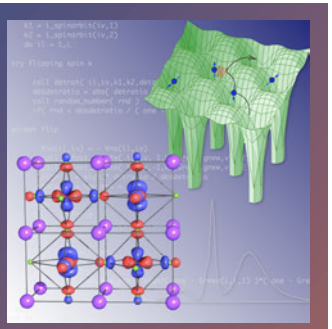
Magnetism in Correlated Matter



Eva Pavarini

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Peter Grünberg Institut

JARA-HPC

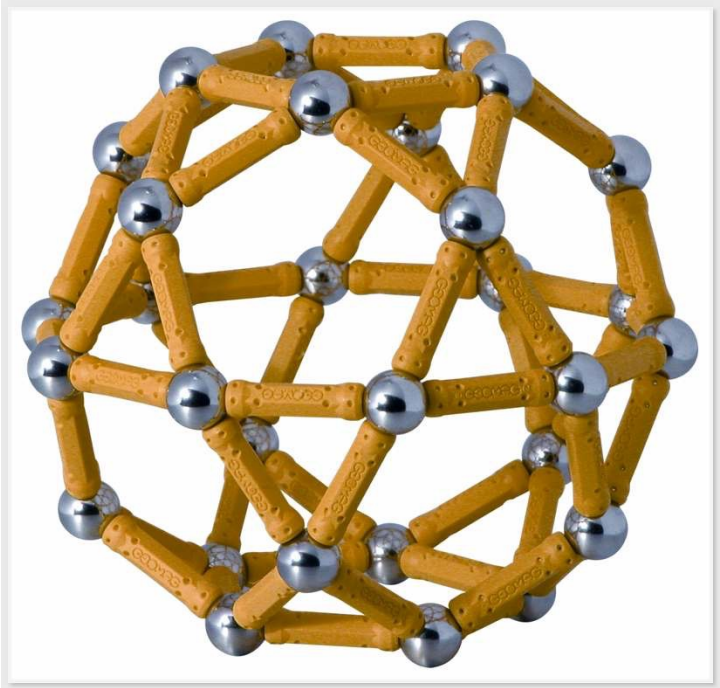
Forschungszentrum Jülich

a short (and very incomplete) history

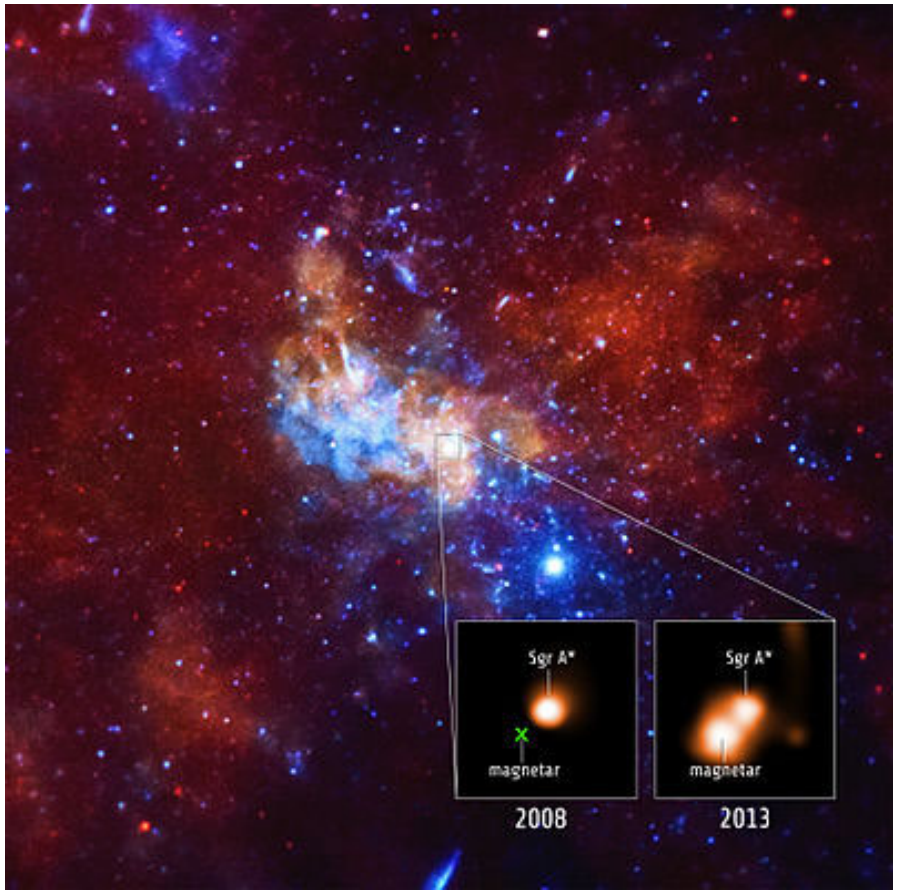
magnetic objects

earth

NdFeB magnetic toy



magnetar



5 10^{-5} T

1 T

10^{8}-10^{11}T

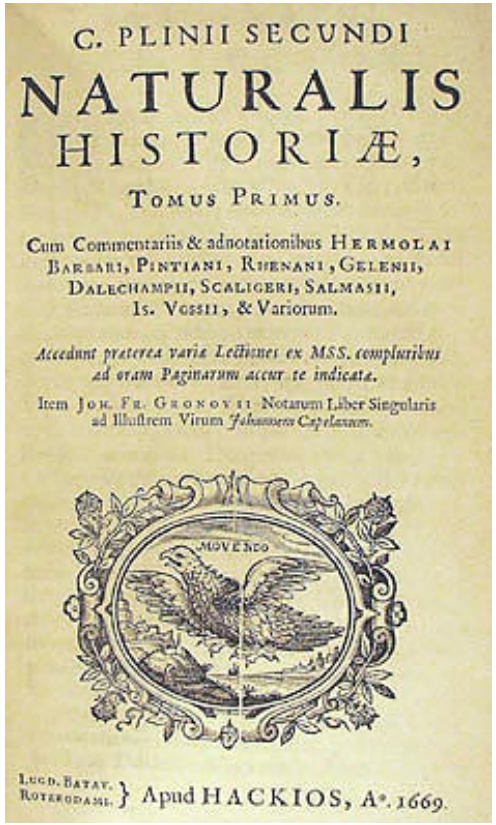
High Magnetic Field Laboratory: 10-100 T

what is magnetism?

Fe_3O_4

T_C=858 K

1000 BC ?


C. PLINII SECUNDI
NATURALIS HISTORIÆ,
TOMUS PRIMUS.
Cum Commentariis & adnotationibus HERMOLAI BARBARI, PINTIANI, RHENANI, GELENII, DALECHAMPII, SCALIGERI, SALMASII, Is. VOSSII, & Variorum.
Accedunt præterea variæ Lectiones ex MSS. compluribus ad oram Paginarum accurate indicatæ.
Item JOH. FR. GRONOVII Notarum Liber Singularis ad Illustrem Virum *Johannem Capelanum.*
MOVENDO
LUGD. BATAV. ROTERODAMI. } Apud HACKIOS, A°. 1669.

Pliny the Elder
23-79 AD

(photos taken from Wikipedia)

magnetic compass, China, Han Dinasty

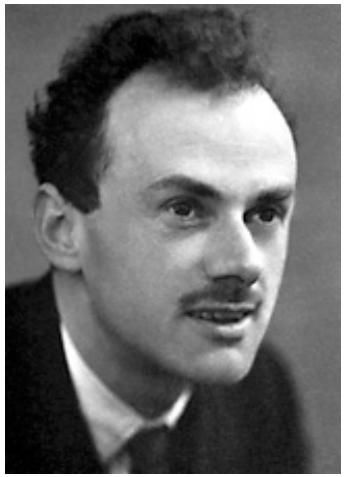
200 BC- 200 AD

(photos taken from Wikipedia)

what is the origin of magnetism
in materials?

the theory of nearly everything

$$\hat{H} = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} - \sum_\alpha \frac{1}{2M_\alpha}\nabla_\alpha^2 + \frac{1}{2}\sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}$$



Paul Adrien Maurice Dirac

Nobel Prize in Physics 1933

The underlying laws needed for the description of all chemistry as well as a large part of physics are now entirely known. The only problem that remains is that the exact equations of quantum mechanics are too difficult to be solved. It is therefore necessary to derive ***approximations*** *that allow us to calculate the properties of complex molecular systems with an acceptable computational effort.*

P.M.A. Dirac 1929

electrons and lattice

Born-Oppenheimer

non-relativistic electronic Hamiltonian

$$\begin{aligned}\hat{H}_e &= -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|} \\ &= \hat{T}_e + \hat{V}_{ee} + \hat{V}_{en} + \hat{V}_{nn}\end{aligned}$$

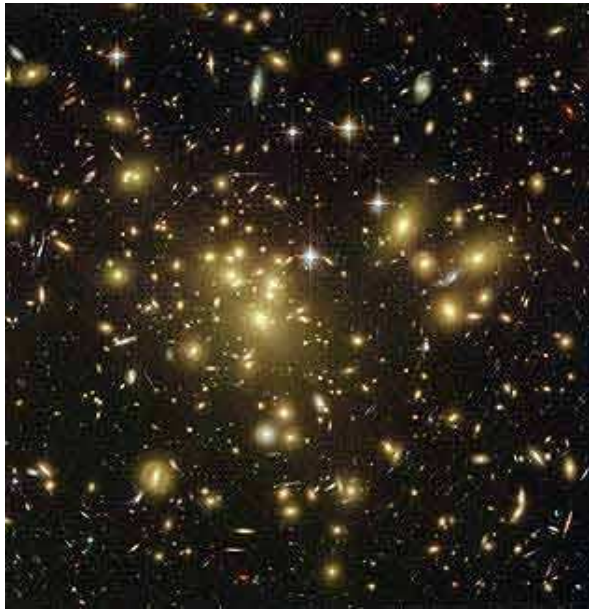
lattice Hamiltonian

$$\begin{aligned}\hat{H}_n &= -\sum_\alpha \frac{1}{2M_\alpha}\nabla_\alpha^2 + \varepsilon(\{\boldsymbol{R}_\alpha\}) \\ &= \hat{T}_n + \hat{U}_n,\end{aligned}$$

if we crystal structure known
we can concentrate on electrons

a single iron atom (not magnetic yet..)

