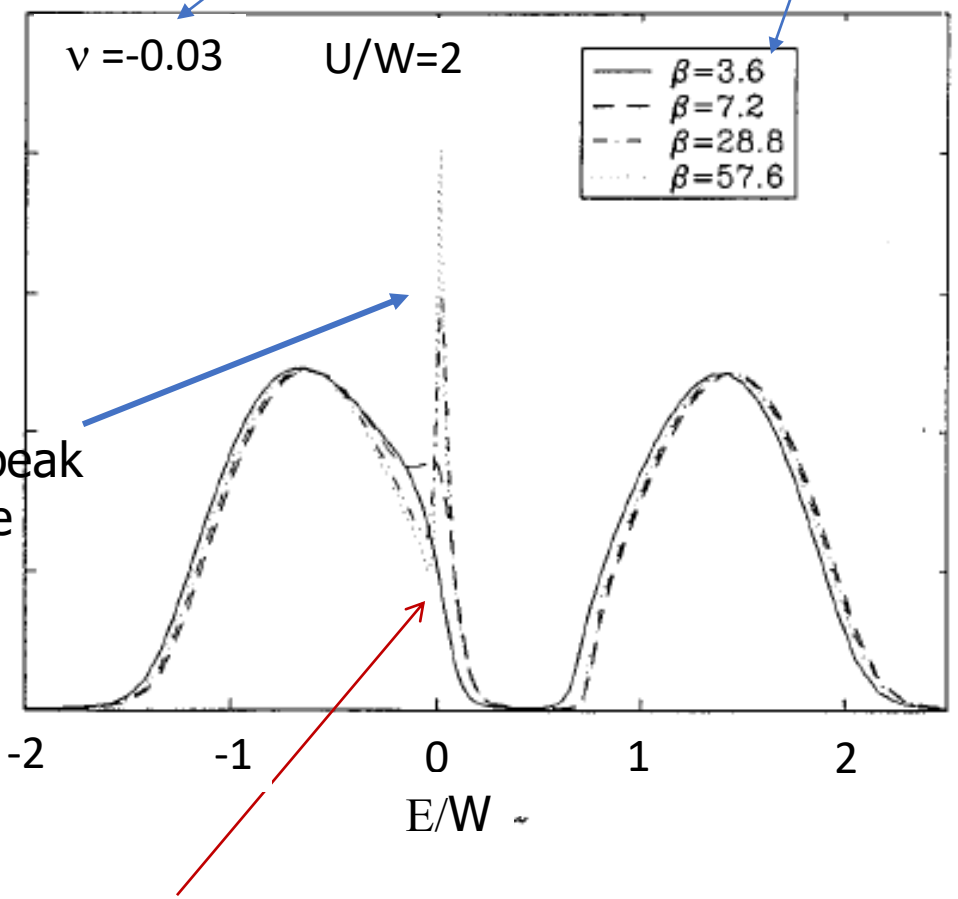
Georges et al , RMP 68, 13 (1996)

Doping dependent Density of States

Single-orbital Hubbard model hole-doped band

Doping with respect to half-filling

Different Temperatures

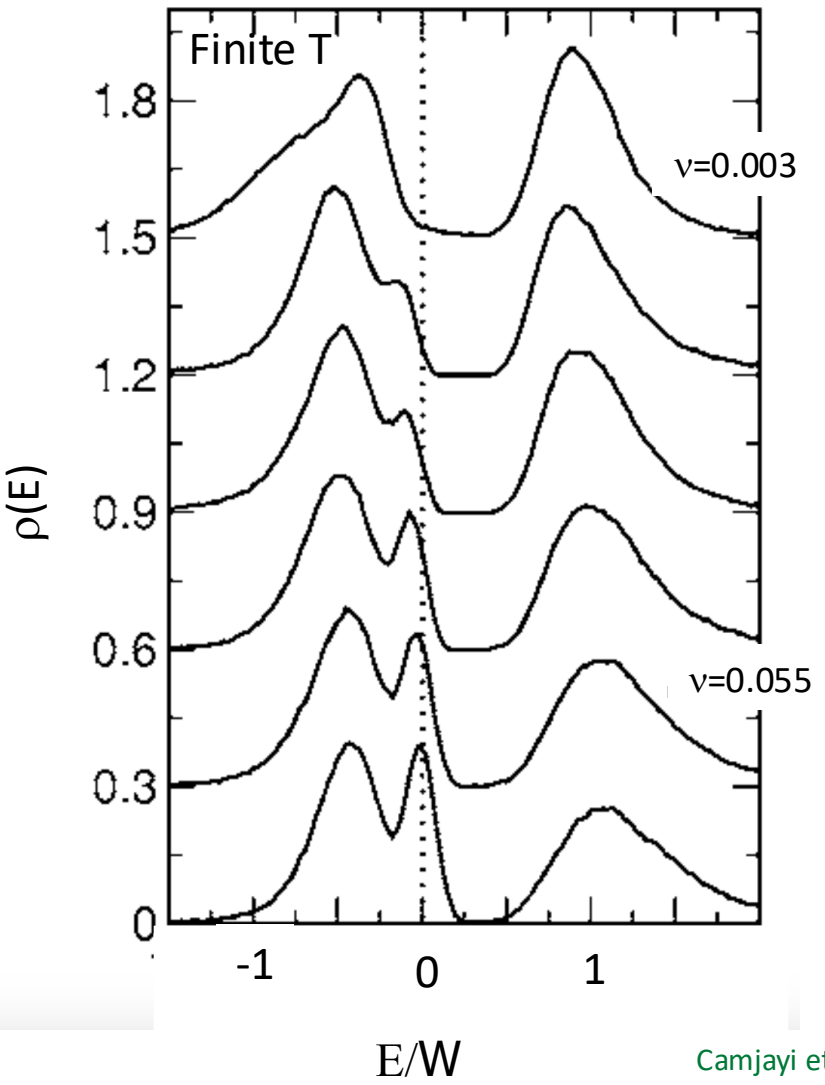


Quasiparticle peak emerges at the Hubbard band

Hubbard band shifts towards the Fermi level

Increasing doping

DMFT



Finite density of states at the Fermi level but correlation features remain

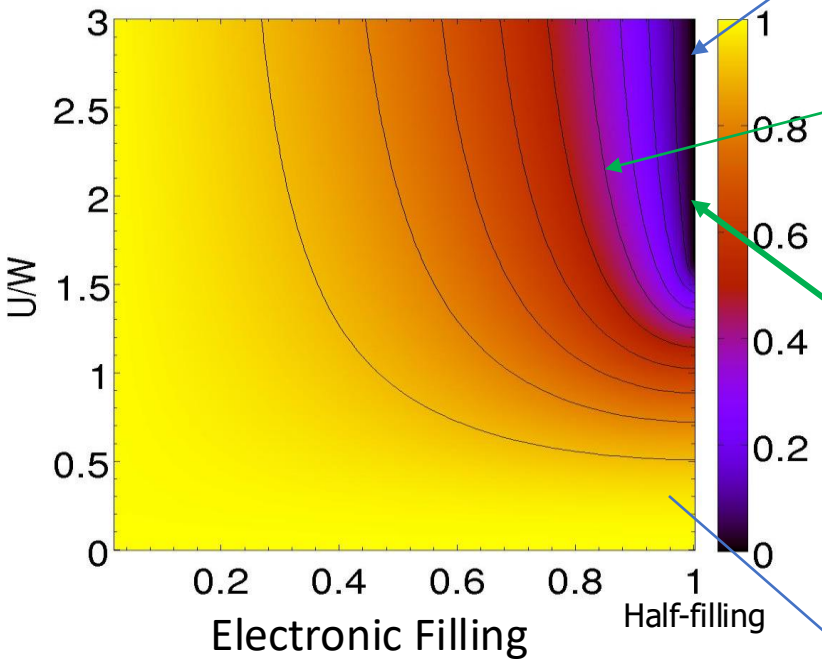
Georges et al , RMP 68, 13 (1996)

Camjayi et al, PRB (2007)

Correlated metal (single orbital Hubbard model)

Quasiparticle weight Z

Band narrowing W*/W



Slave-spin calculation
Single orbital Hubbard in
2D square lattice
Fig: Fanfarillo & EBascones

Mott insulator

Important effect of correlations at intermediate/large U at half-filling but also in a range of doping away from it

Z vanishes in the Mott state

The quasiparticle weigth depends on doping
Doping dependent bandwidth (non-rigid band shift)
The spectrum depends on doping

The strength of the electronic correlations decreases with increasing doping, away from the Mott insulator

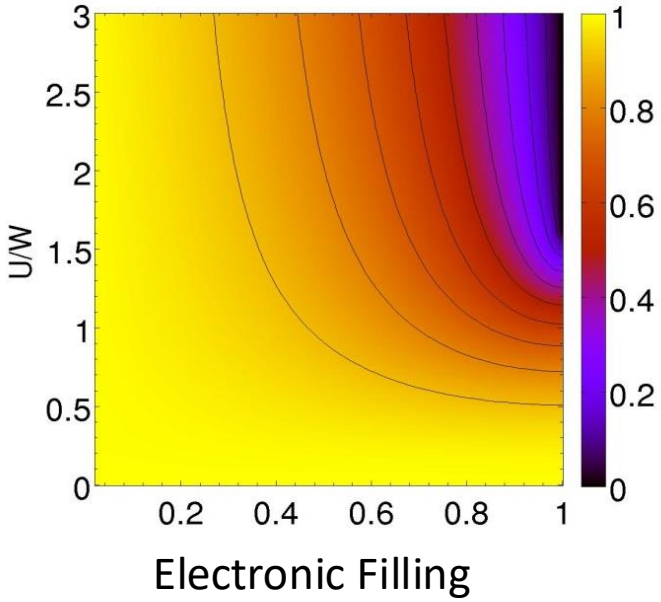
Correlated metal: Local moments & suppression of charge fluctuations

$$C_T = \langle n^2 \rangle - \langle n \rangle^{2=} \langle (\delta n)^2 \rangle$$

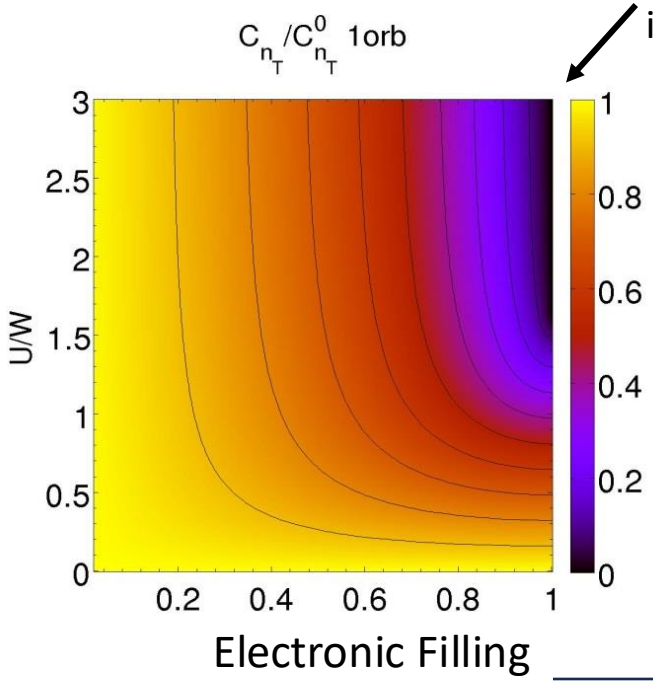
$$n = \langle n \rangle + \delta n$$

Quasiparticle weight Z

Band narrowing W*/W



Suppression of charge fluctuations in the Mott insulator



Localization

Charge fluctuations

Measurement of the degree of localization of the charge

Slave-spin calculation
Single orbital Hubbard in 2D square lattice
Fig: Fanfarillo & EBascones

In the single orbital Hubbard model

Smaller Quasiparticle weight (Larger Correlations) → Charge fluctuations are more strongly suppressed

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Correlated metal: Local moments & suppression of charge fluctuations

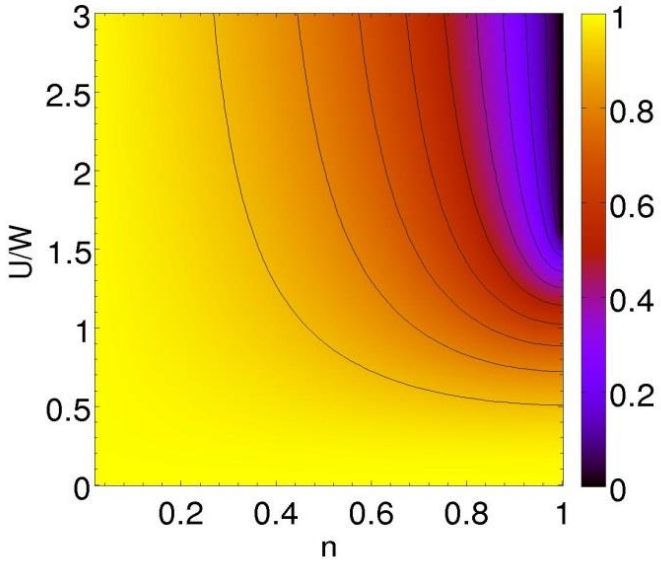
$C_T = \langle n^2 \rangle - \langle n \rangle^{2=} \langle (\delta n)^2 \rangle$