26 electrons, 78 arguments,
10^{78} values
10 X 10 X 10 grid



$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{26})$$

electronic Hamiltonian

non relativistic electronic Hamiltonian

$$H_e^{\mathrm{NR}} = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_{i'}|} - \sum_{i\alpha} \frac{Z_\alpha}{|\boldsymbol{r}_i - \boldsymbol{R}_\alpha|} + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\boldsymbol{R}_\alpha - \boldsymbol{R}_{\alpha'}|}$$

kinetic **Coulomb** **potential** constant

magnetism is a quantum mechanical effect

interplay between Coulomb interaction, Pauli principle, crystal field and hoppings

from the general Hamiltonian to effective simple models

Heisenberg model
Hubbard model
Anderson and Kondo model

(and some successes of mean-field theories)

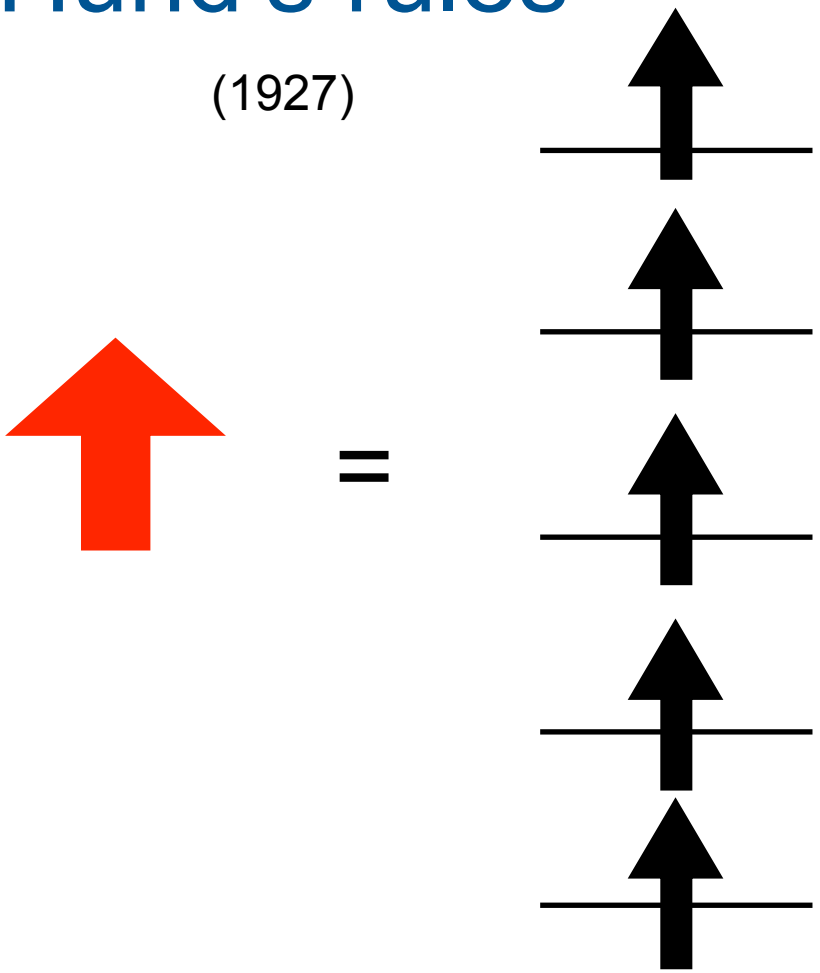
local spins and their interactions

effective elementary objects

Friedrich Hund

Hund's rules

(1927)



Fe^{3+}

S=5/2

local moments

interaction?

inter-site Coulomb exchange

$$J^{i,i'} = U^{ii'i'i}_{mmmm} = \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 \, \frac{\overline{\psi_{im\sigma}}(\boldsymbol{r}_1)\overline{\psi_{i'm\sigma}}(\boldsymbol{r}_2)\psi_{im\sigma}(\boldsymbol{r}_2)\psi_{i'm\sigma}(\boldsymbol{r}_1)}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|},$$

ferromagnetic!

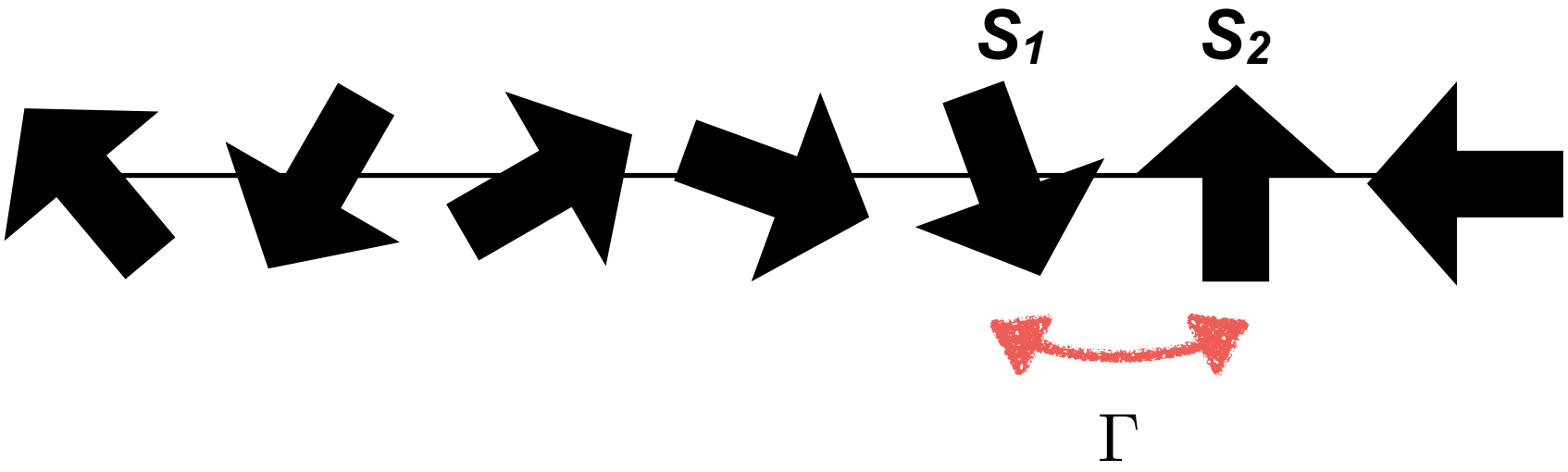
Heisenberg model

Coulomb exchange (FM) + direct- and super-exchange (FM or AFM)

local spins: effective emergent elementary particles

Heisenberg model: effective interaction

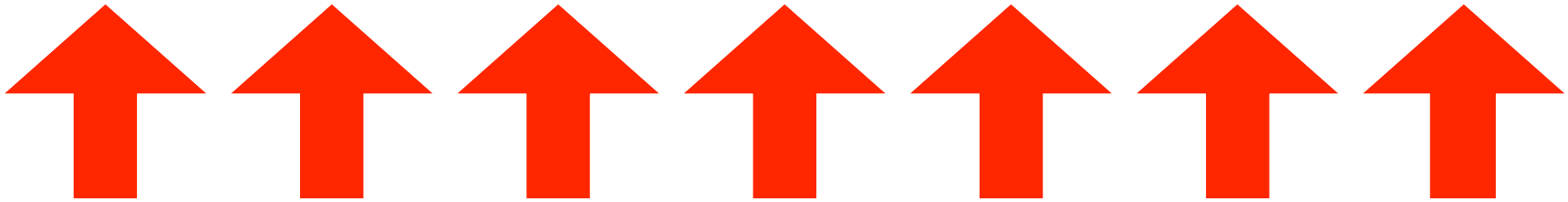
$$H = \frac{1}{2}\,\Gamma \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