$n = \langle n \rangle + \delta n$

$C_S = \langle S^2 \rangle - \langle S \rangle^2 = \langle S^2 \rangle$

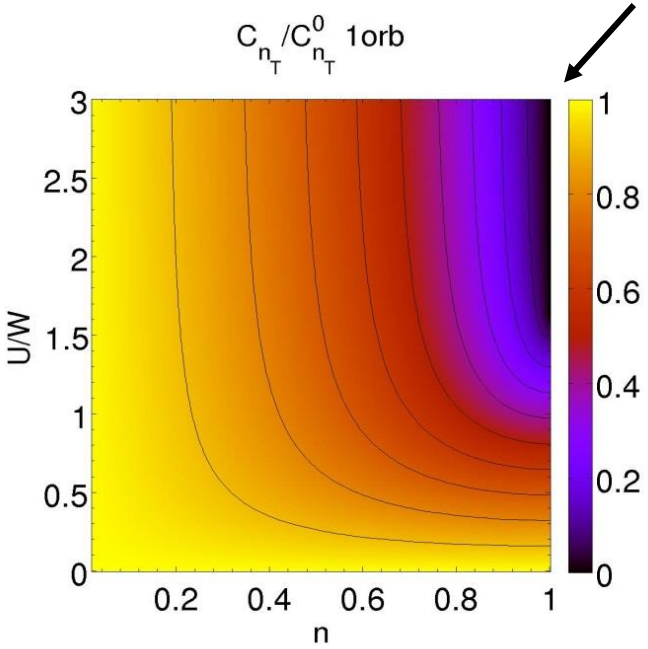
Quasiparticle weight Z

Band narrowing W*/W

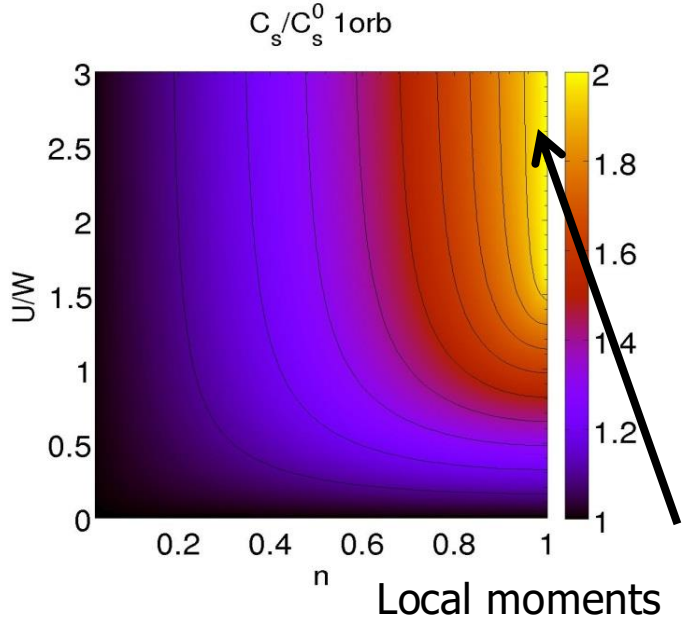


Suppression of charge fluctuations

Localization



C_s larger when atoms are spin polarized even if there is no long range order



Local moments maximally formed in the Mott insulator

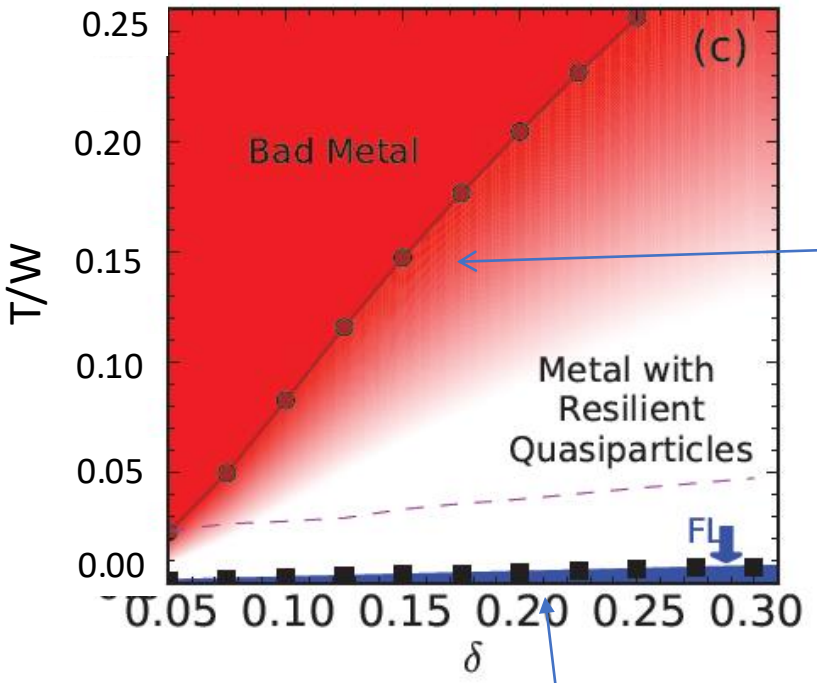
Slave-spin calculation
Single orbital Hubbard in 2D square lattice

Fig: Fanfarillo & EBascones

(Paramagnetic)

Transport properties of a Doped Mott insulator

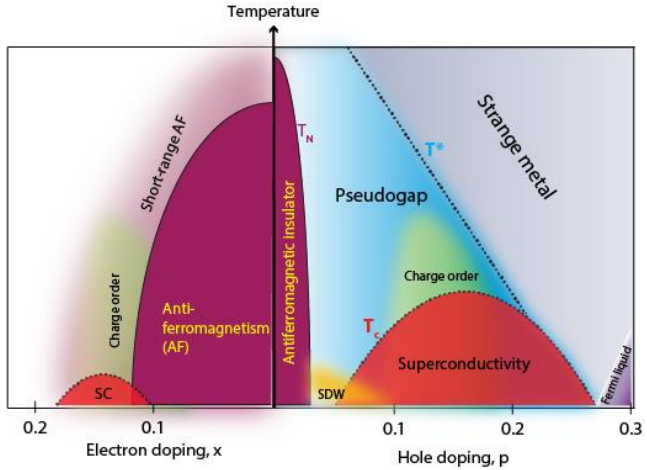
DMFT



Bad metal: the electronic scattering mean free path is smaller than the lattice constant

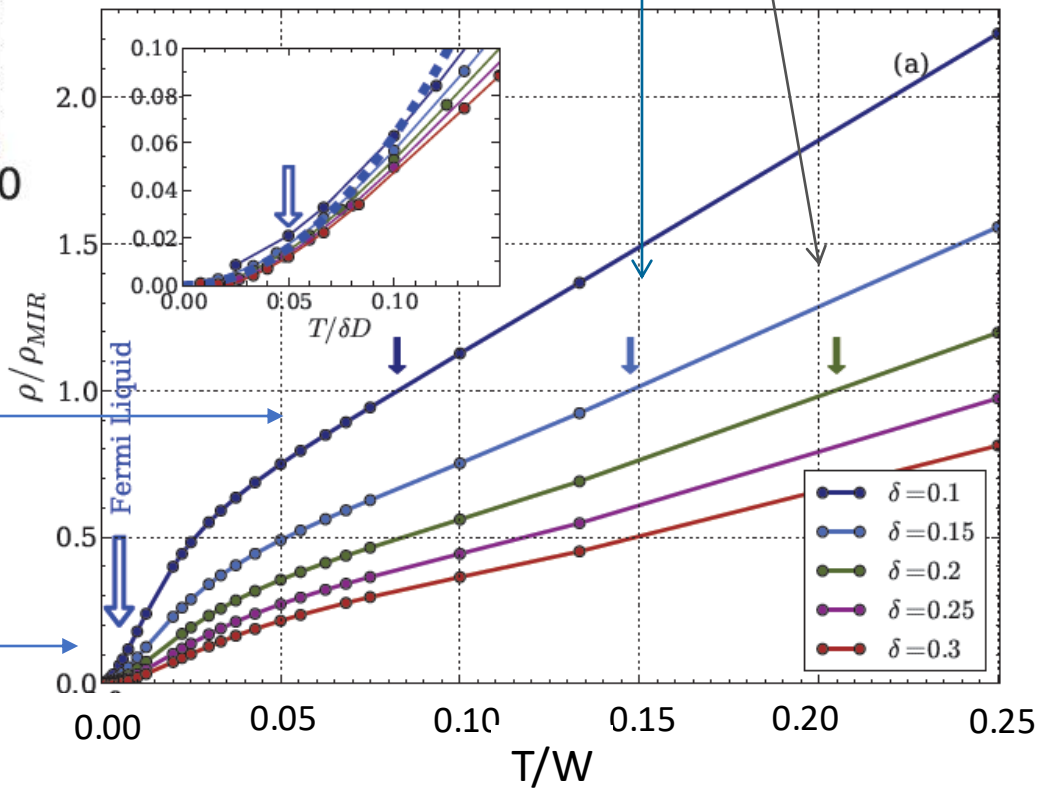
$\rho > \rho_{MIR}$

Mott-Ioffe-Regel limit



Range of temperatures with resistivity linear in temperature

Fermi liquid behavior at very low temperatures



Both the scattering rate and the quasiparticle weight depend on temperature

Deng et al, PRL 110, 086401 (2013)

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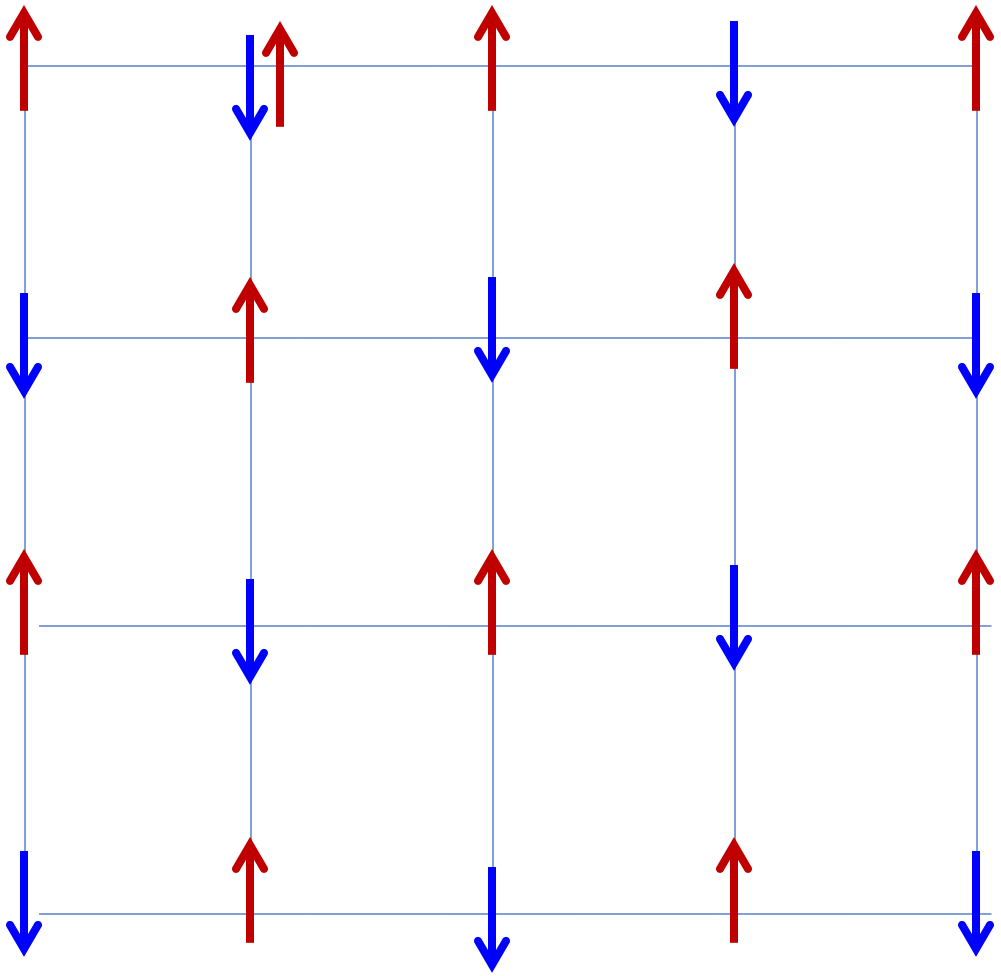
Doping a Mott insulator. Disappearance of Antiferromagnetic Order