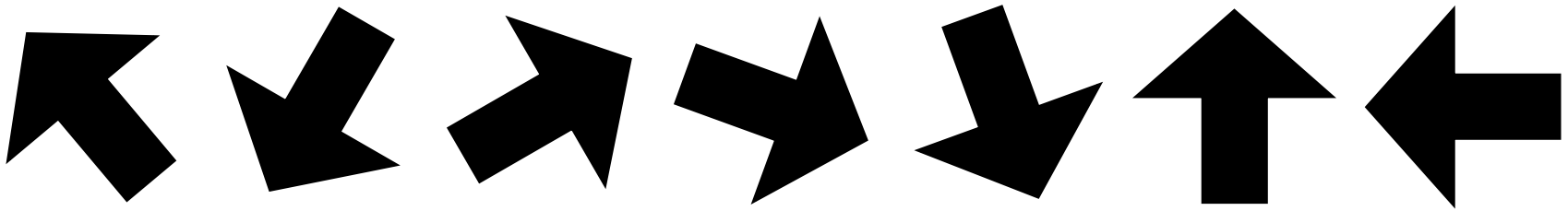
Weiss molecular theory

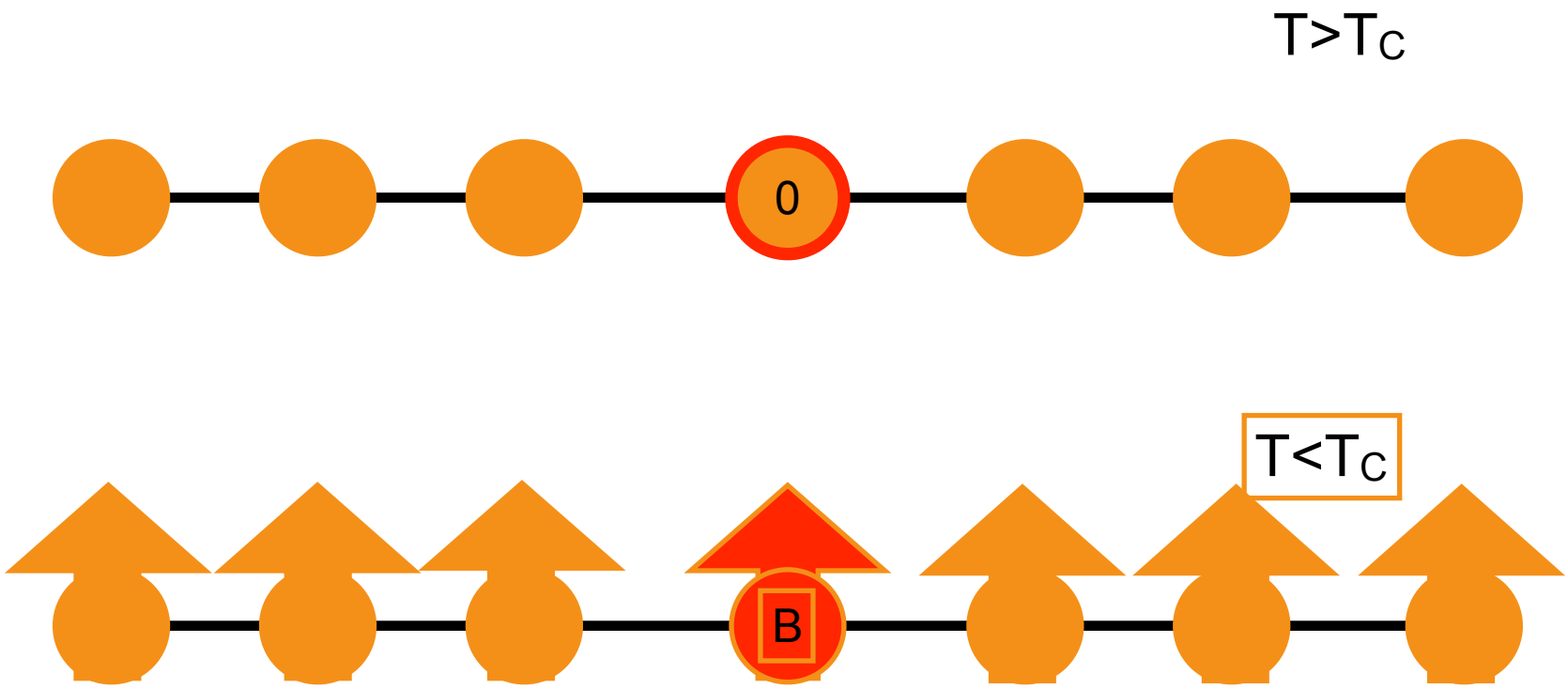
Pierre Weiss

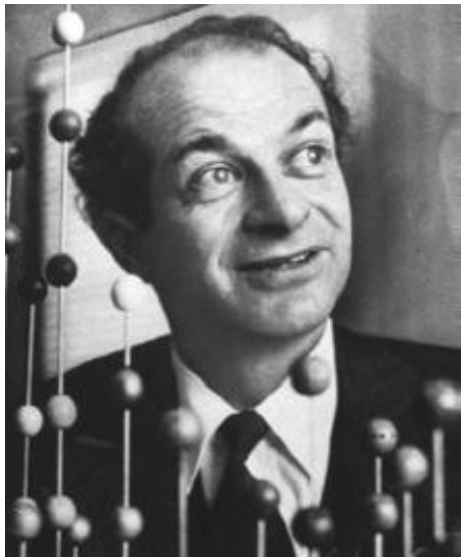
Reduce many-body problem to single-body problem in **effective mean field**



static mean-field theory







Linus Pauli

A THEORY OF FERROMAGNETISM

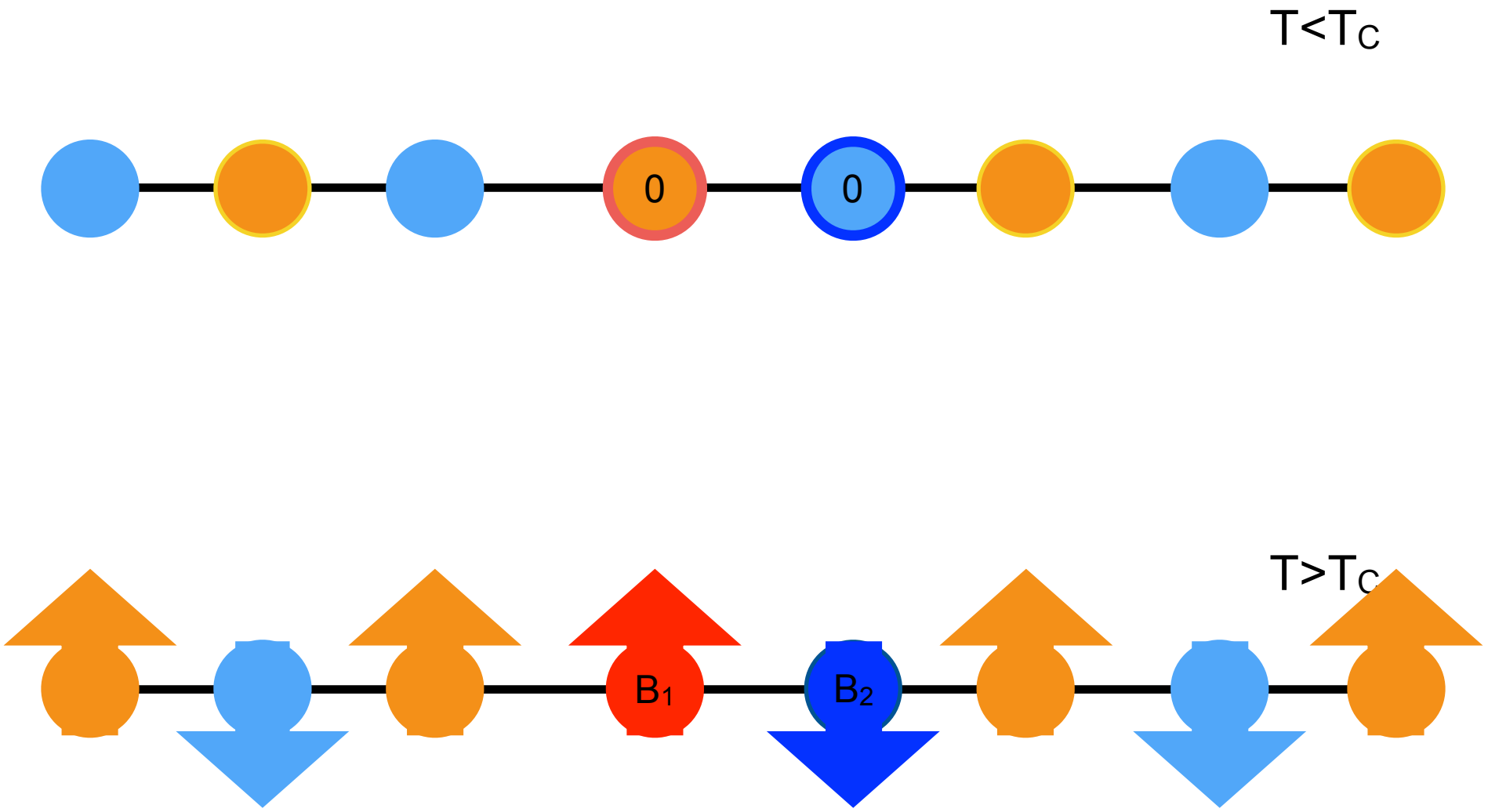
By Linus Pauling

Gates and Crellin Laboratories of Chemistry,* California Institute of Technology

Communicated April 1, 1953

The properties of ferromagnetic substances are in reasonably good accord with the theory of Weiss.[1] In this theory it is postulated that the atomic magnets tend to be brought into parallel orientation not only by an applied magnetic field but also by an inner field which is proportional to the magnetization of the substance. The inner field is not due to magnetic interaction of the magnetic moments of the molecules, but to electrostatic interactions, which are related to the orientation of the magnetic moments of electrons through the Pauli principle. During the past twenty-five years many efforts have been made to develop a precise theory of the interactions that produce the inner field, and to account in this way for the observed magnetic properties of ferromagnetic substances, but these attempts have not been successful—no one has published a theory of the electronic structure of ferromagnetic substances that permits reasonably good predictions to be made of the values of the saturation magnetic moment and the Curie temperature.