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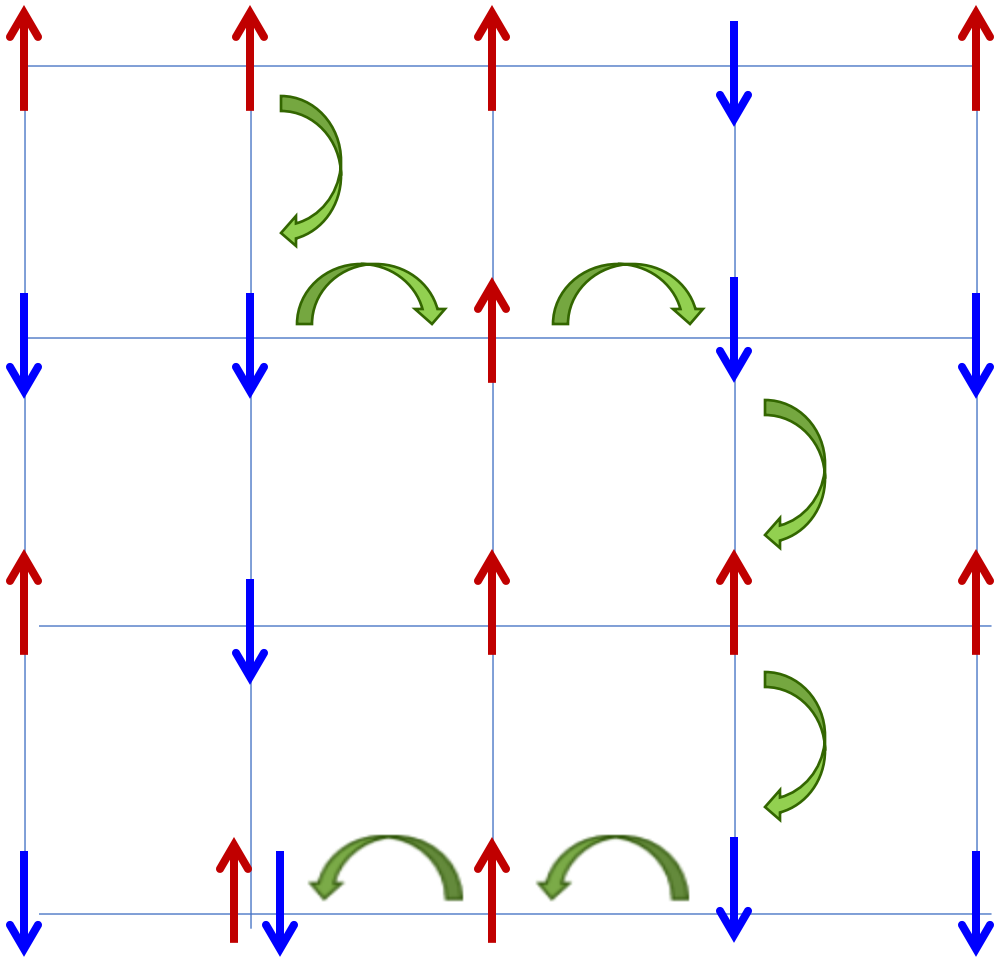
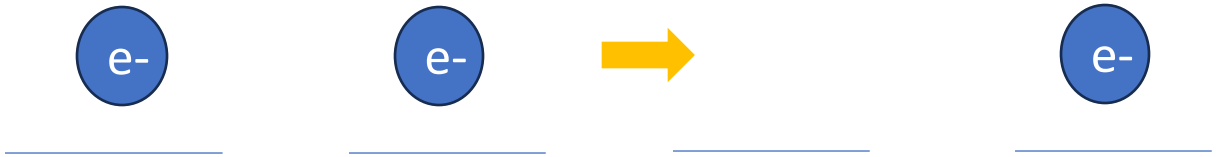
Doping a Mott insulator. Disappearance of Antiferromagnetic Order



Mass enhanced
by AF correlation
Tendency to
Localization due to AF
(Spin bags)

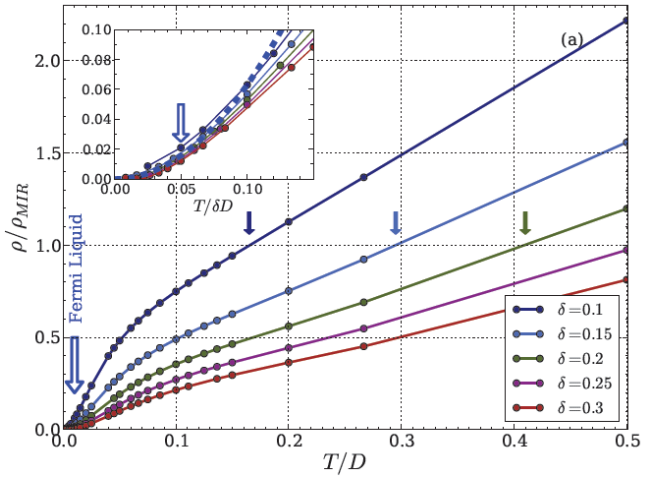
Antiferromagnetic ordering is destroyed by doping

Doped Mott insulator



Partial electronic filling per site/atom

A doped Mott insulator is metallic
(if no symmetry breaking) but the effect of correlations (small quasiparticle weight, Hubbard bands, tendency to localization…) remain if the doping is not too large.

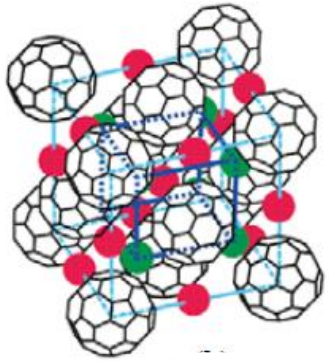


Deng et al, PRL 110, 086401 (2013)

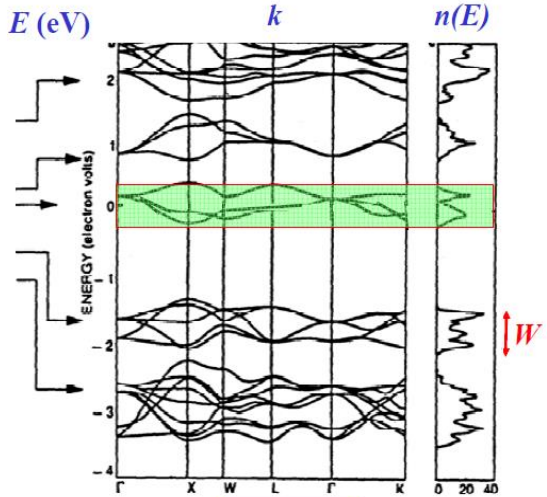
The resistivity in doped Mott insulators is large and presents an anomalous temperature dependence

Doping the Mott insulator tends to suppress the antiferromagnetic tendencies

Multi-orbital systems



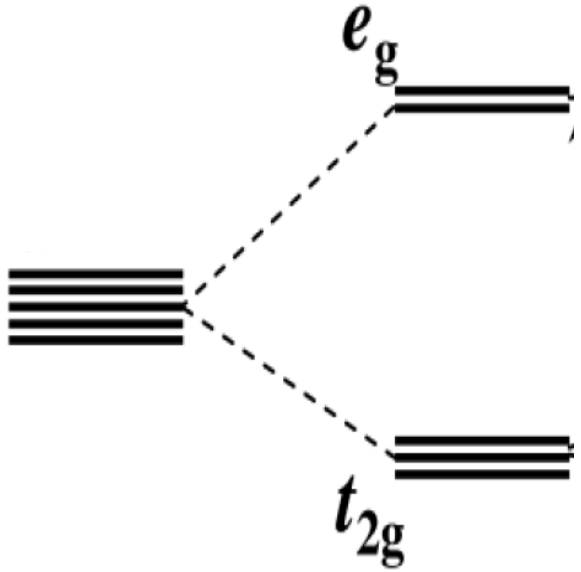
A_3C_{60}



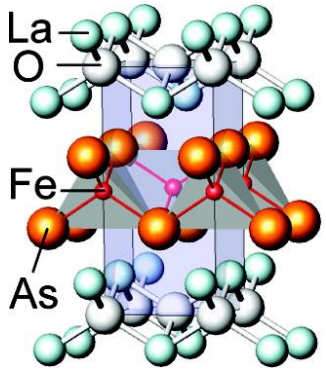
Alloul, EPJ Web of Conf. 23, 15 (2012)

Erwin & Pickett, Science 254, 842 (1991)

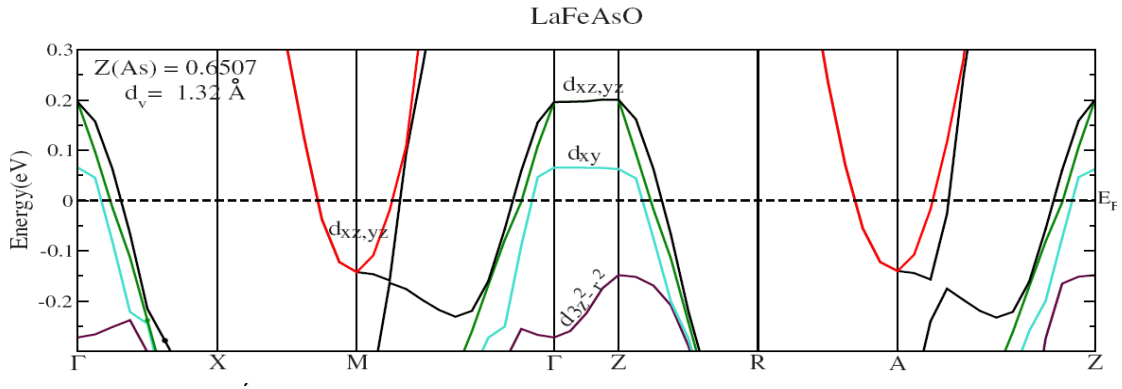
Oxides with cubic symmetry



Iron superconductor



Kamihara et al, JACS, 130, 3296 (2008)



Vildosola et al, PRB 78, 064518 (2008)

Multi-orbital systems: New Interaction Scales

Simplified Hamiltonian for interactions in multi-orbital systems

Interactions restricted to electrons in the same atom. Only density-density interactions

Intra-orbital repulsion

Inter-orbital Repulsion (different spin)

Inter-orbital Repulsion (same spin)

N orbitals

$$U\sum_{m}\hat{n}_{m\uparrow}\hat{n}_{m\downarrow}+U'\sum_{m\neq m'}\hat{n}_{m\uparrow}\hat{n}_{m'\downarrow}+(U'-J_{H})\sum_{m<m',\sigma}\hat{n}_{m\sigma}\hat{n}_{m'\sigma}$$

Intraorbital interaction U

m, m' label the orbitals

Interorbital interaction U'

Hund's coupling

Reduces the repulsion between electrons with parallel spin

spin

Assume all orbitals are equivalent

Multi-orbital systems: New Interaction Scales

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Intraorbital interaction U

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Interorbital interaction U'

Hund's coupling

spin

Hund's coupling reduces the repulsion between electrons with parallel spin

With rotational invariance

$U' = U - 2J_H$

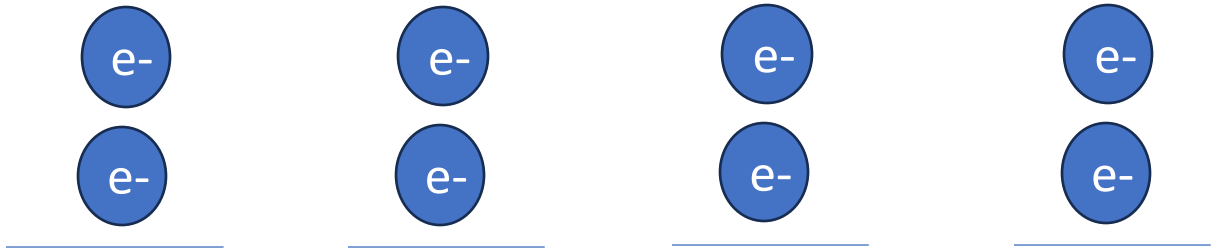
Two interaction parameters in the model U, J_H

Maximum $J_H = U/3$

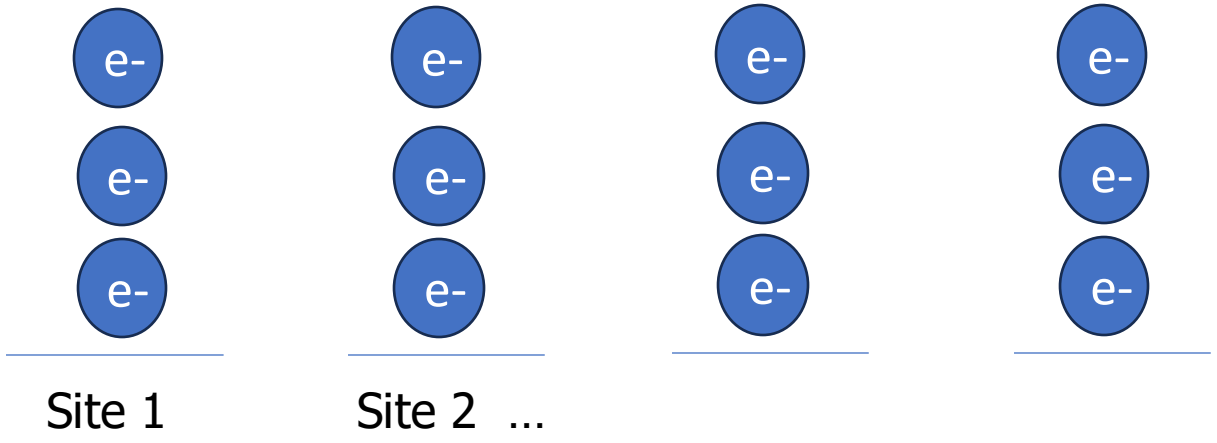
Assume all orbitals are equivalent

Multi-orbital systems: Insulators also away from half-filling

1 electron/site



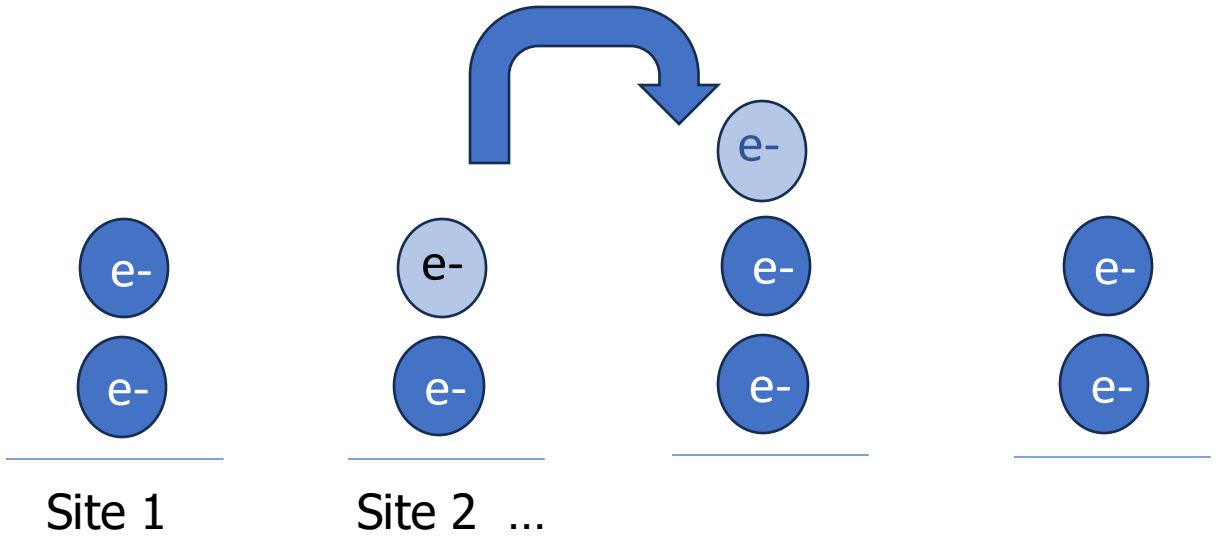
2 electrons/site



3 electrons/site

Mott insulators for each
integer number of electrons per unit cell
if interaction U is large enough
(except full filling = band insulator)

Multi-orbital systems: Interaction at which the Mott transition takes place



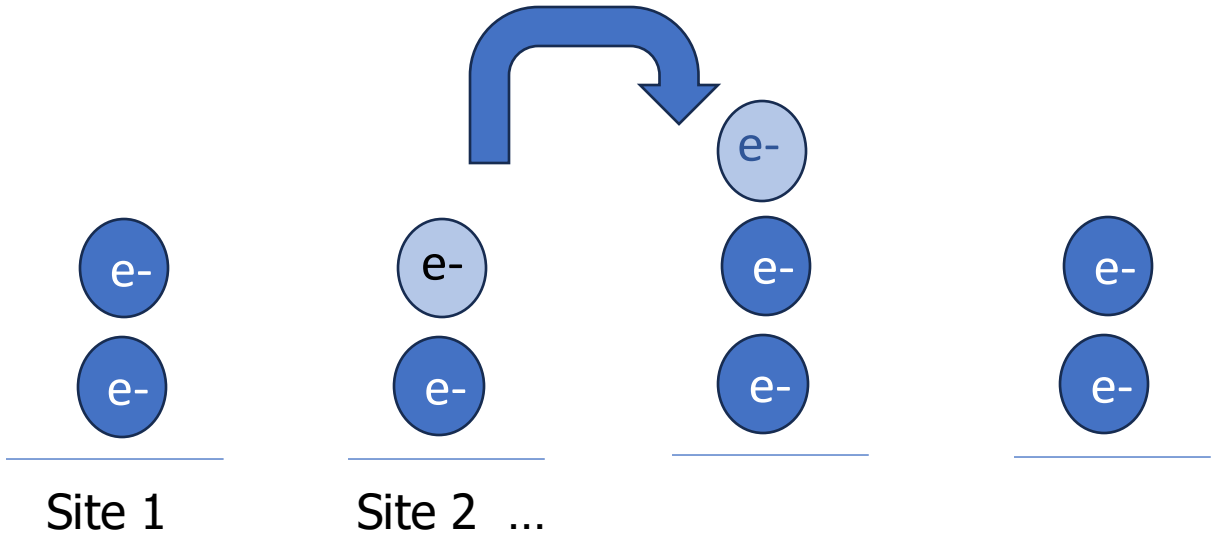
Interaction Gap for Hopping

$$E(n+1)+E(n-1)-2\,E(n)$$

n: integer
(number of electrons/site)

Assume all orbitals are equivalent

Multi-orbital systems: Interaction at which the Mott transition takes place



Interaction Gap for Hopping

$$E(n+1)+E(n-1)-2\,E(n)$$

n: integer
(number of electrons/site)

Half-filling: $n=N/2$

$U+(N-1)J_H$

N number of orbitals

Away from half-filling but n integer:

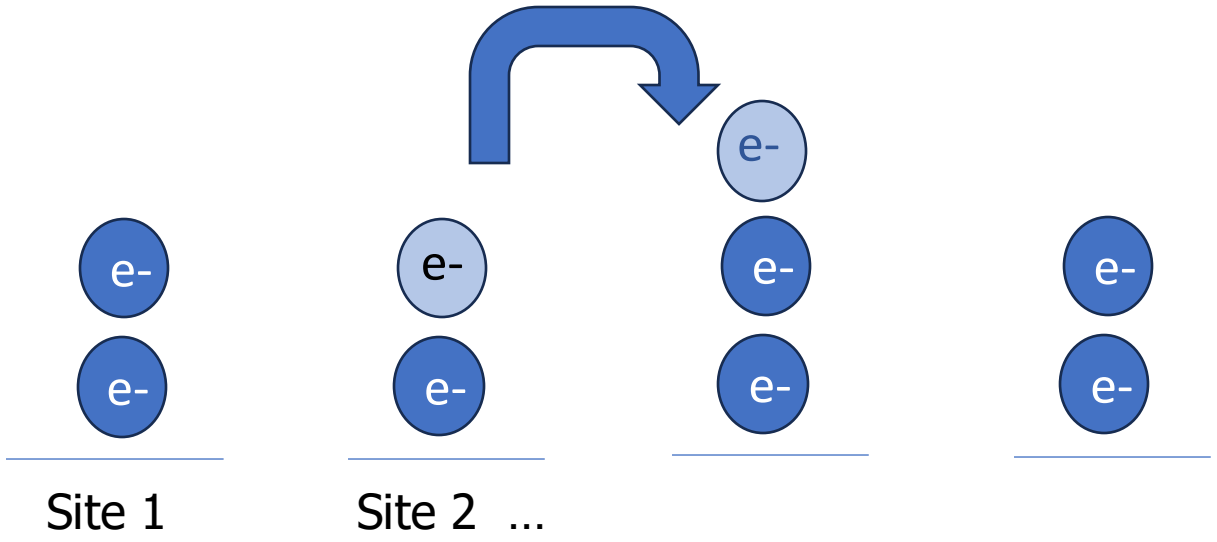
$U-3J_H$

The interaction U at which the Mott transition will take place will depend on the number of orbitals N, number of electrons/site n and Hund's coupling J_H

Han et al PRB 58, R4199 (1998)

Assume all orbitals are equivalent

Multi-orbital systems: Interaction at which the Mott transition takes place



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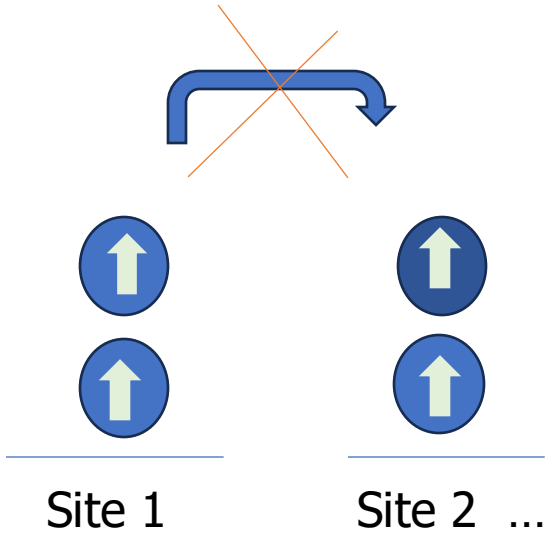
Away from half-filling but n integer:

$U-3J_H$

Opposite effect of Hund's coupling at half-filling and away from it

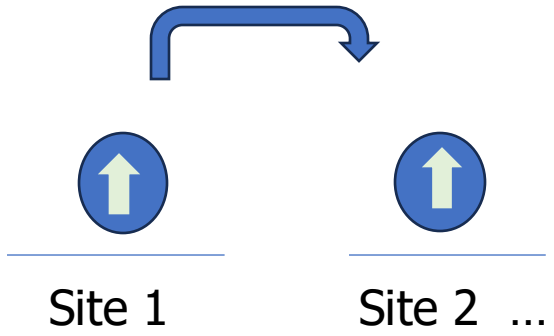
Multi-orbital systems: Interaction at which the Mott transition takes place

Example: 2 orbital system



Hund's coupling polarizes the spins

At half-filling, it is only posible to add an electron with opposite spin



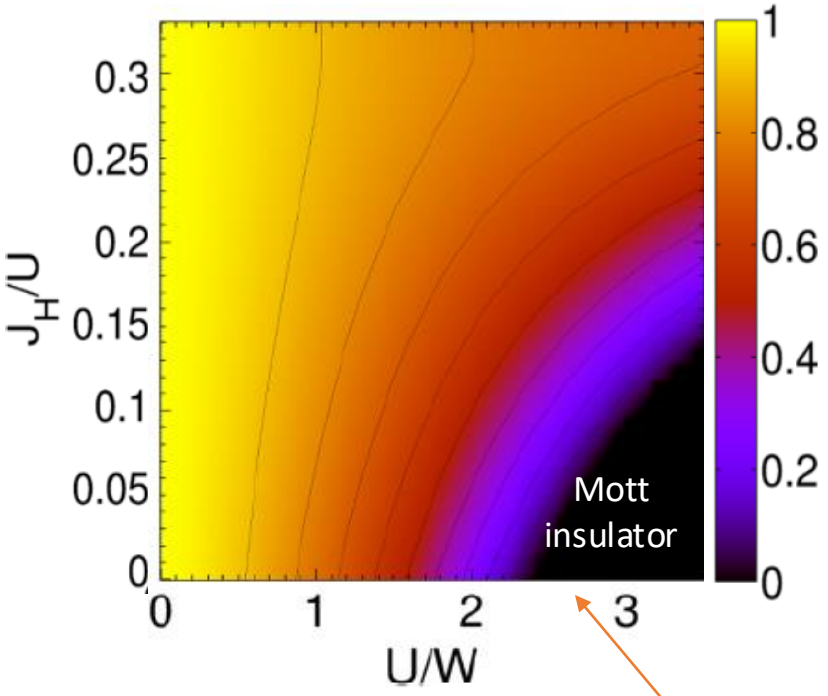
Away from half-filling, the hopping does not act against Hund's tendencies