generalized mean-field theory

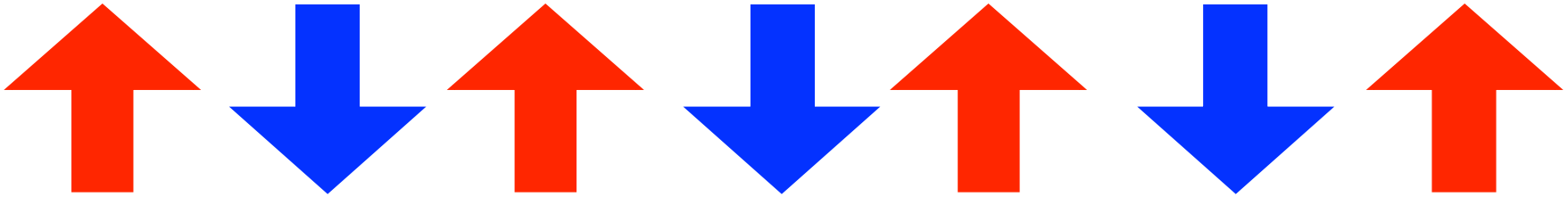


prediction: antiferromagnetism

Louis Néel

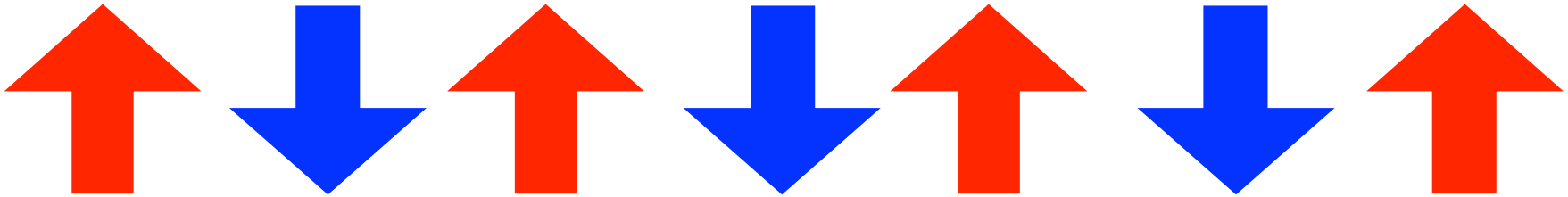
prediction: Néel (1932)

Reduce many-body problem to single-body problem in effective field
Generalize to more complicated situations



antiferromagnetism

prediction: Néel (1932)



experiment: Shull and Smart (1949)

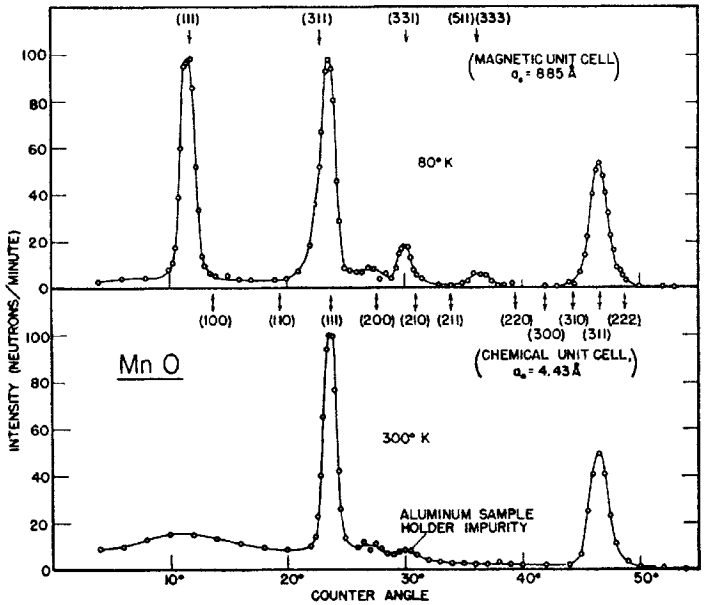
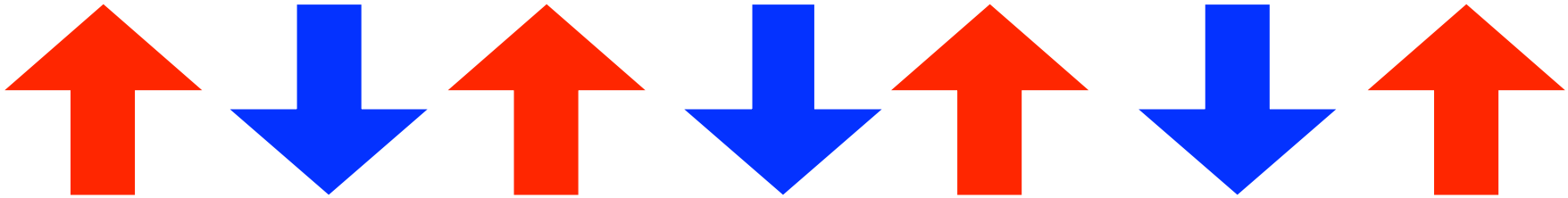


FIG. 1. Neutron diffraction patterns for MnO at room temperature and at 80°K.

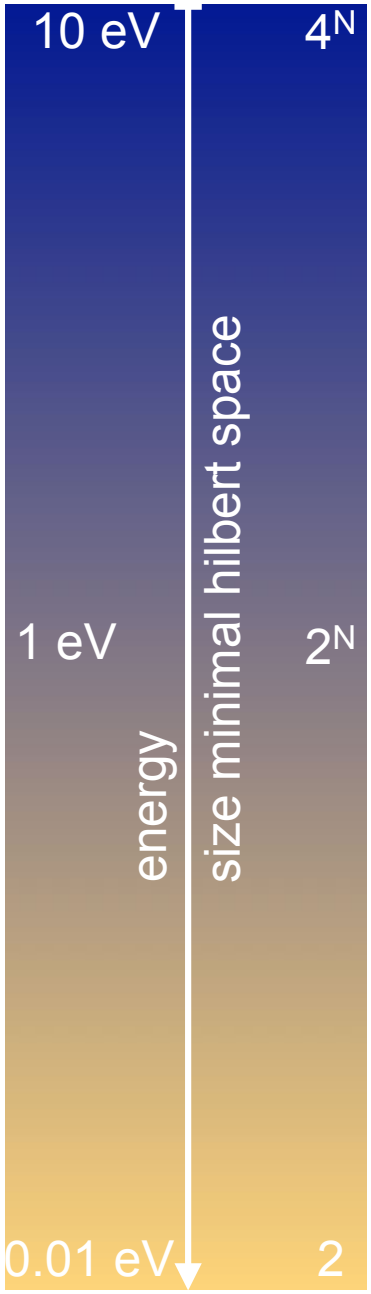
exact solution?

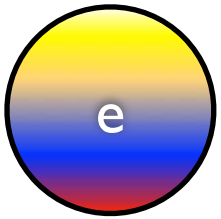
H. Bethe: ground state of linear Heisenberg chain has S=0



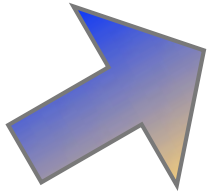
P.W. Anderson: broken symmetry & quantum fluctuations