Opposite effect of Hund's coupling at half-filling and away from it

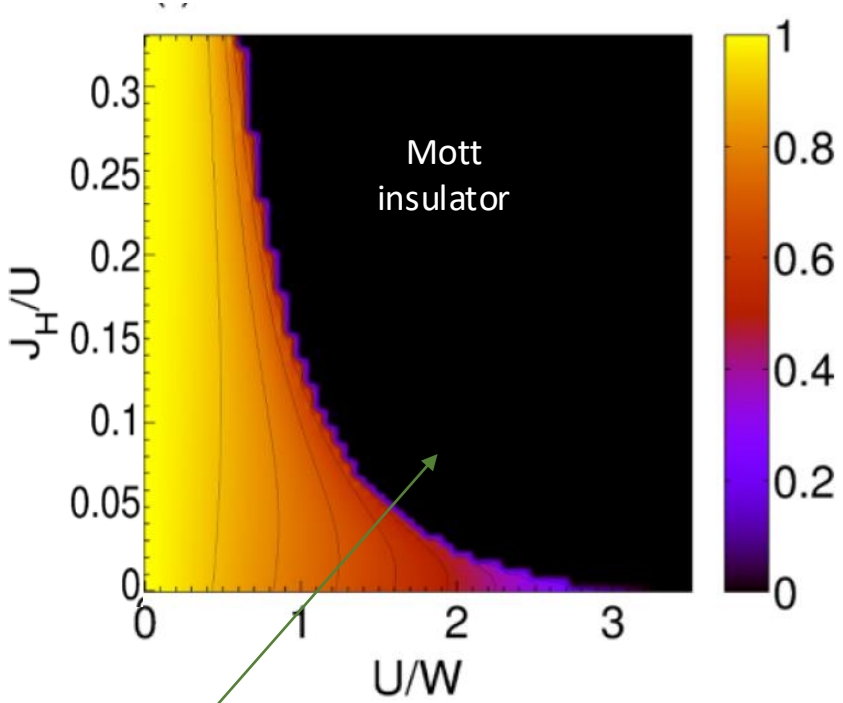
Multi-orbital systems: Interaction at which the Mott transition takes place

Color Plot: Quasiparticle weight as a function of interactions U and J_H for 3 orbital system

1 electron/site



3 electrons/site (Half-filling)



W: bandwidth

Opposite dependence on Hund's coupling J_H
for the emergence of Mott insulating state (black)

Fanfarillo & Bascones PRB 92, 075136 (2015)
De'Medici et al PRL 107, 255701 (2011)

leni.bascones@csic.es

Multi-orbital systems: Interaction at which the Mott transition takes place

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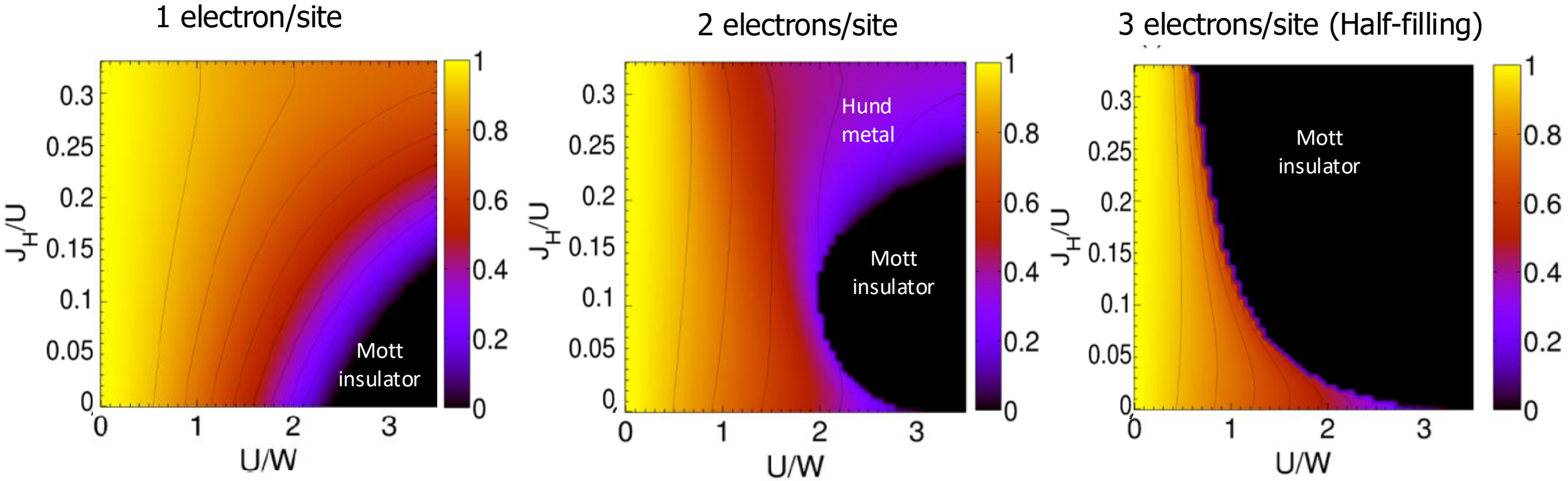

W: bandwidth

Fanfarillo & Bascones PRB 92, 075136 (2015)
De'Medici et al PRL 107, 255701 (2011)

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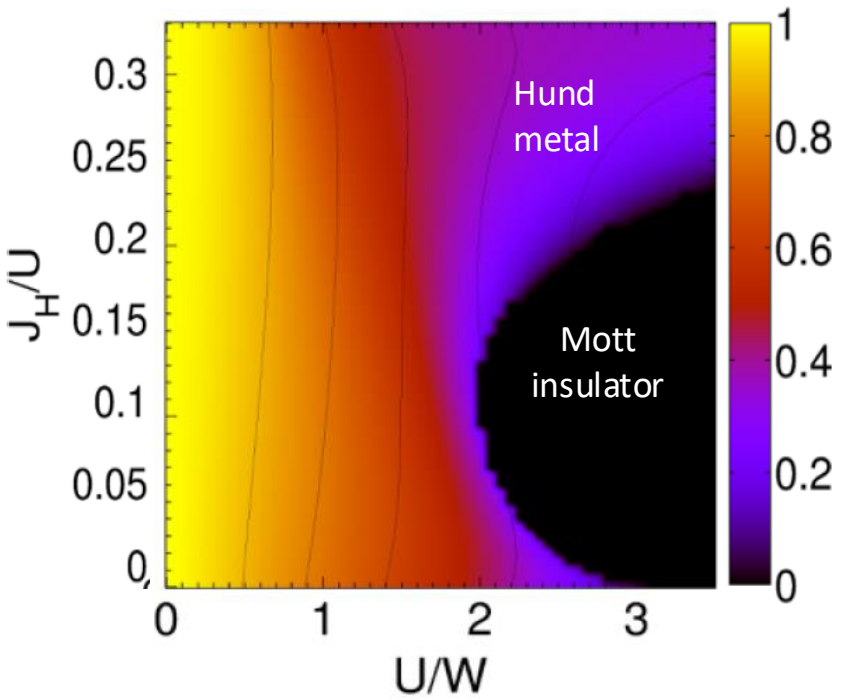
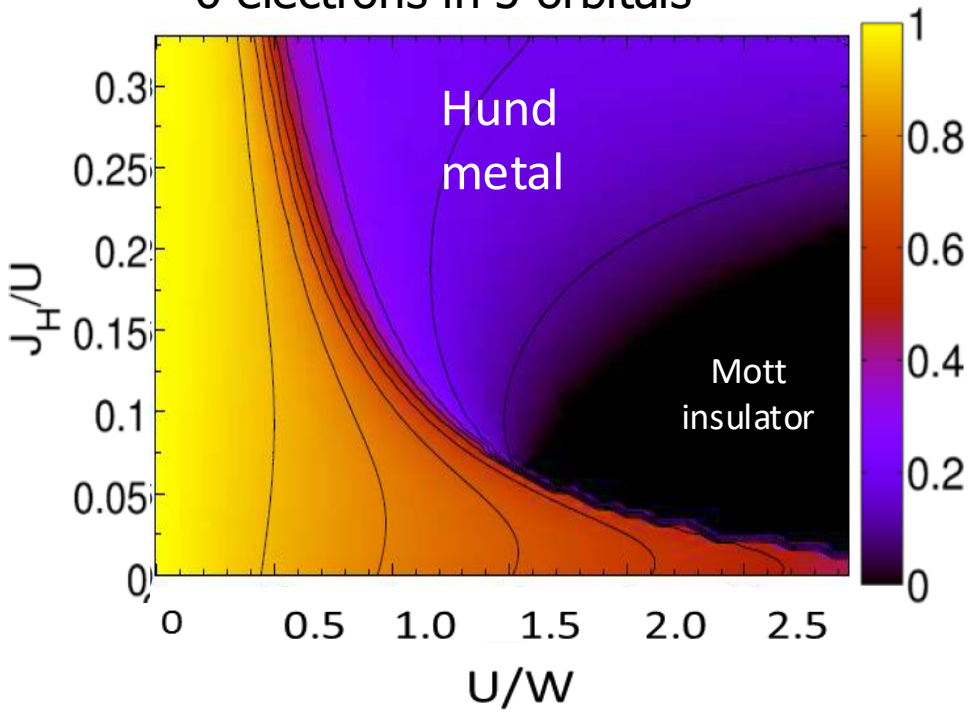
Multi-orbital systems: Interaction at which the Mott transition takes place

Color Plot: Quasiparticle weight as a function of interactions U and J_H

2 electrons in 3 orbitals



6 electrons in 5 orbitals



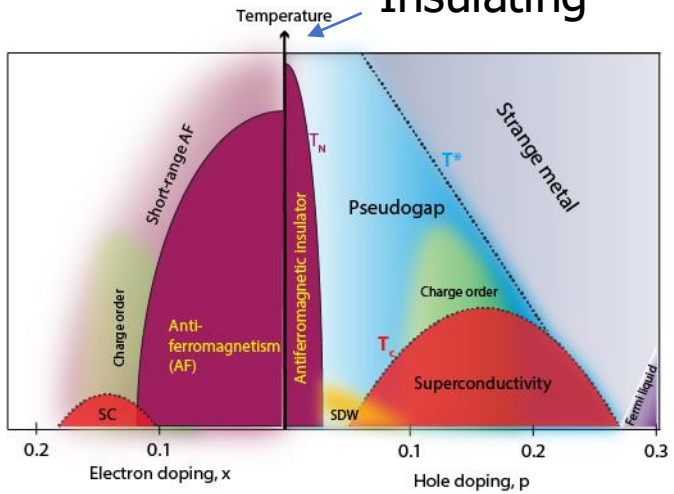
Fanfarillo & Bascones
PRB 92, 075136 (2015)
De'Medici et al PRL 107, 255701 (2011)

Hund metal:

Strongly correlated metal (small Z) due to the formation of local moments but charge fluctuations are only partially suppressed (more metallic than a priori expected for this small Z)

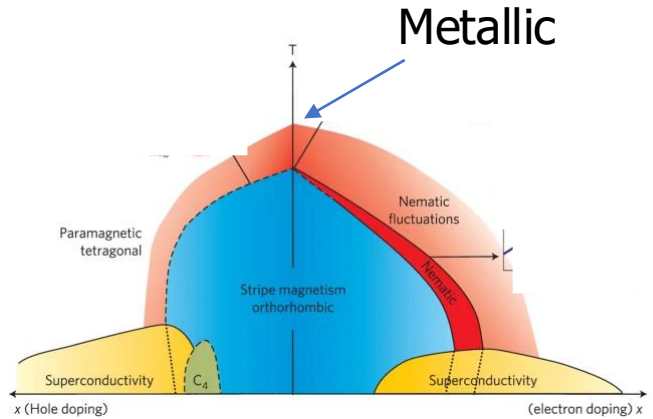
High-Tc Iron superconductors: (at the verge of) Hund metals

High-Tc Cuprates



Single orbital Hubbard model
& Mott insulators when undoped

High-Tc Iron superconductors



6 electrons in 5 orbitals
(5 Fe-d orbitals)