magnetism & emergence



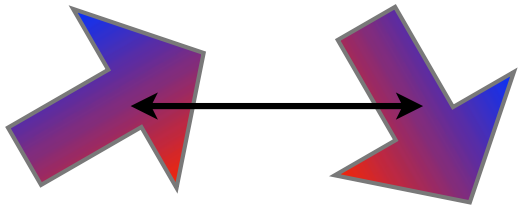


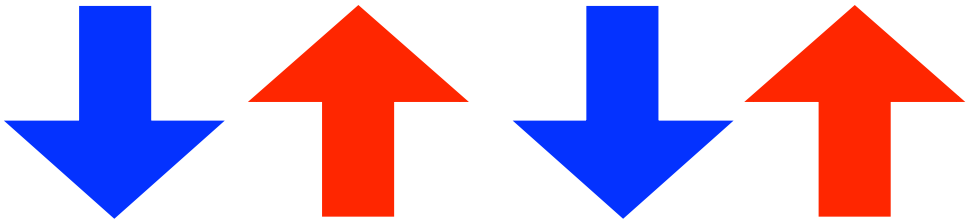
from electrons emerge spins



effective elementary entities

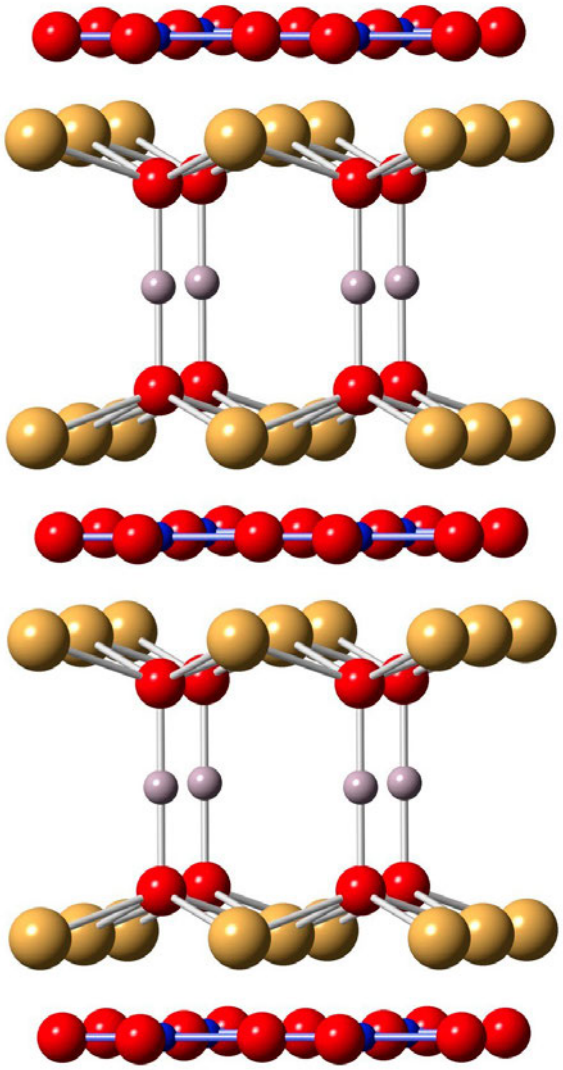
spins interact



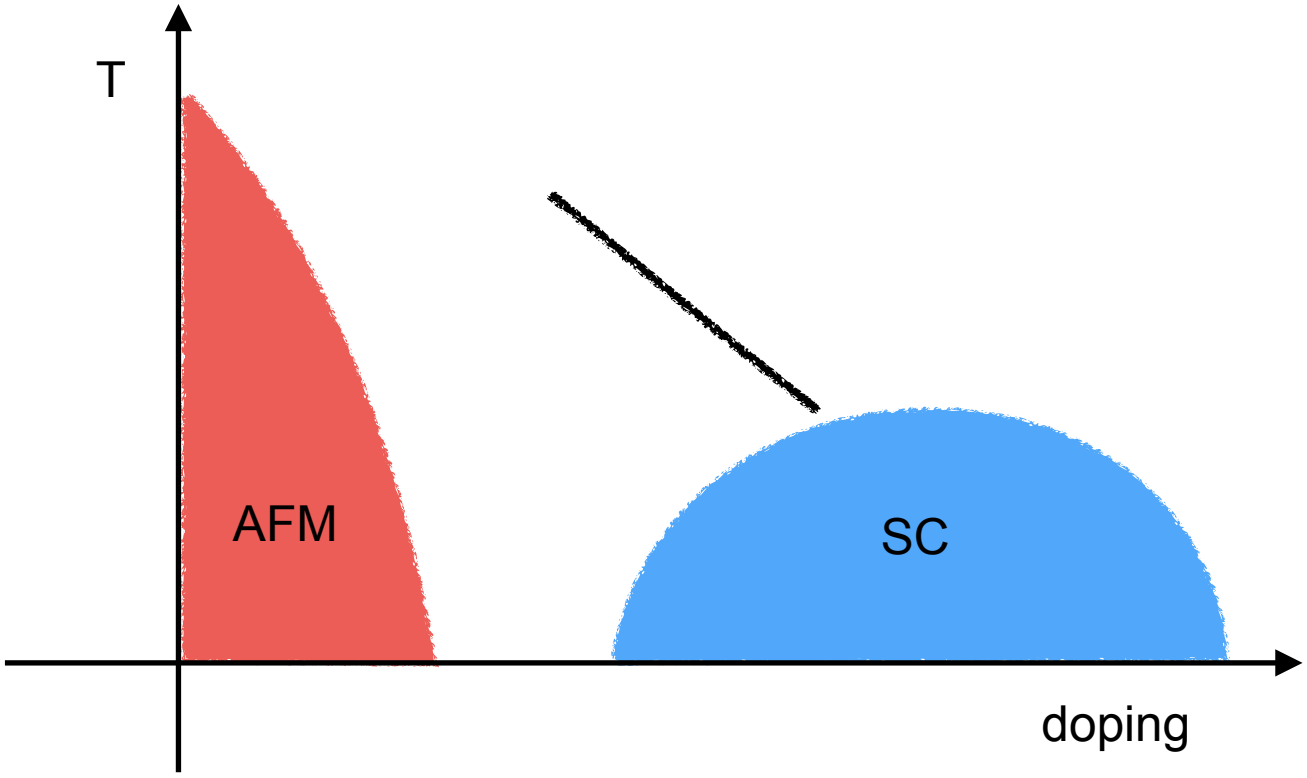


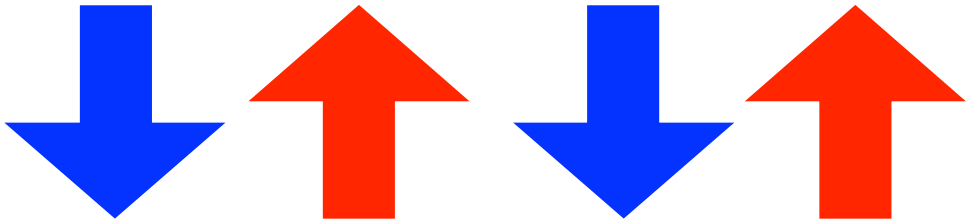
cooperative state

Mott insulators & high-T_c cuprates



$HgBa_2CuO_4$



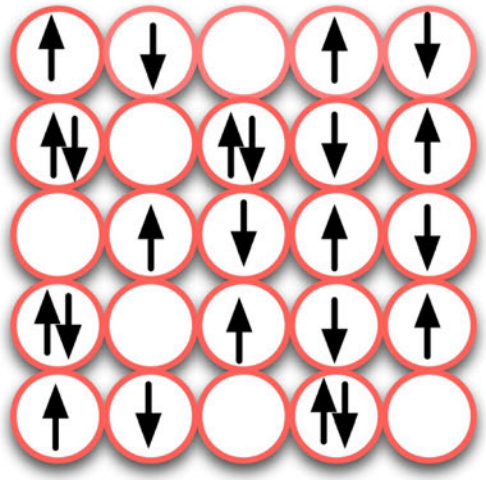


Hubbard model

$$\begin{cases} \varepsilon_d &= -t_{1,1}^{i,i} \\ t &= t_{1,1}^{\langle i,i' \rangle} \\ U &= U_{1111}^{iiii} \end{cases}$$

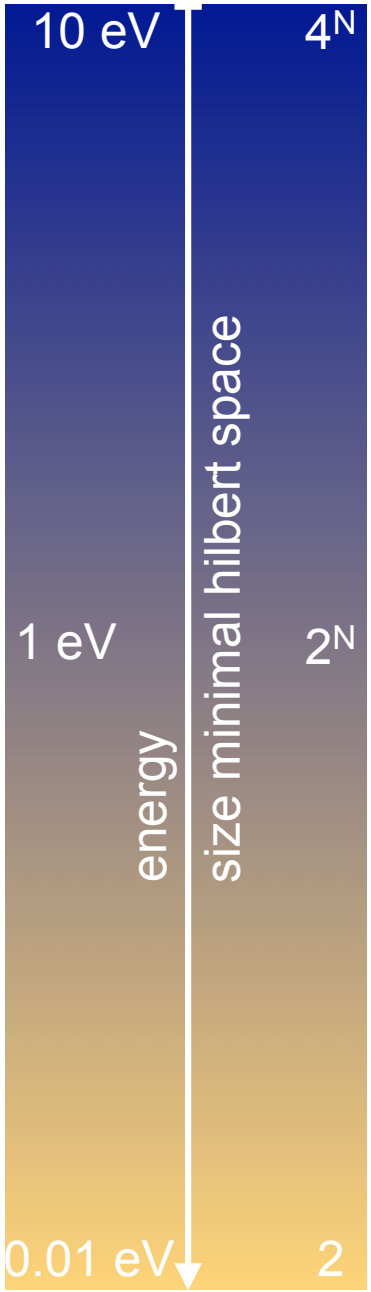
atomic hoppings atomic

$$H = \varepsilon_d \sum_i \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c_{i\sigma}^\dagger c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U$$



t=0: collection of atoms, insulator

U=0: half-filled band, metal



$$\begin{cases} \varepsilon_d &= -t_{1,1}^{i,i} \\ t &= t_{1,1}^{\langle i,i' \rangle} \\ U &= U_{1111}^{iiii} \end{cases}$$

atomic hoppings atomic

$$H = \varepsilon_d \sum_i \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c_{i\sigma}^\dagger c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U$$

perturbation theory
or canonical transformation

large U limit, n=1

$$H = \frac{1}{2} \Gamma \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

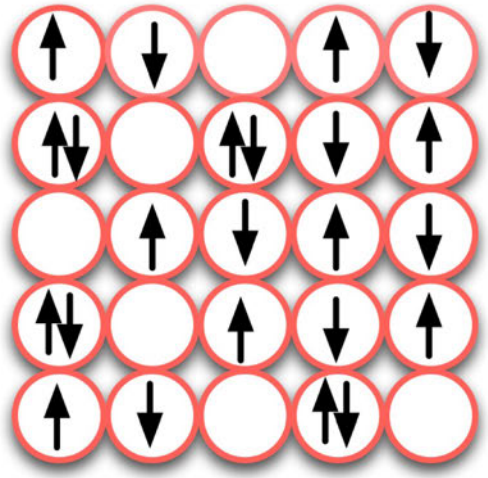
$$\Gamma \propto -t^2/U$$

metal-insulator transition

$$\begin{cases} \varepsilon_d &= -t_{1,1}^{i,i} \\ t &= t_{1,1}^{\langle i,i' \rangle} \\ U &= U_{1111}^{iiii} \end{cases}$$

atomic hoppings atomic

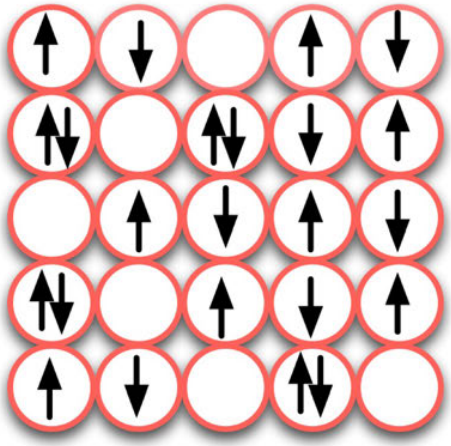
$$H = \varepsilon_d \sum_i \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c_{i\sigma}^\dagger c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U$$



t=0: collection of atoms, insulator

U=0: half-filled band, metal

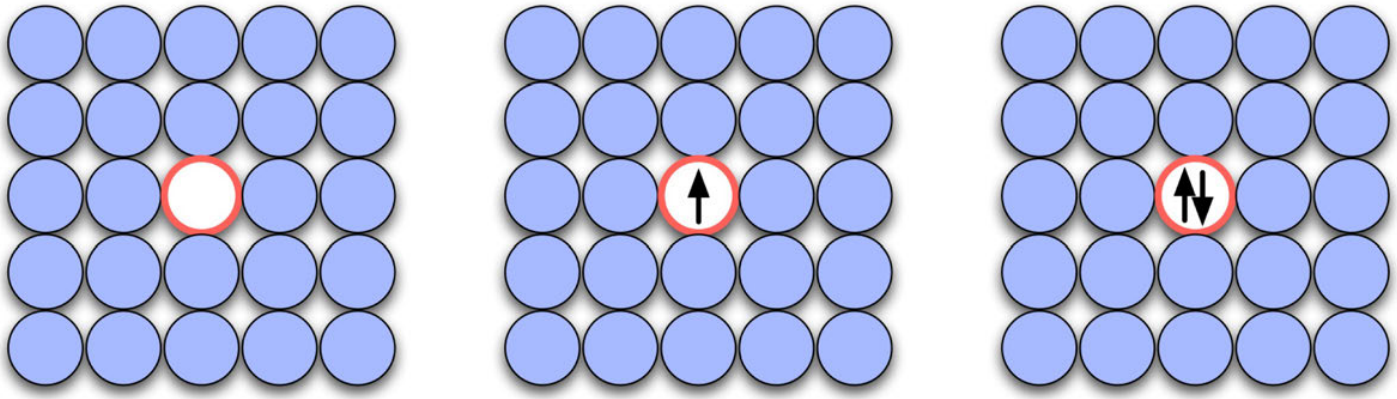
dynamical mean-field theory



$G^{i,j}$

H^{LDA}

$U^{i,i}$



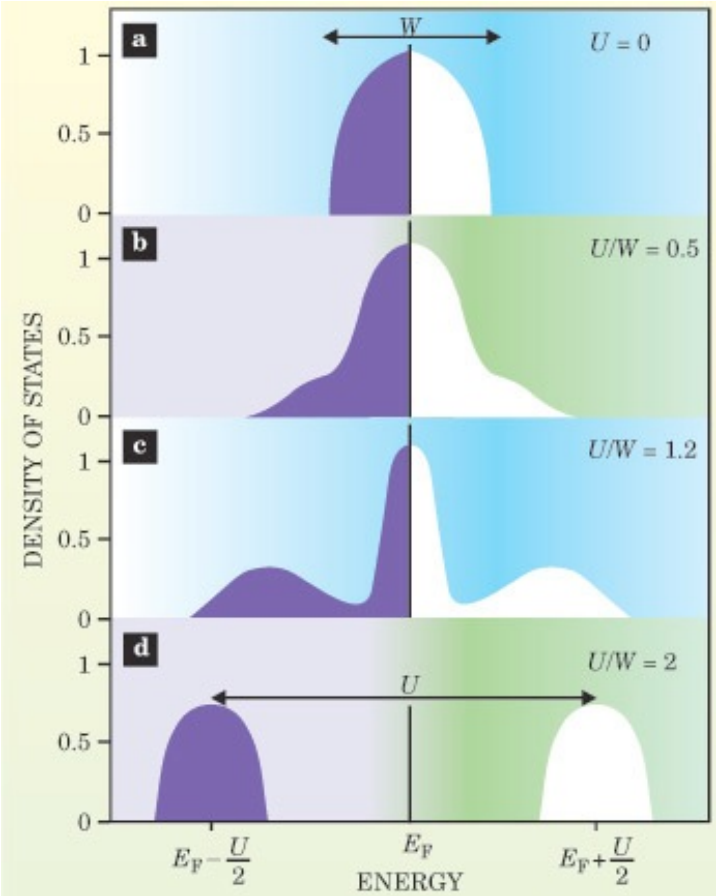
$$\mathcal{G}^{-1} = G^{-1} + \Sigma$$

$$G = G^{i,i}$$

Metzner and Vollhardt, PRL **62**, 324 (1989); Georges and Kotliar, PRB **45,** 6479 (1992)

metal-insulator transition

Bethe lattice



G. Koltiar and D. Vollhardt
Physics Today **57,** 53 (2004)

metallic phase

$$\mathrm{Re}\Sigma(\omega + i0^+) = U/2 + (1 - 1/Z)\omega + O(\omega^3), \qquad (226)$$

$$\mathrm{Im}\Sigma(\omega + i0^+) = -B\omega^2 + O(\omega^4). \qquad (227)$$

The quasiparticle residue Z defines the renormalized Fermi energy of the problem:

$$\epsilon_F^* \equiv ZD \qquad (228)$$

This is also the Kondo temperature of the impurity model. Since the self-energy is momentum independent, Z directly yields the effective mass of quasiparticles (Müller-Hartmann, 1989c):

$$\frac{m^*}{m} = \frac{1}{Z} = 1 - \frac{\partial}{\partial\omega}\,\mathrm{Re}\Sigma(\omega + i0^+)\big|_{\omega=0}. \qquad (229)$$

insulating phase

$$\mathrm{Im}\Sigma(\omega + i0^+) = -\pi\rho_2\delta(\omega) \quad \text{for} \quad \omega \in [-\Delta_g/2, \Delta_g/2] \qquad (235)$$

and that $\mathrm{Re}\Sigma$ has the following low-frequency behavior:

$$\mathrm{Re}\Sigma(\omega + i0^+) - U/2 = \frac{\rho_2}{\omega} + O(\omega). \qquad (236)$$

A.Georges et al. RMP **63**, 13 (1996)

dmft

lattice model

$$H = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U$$

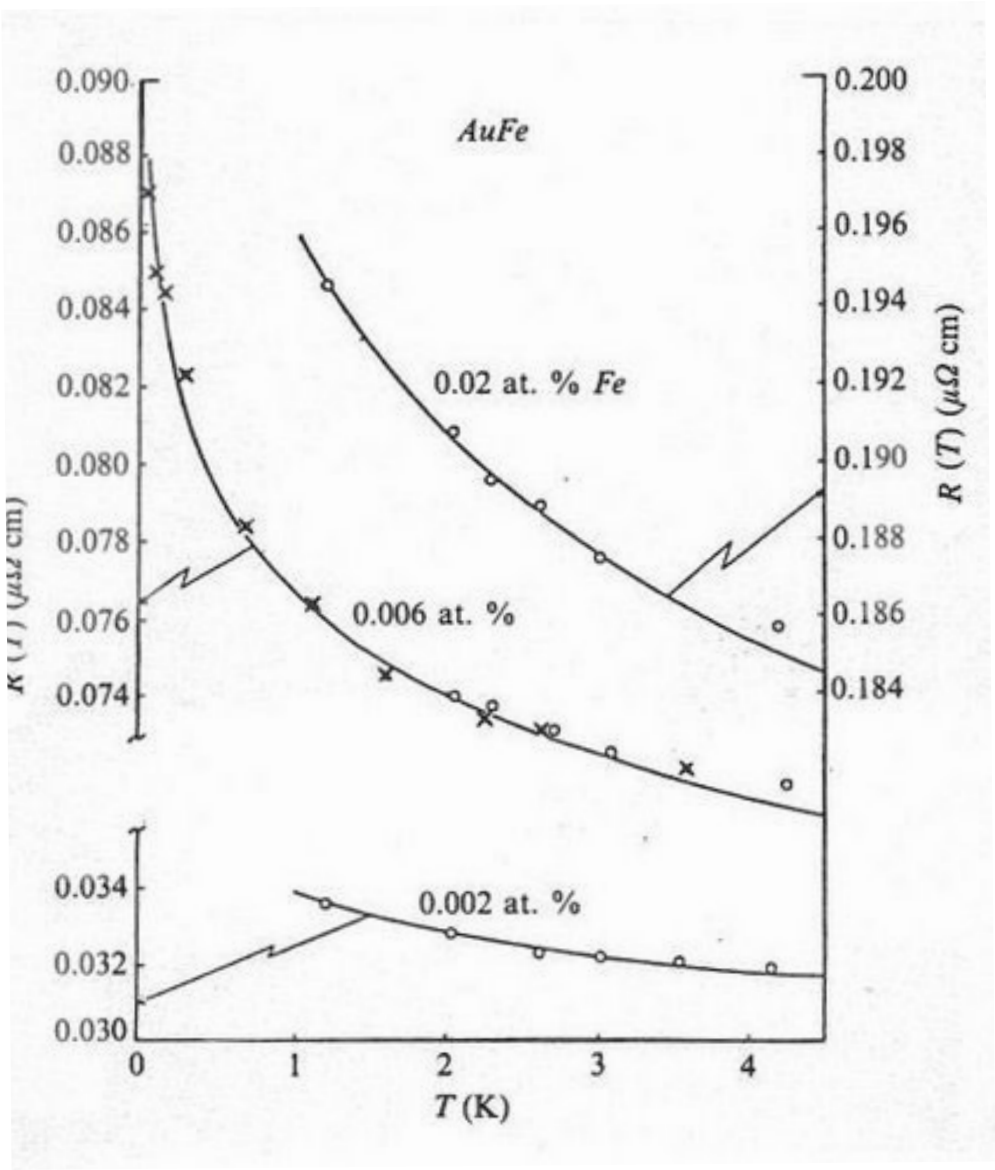
quantum impurity model

$$H_{\mathrm{A}} = \sum_\sigma \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_\sigma \varepsilon_f n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow}$$

$$+ \sum_\sigma \sum_{\boldsymbol{k}} \left[V_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{f\sigma} + h.c. \right]$$