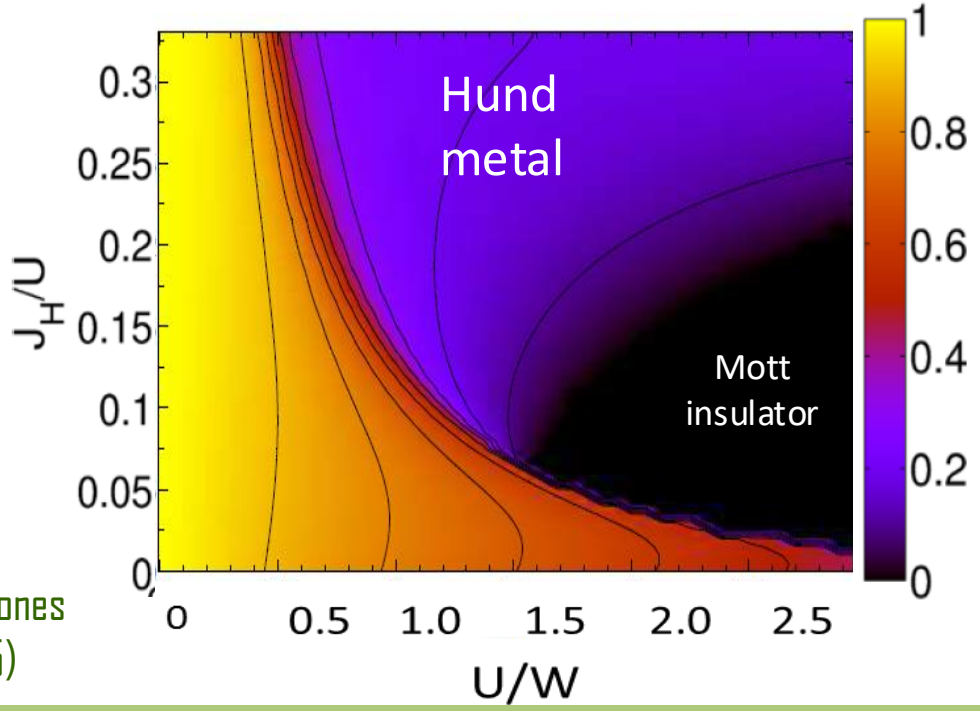


Fig: Fanfarillo & Bascones
PRB 92, 075136 (2015)

In iron superconductors
not all the orbitals
are equivalent

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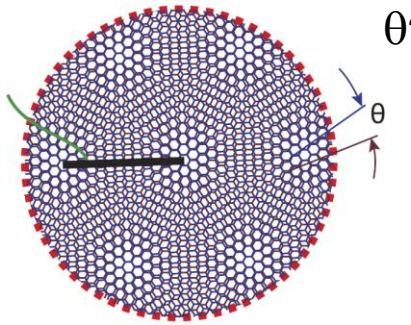
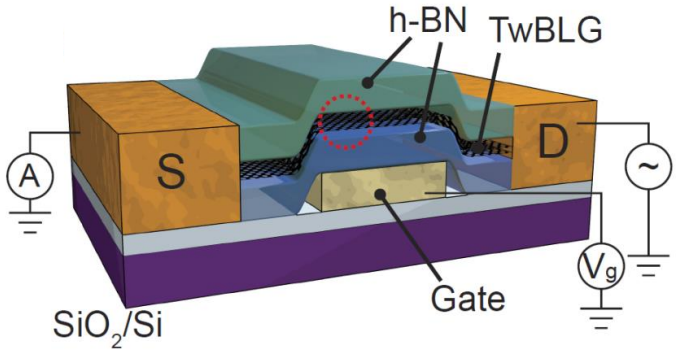
Flat bands and Gate Doping in Magic Angle Twisted Bilayer Graphene

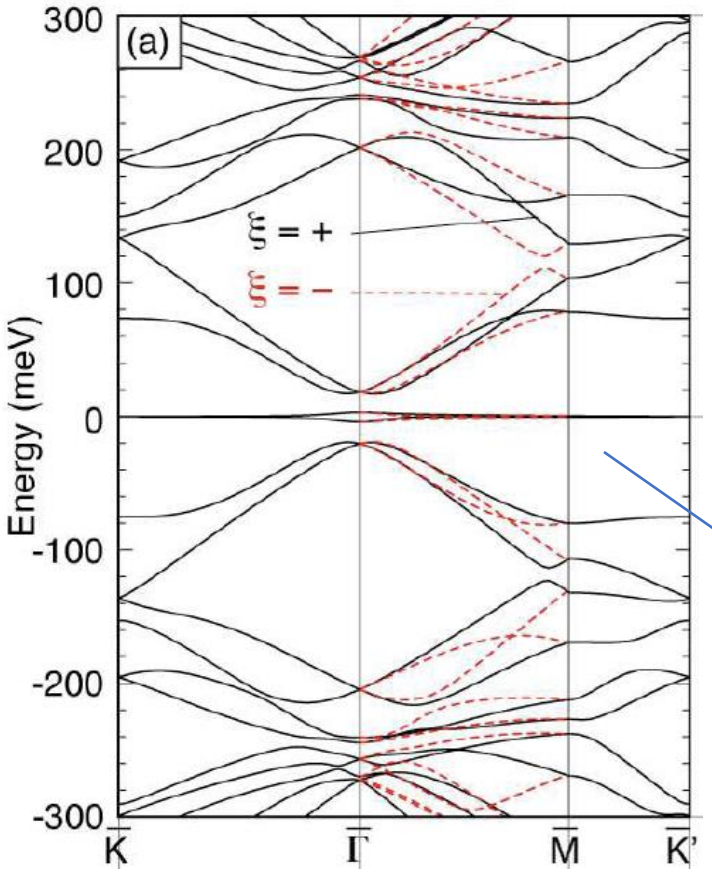


θ~1.1º

Large moiré unit cell
(λ ~13 nm)

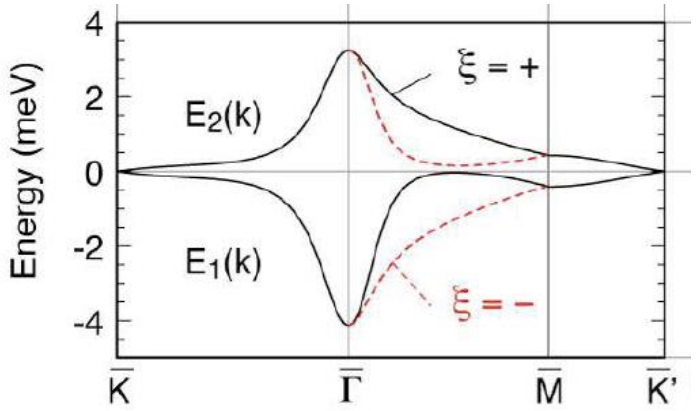


2 valleys from Diracs at K and K' in graphene



CNP
(undoped)

4 flat bands (2 per valley)



Up to 4 electrons or 4 holes per unit cell

Bands very flat: sensitivity to electronic correlations

Plethora of correlated states (including superconductivity)

Cao et al, Nature 556, 43 and 80 (2018) Cao et al, PRX 8, 031087 (2016),
Suarez Morell et al, PRB 82, 121407 (2010), Bistritzer & Macdonald,. PNAS 108, 12233 (2011), Koshino et al, PRX 031037 (2018)

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Flat bands and Gate Doping in Magic Angle Twisted Bilayer Graphene

Resistivity as a function of doping and temperature

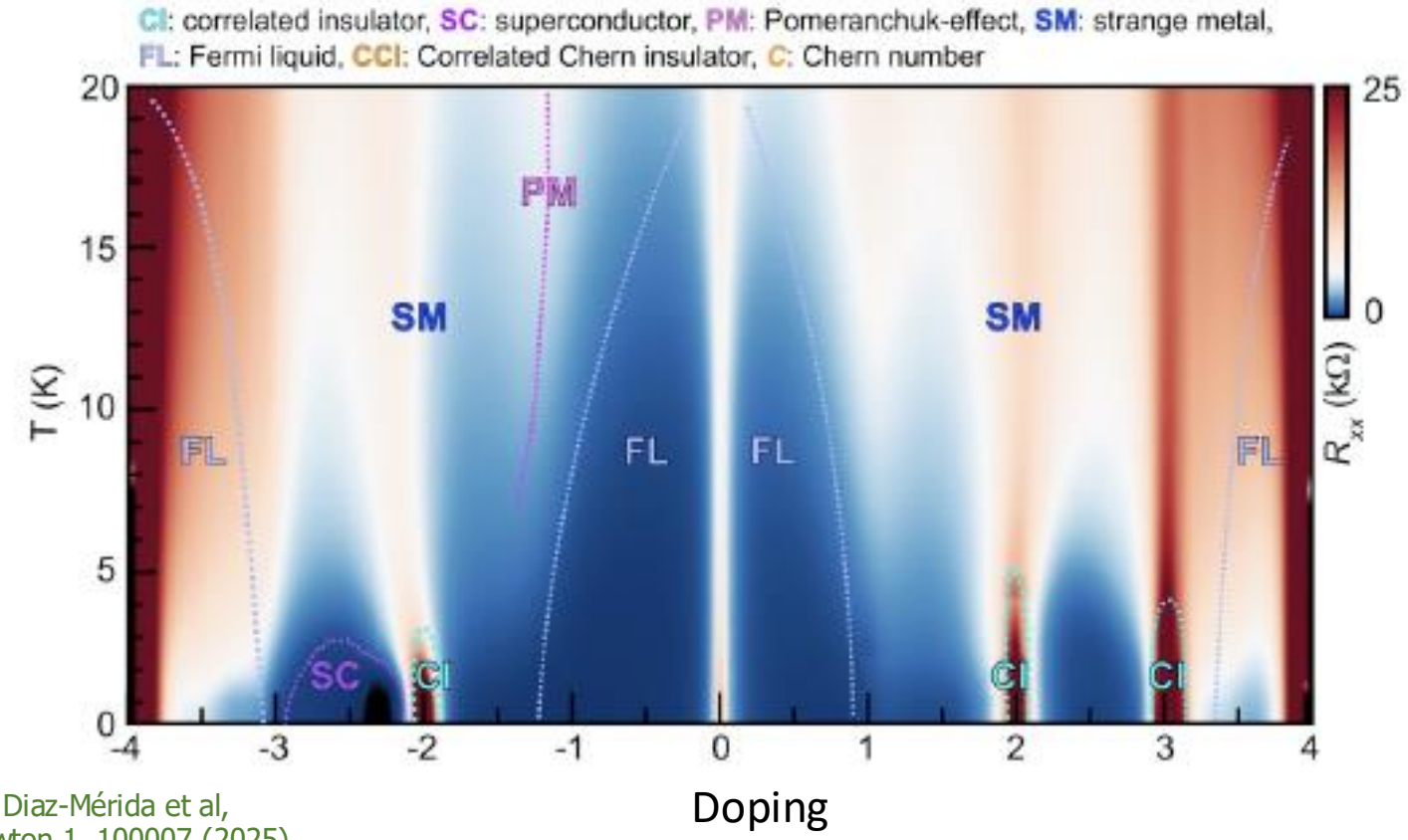
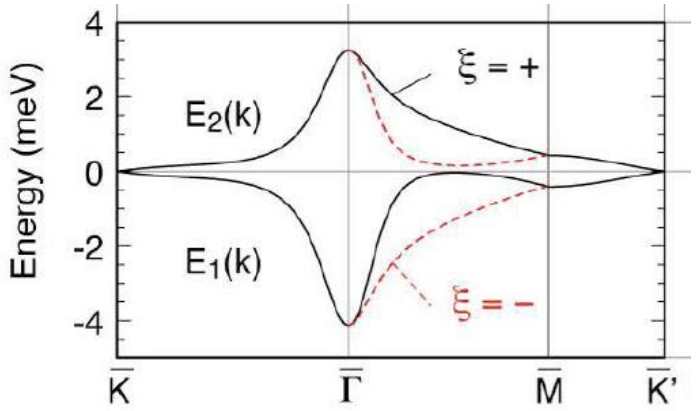


Fig:Diaz-Mérida et al,
Newton 1, 100007 (2025)

4 flat bands (2 per valley)



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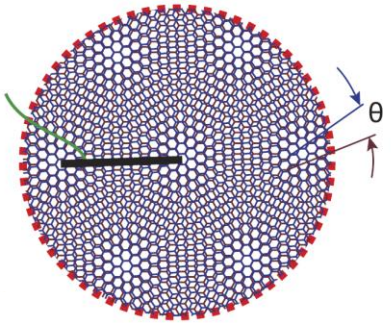

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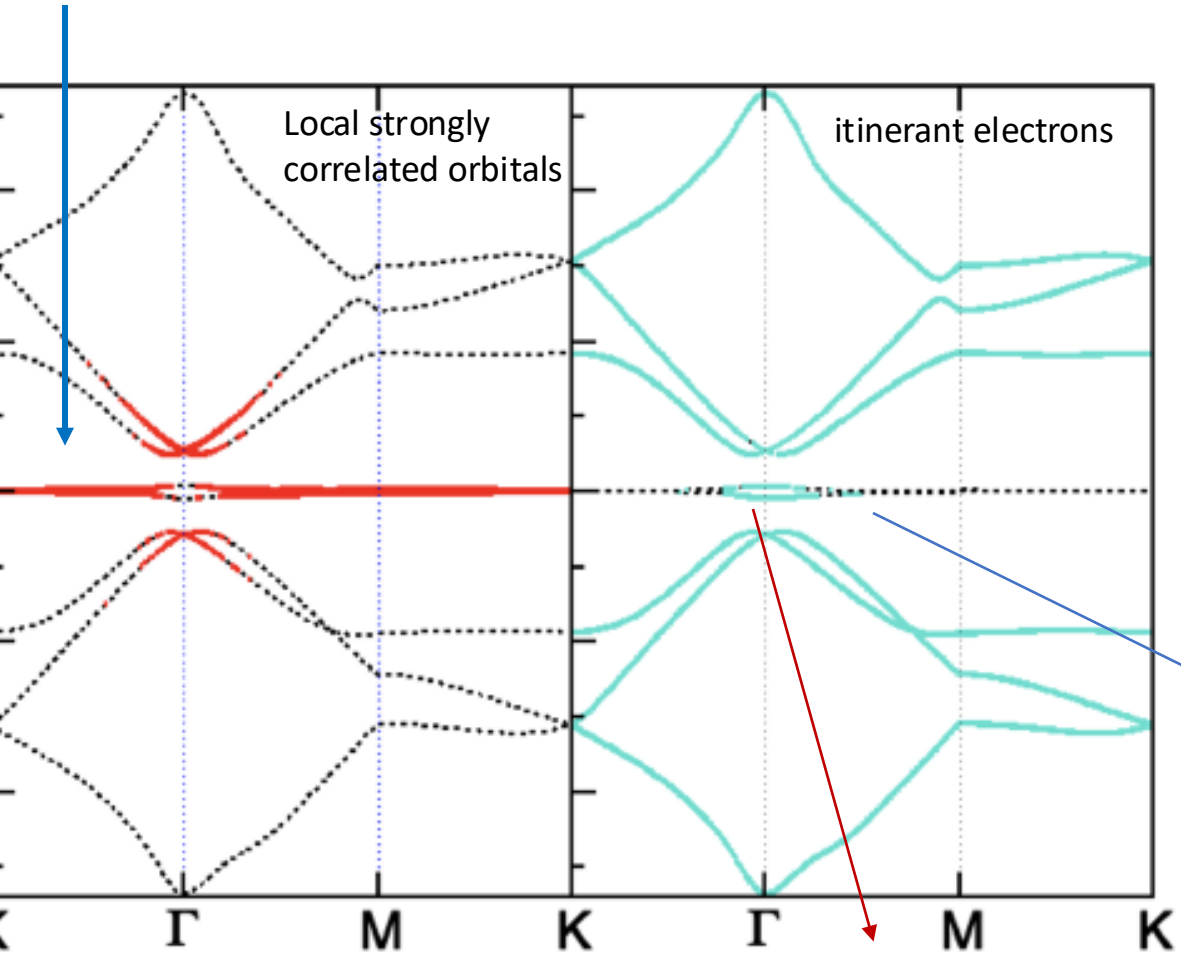
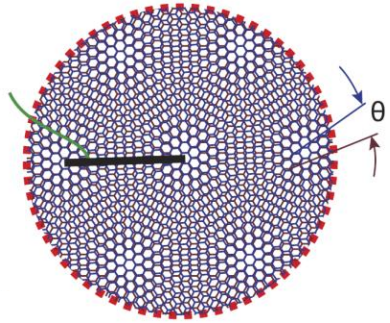
Heavy Fermion description of Magic Angle Twisted Bilayer Graphene (TBG)

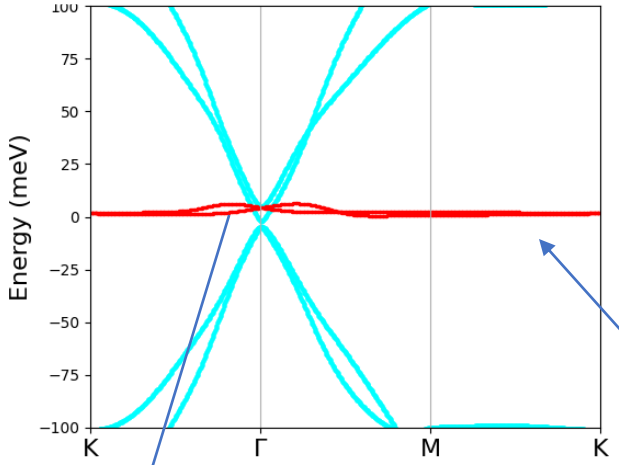
Local electrons: Flat and strongly correlated orbitals centered at the center of the moiré unit cell in the flat bands except around Γ (topology of TBG).



Itinerant electrons at Γ



Before hybridization



Topology of the Flat Bands

The Flat electrons want to be Mott

See:
Haule et al, arXiv:1901.09852 (2019)
Jiang et al, Nature 573, 91 (2019)

Calderón & Bascones, PRB 102, 155149 (2020),
Song and Bernevig, PRL 129, 047601 (2022)

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Momentum selective incoherence in the band spectrum at CNP (undoped)

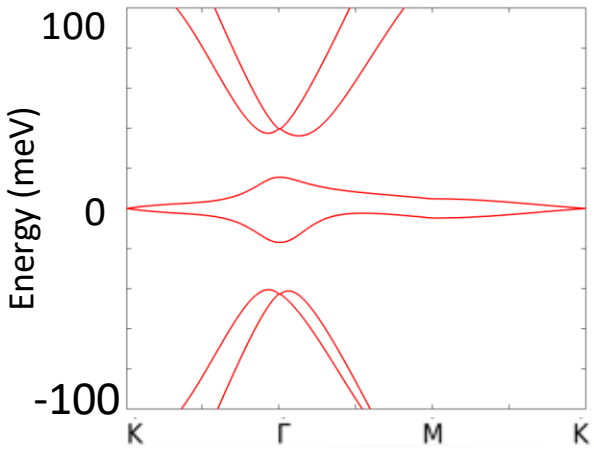
w_0/w_1=0.85

U=32 meV

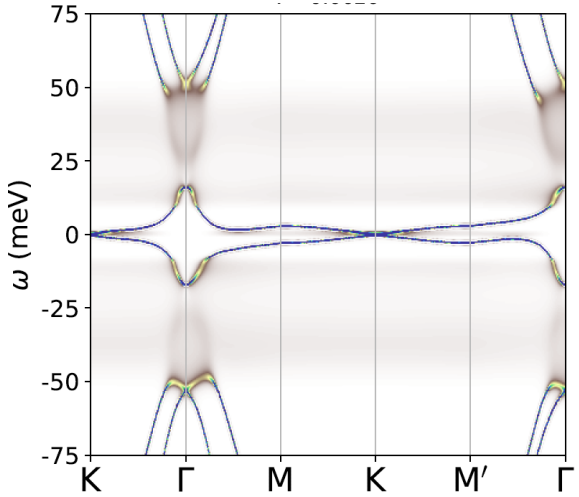
@ T=5.8 K

No symm breaking

θ~1.25º Non-interacting



DMFT + H (theory)



Not very narrow bands. Little incoherence

Band shape similar to non-interacting bands (a bit renormalized)

Momentum selective incoherence in the band spectrum at CNP (undoped)

w_0/w_1=0.7

ε=16

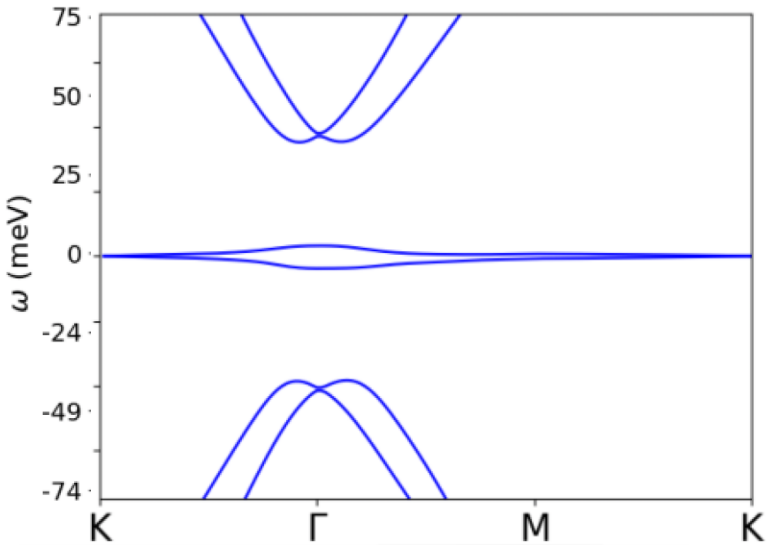
U=32 meV

@ T=5.8 K

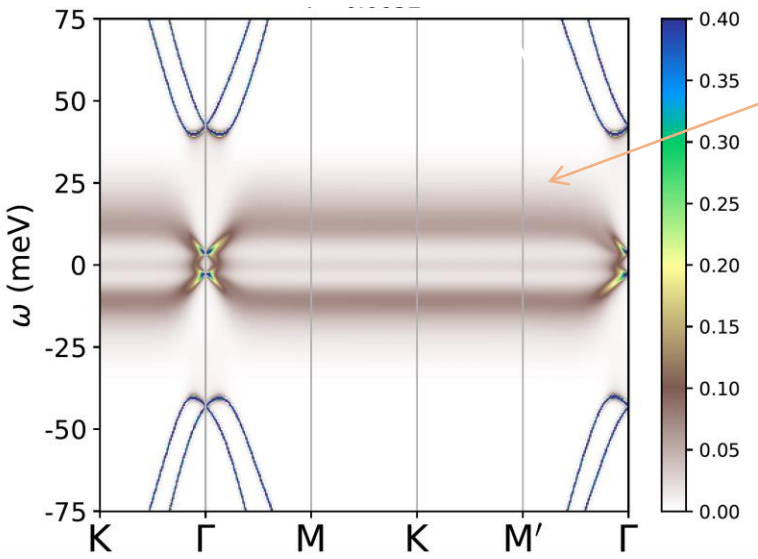
No symm breaking

1.08º

Non-interacting



DMFT +H



Incoherent (Hubbard band) Local moment

~ U

A.Datta, MJ Calderón, A. Camjayi, EBascones, Nature Comms 14, 5036 (2023)

MJ Calderón, A Camjayi, A Datta, EBascones, PRB 112 L041126 (2025)

See also:
M. Haule, E. Andrei, K. Haule, arXiv:1901.09852 (2019),
Rai et al, PRX 14, 031045 (2024)

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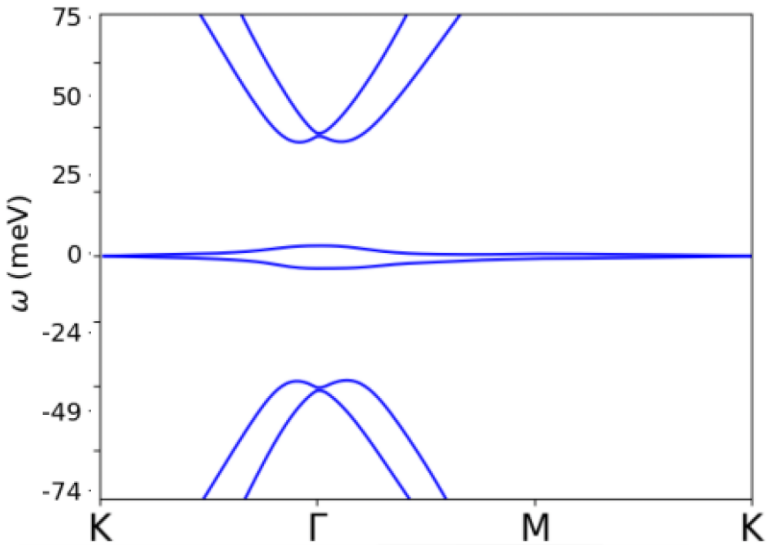
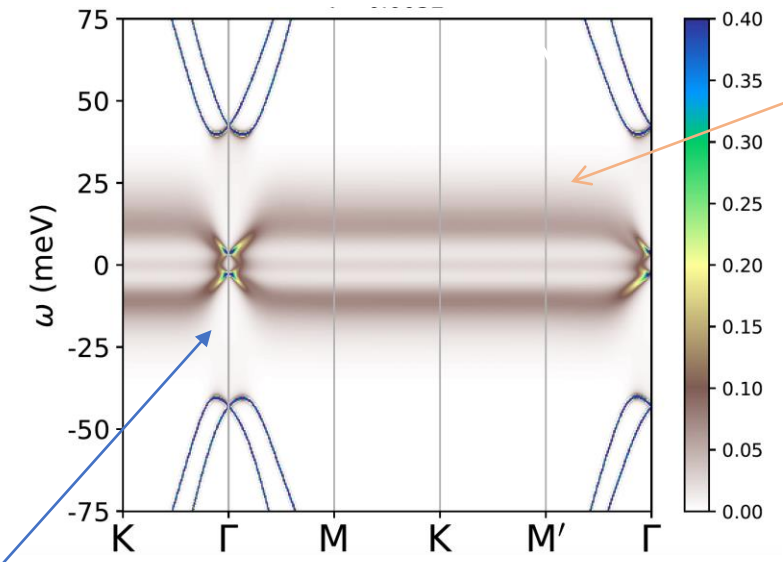