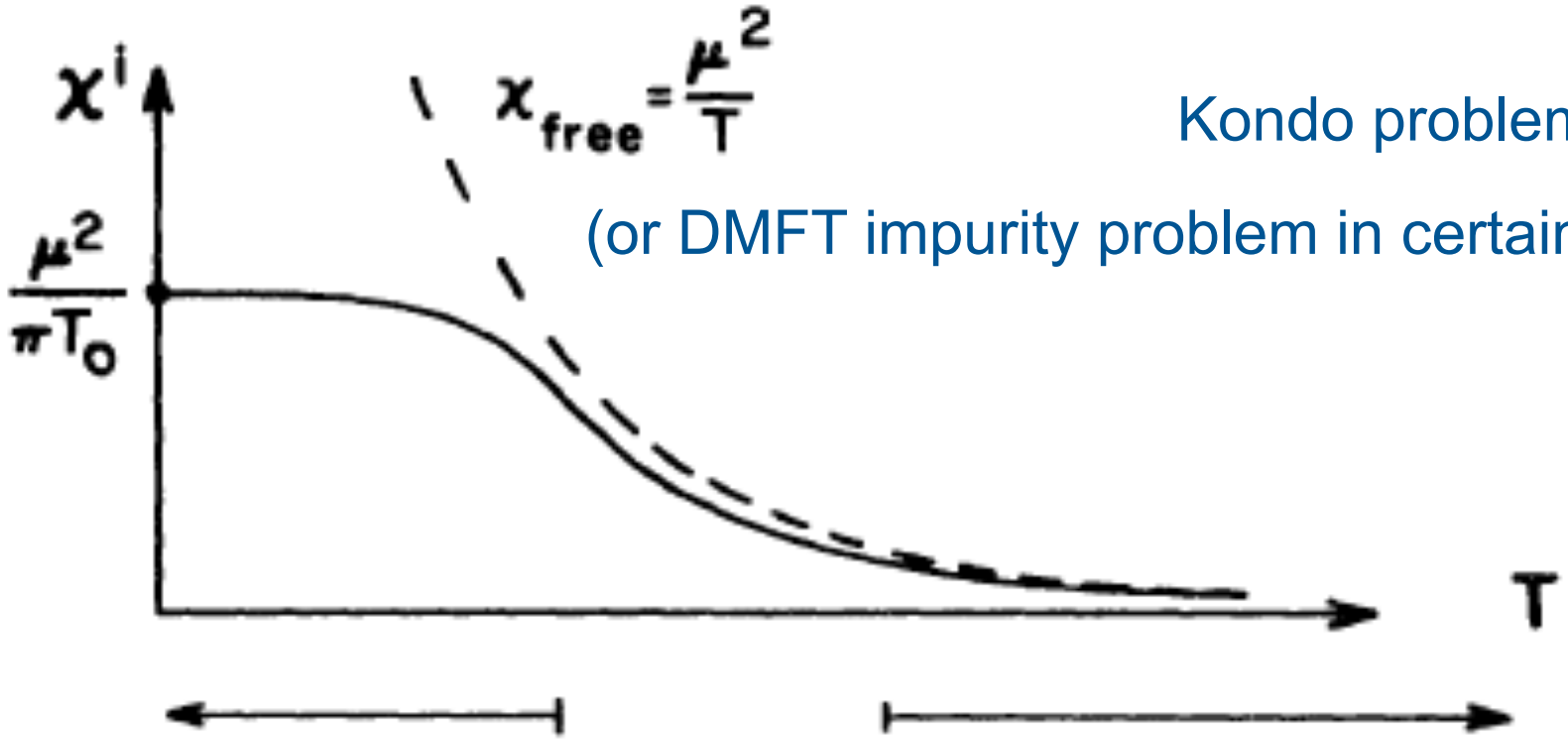
self-consistency loop

Kondo effect



screening of local moments

linear magnetic susceptibility



Kondo problem

(or DMFT impurity problem in certain regime)

Anderson model & Kondo model

metal

impurity

$$H_{\mathrm{A}} = \sum_{\sigma}\sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_{\sigma} \varepsilon_f n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow}$$

$$+ \sum_{\sigma}\sum_{\boldsymbol{k}} \left[V_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{f\sigma} + h.c. \right]$$

hybridization

perturbation theory
or canonical transformation

large U limit, n=1

$$H = \Gamma\, \mathbf{S}_f \cdot \mathbf{s}_c(\mathbf{0})$$

dmft

lattice model

$$H = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U$$

large U limit, n=1

$$H = \frac{1}{2} \Gamma \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

quantum impurity model

$$H_{\mathrm{A}} = \sum_\sigma \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_\sigma \varepsilon_f n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow}$$

$$+ \sum_\sigma \sum_{\boldsymbol{k}} \left[V_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{f\sigma} + h.c. \right]$$

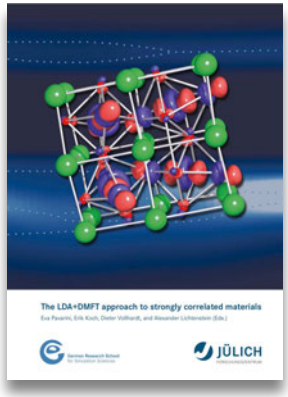
large U limit, n=1

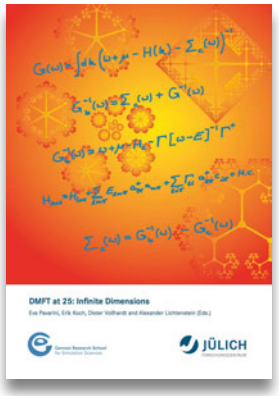
$$H = \Gamma \, \mathbf{S}_f \cdot \mathbf{s}_c(\mathbf{0})$$

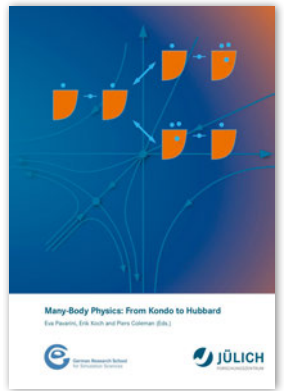
self-consistency loop

scheme of the lecture

- emergence of local moments
- from the many-body problem to simple models
- the Hubbard model
  - itinerant and Fermi-liquid limit
  - atomic limit
- the metal-insulator transition
  - Hartree-Fock
  - DMFT
  - Hubbard and Anderson model
- the Anderson model
  - Kondo effect
  - atomic limit
- conclusions



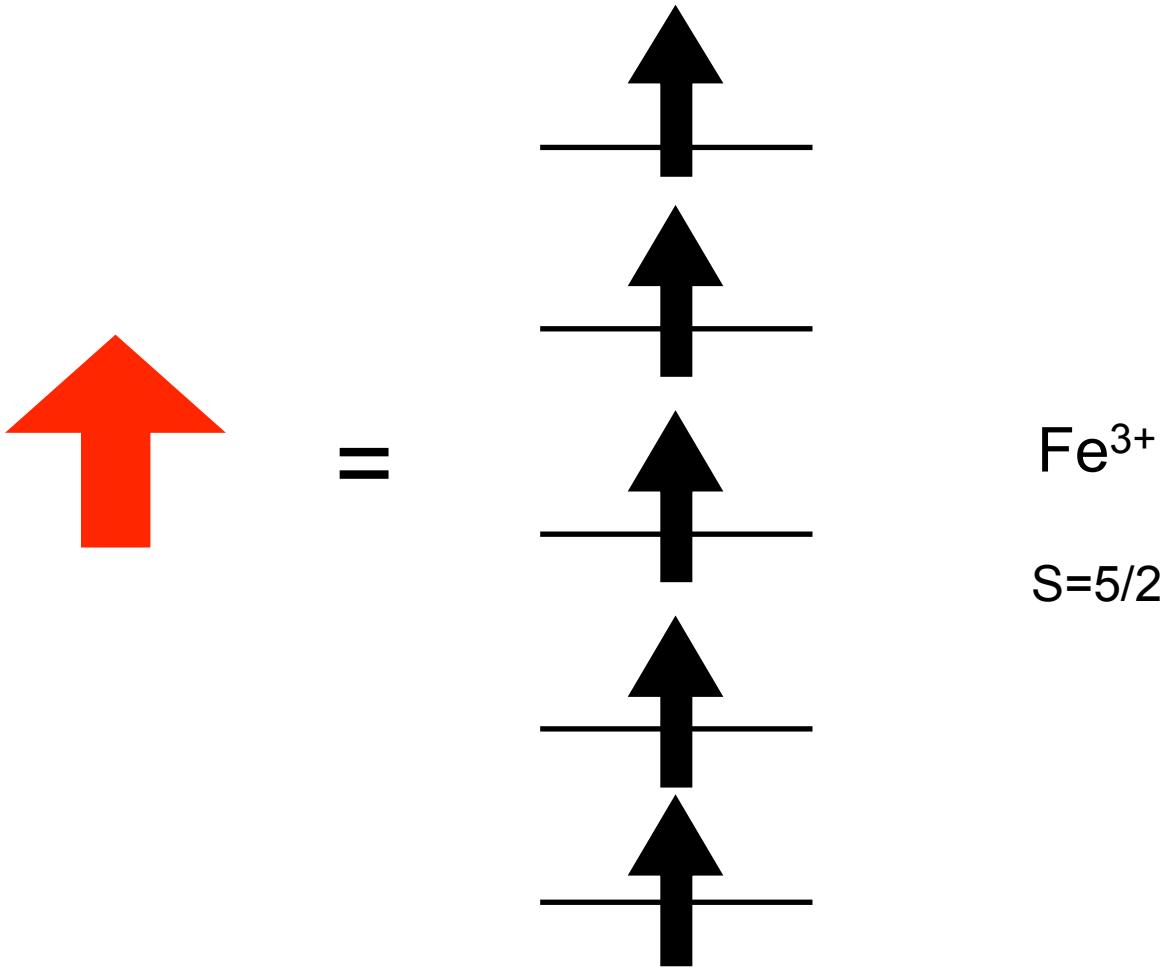




let us start from local moments

what are local moments?