DMFT +H



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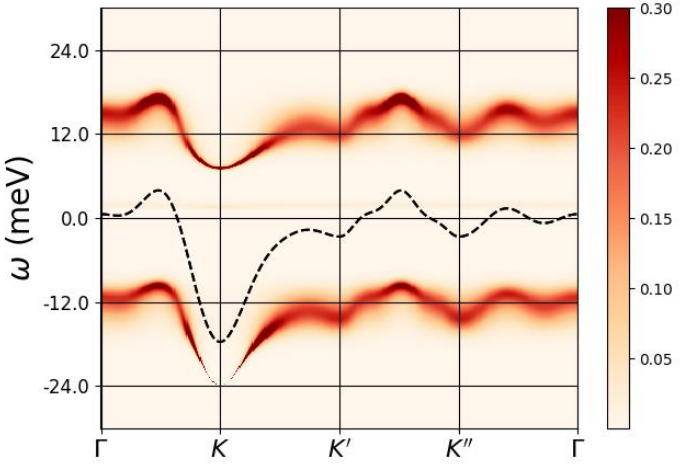
Momentum selective incoherence: (different around Γ)



Mott insulator

See also:
M. Haule, E. Andrei, K. Haule, arXiv:1901.09852 (2019),
Rai et al, PRX 14, 031045 (2024)

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ε=16

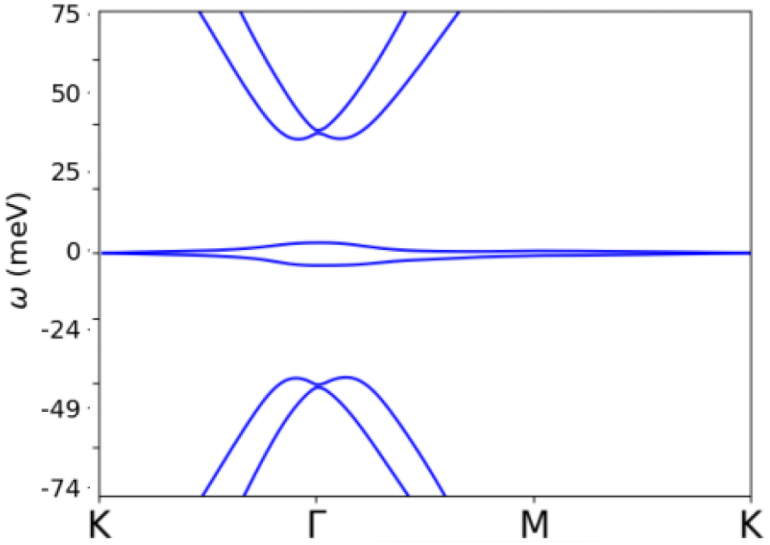
U=32 meV

@ T=5.8 K

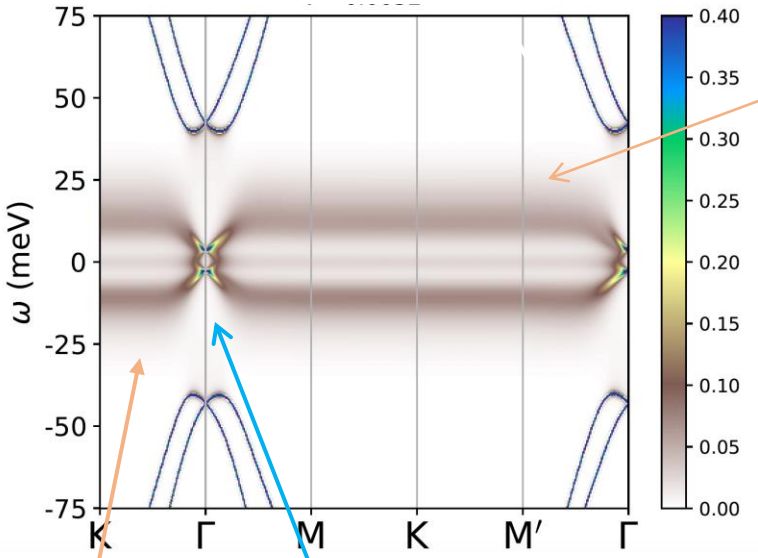
No symm breaking

1.08º

Non-interacting



DMFT +H



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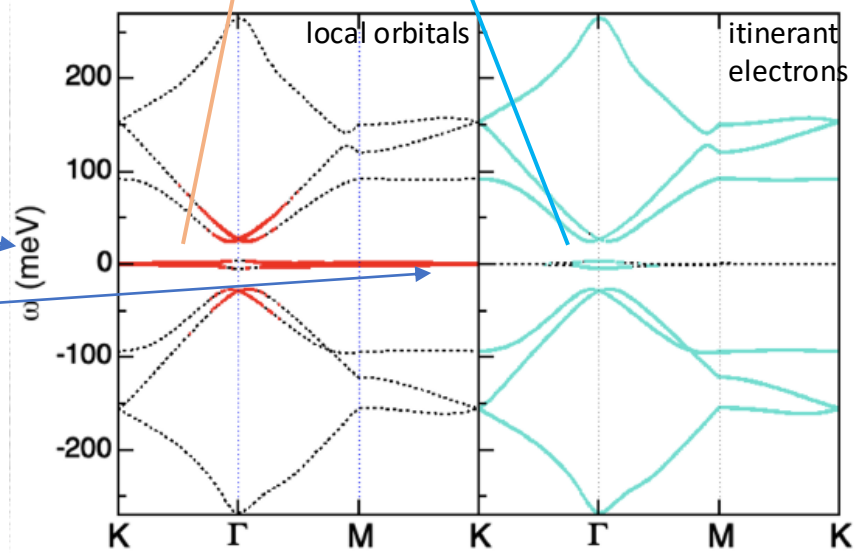
MJ Calderón, A Camjayi, A Datta, EBascones, PRB 112 L041126 (2025)

Momentum selective incoherence: (different around Γ) Two types of electrons

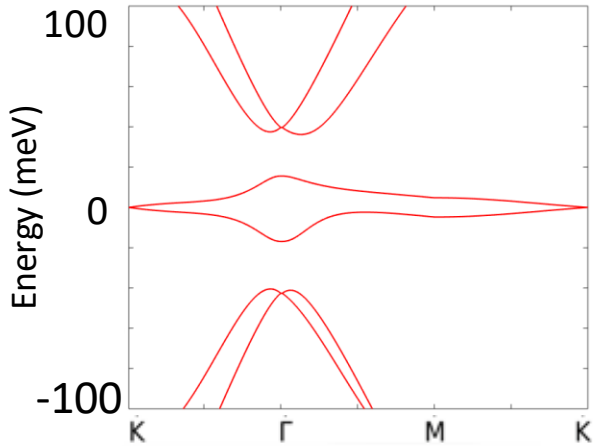


See also:
M. Haule, E. Andrei, K. Haule, arXiv:1901.09852 (2019),
Rai et al, PRX 14, 031045 (2024)

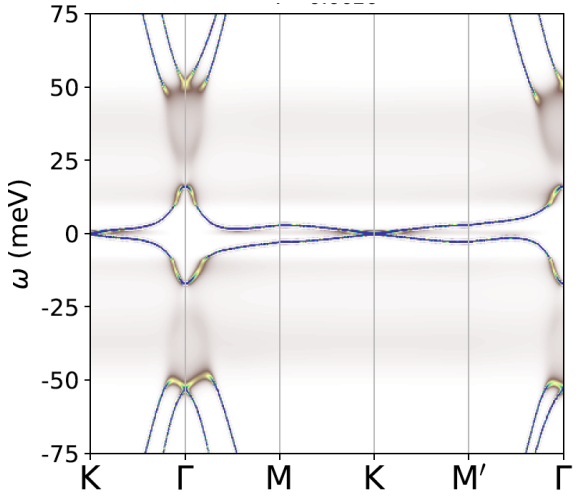
Spectral function of TBG at CNP: Comparison between theory and experiment

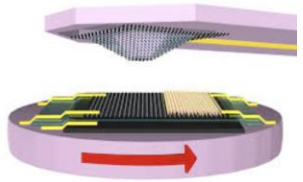
1.25º w_0/w_1=0.85

Non-interacting



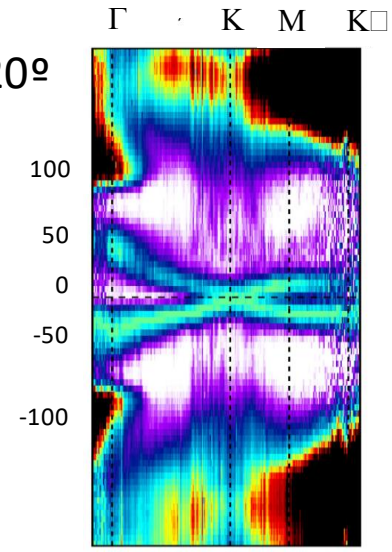
DMFT + H (theory)





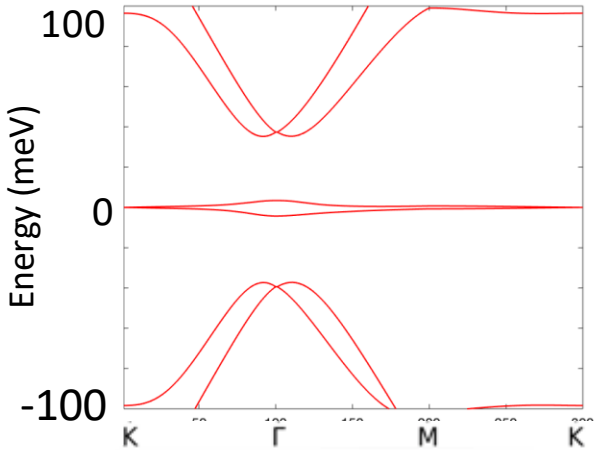
QTM @4.2 K (experiment)

θ~1.20º

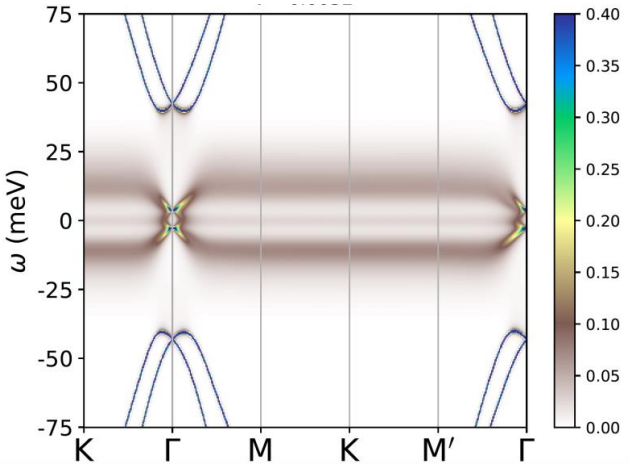


1.08º e, w_0/w_1=0.70

Non-interacting

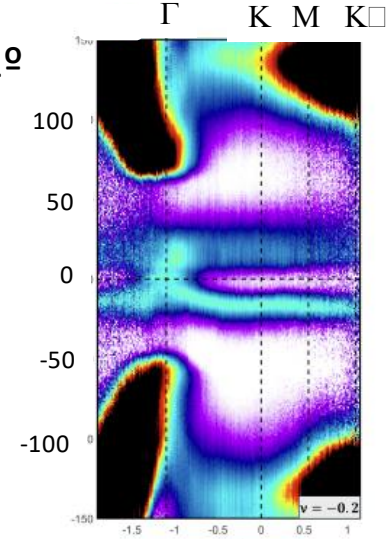


DMFT + H (theory)



QTM @4.2 K (experiment)

θ~1.1º



A.Datta, et al Nature Comms 14, 5036 (2023)

MJ Calderón, et al. PRB 112 L041126 (2025)

Xiao et al, arXiv:2506.20738

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Mott physics beyond single band

- In multi-orbital systems Mott insulators can appear not only at half-filling but at any integer filling/site
- Hund's coupling: new scale for interactions. Hund metals. Correlated metals due to the formation of local moment, but charge not so much localized.
- High-Tc iron superconductors are Hund metals
- Orbitals can feel different correlation strengths (different bandwidths, different interactions)
- Very flat correlated orbitals hybridized to weakly correlated electrons: heavy fermion systems
- Twisted bilayer Graphene: Topological flat bands.
  Heavy fermion description with flat orbitals (4 spin degenerate) coupled to itinerant electrons only around Γ