Friedrich Hund



local moments

how do magnetic moments emerge?

let us consider one atom or ion

Atom

Fe

Magnetite

Fe^{2+} (octahedral)

Fe^{3+} (octahedral)
(tectrahedral)

what does it mean that it has a magnetic moment?

electronic Hamiltonian

Fe, 26 electrons

$$H_e^{\mathrm{NR}} = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_i \frac{Z}{r_i} + \sum_{i>j} \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

one-electron part Coulomb repulsion

self-consistent potential

$$H_e^{\mathrm{NR}} = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_i \frac{Z}{r_i} + \sum_{i>j} \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

$$H_e^{\mathrm{NR}} = -\frac{1}{2}\sum_i \nabla_i^2 + \sum_i v_R(r_i)$$

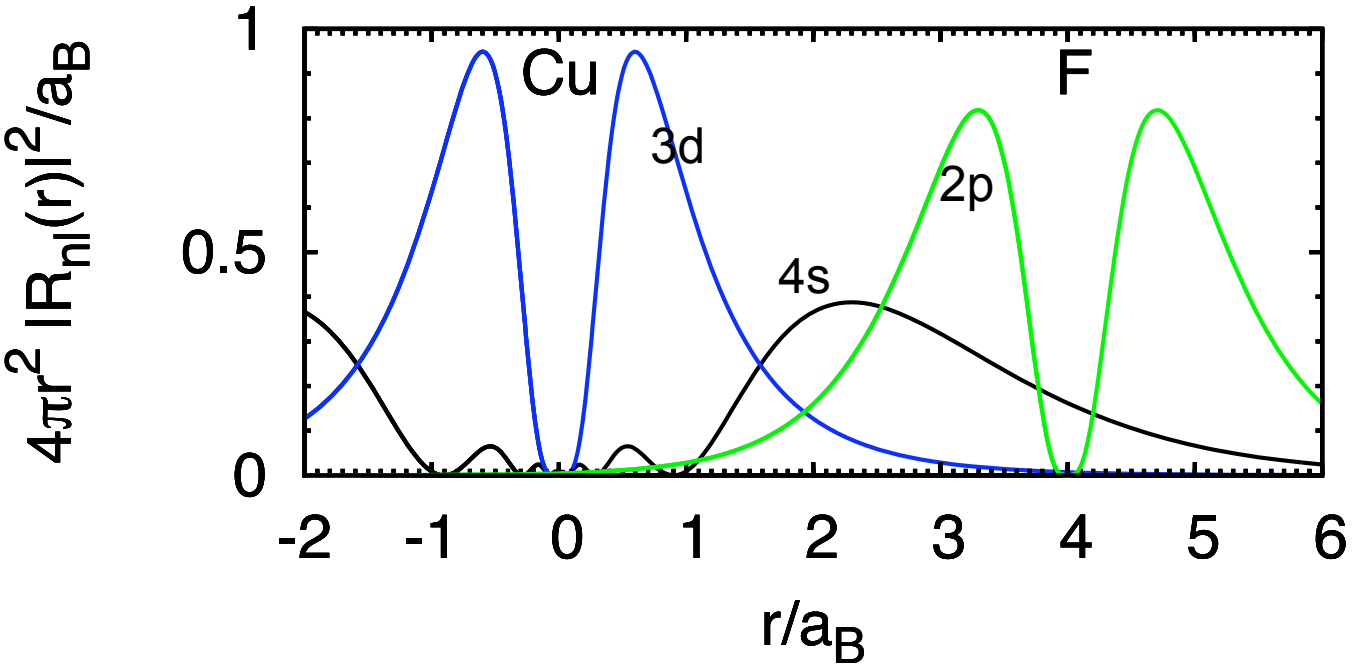
e.g., DFT/LDA

contains e.g. Hartree term

hydrogen-like atom

$$H_e^{\mathrm{NR}} = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_i Z_{\mathrm{eff}}/r_i$$

atomic functions



$$\psi_{nlm}(\rho,\theta,\phi) = R_{nl}(\rho)Y_l^m(\theta,\phi)$$

(hydrogen-like atom)

$$R_{nl}(\rho) = \sqrt{\left(\frac{2Z}{n}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}} e^{-\rho/n} \left(\frac{2\rho}{n}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2\rho}{n}\right)$$

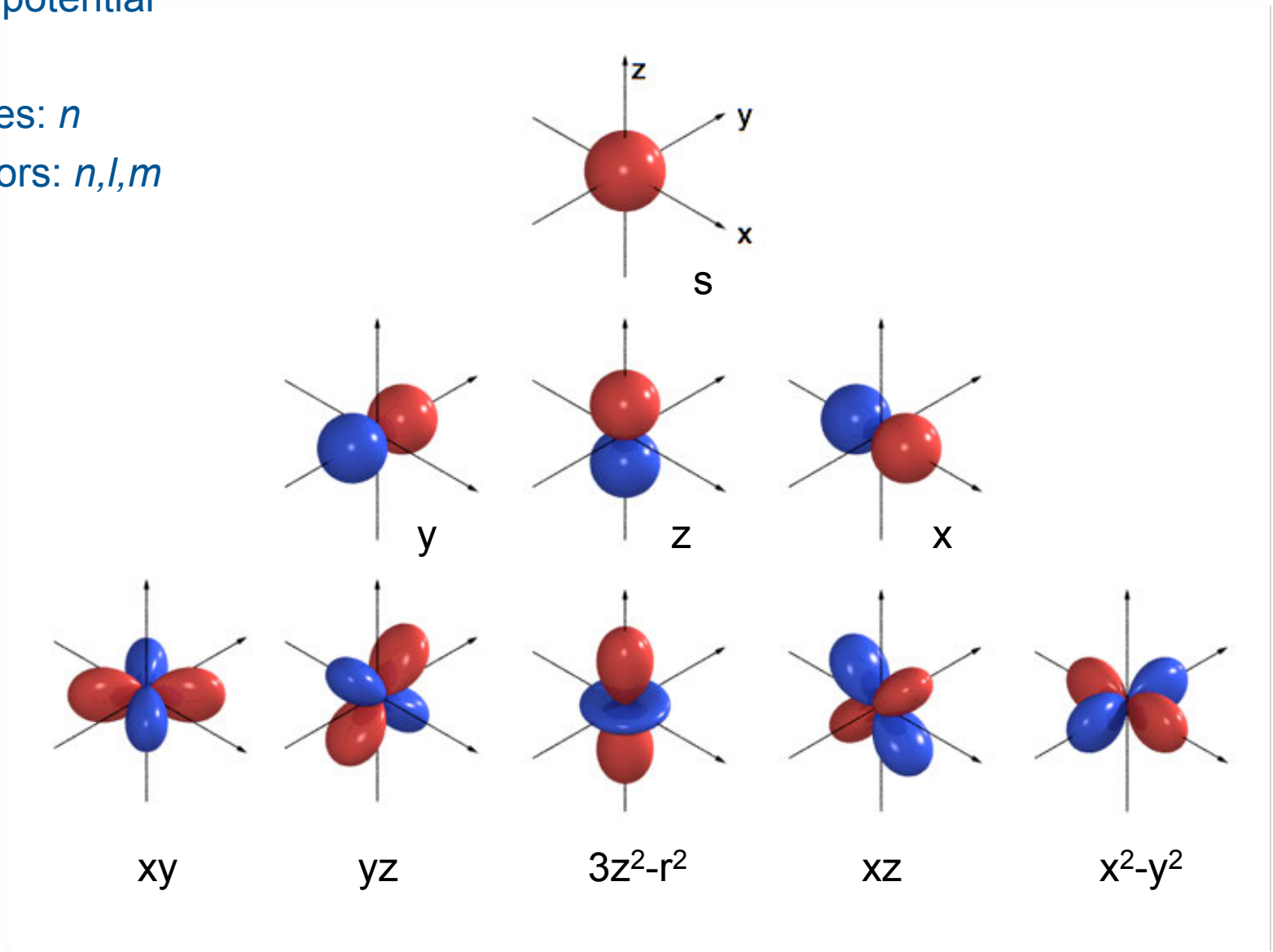
Laguerre polynomials

real harmonics

spherical potential

eigenvalues: *n*

eigenvectors: *n,l,m*

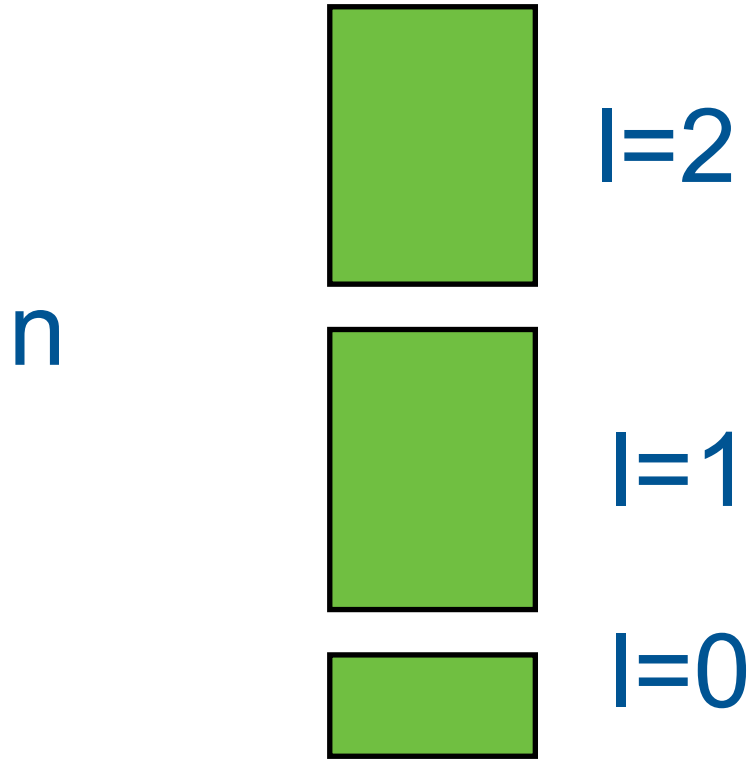


l=0

l=1

l=2

atomic states (radial potential)



high-degeneracy,
no magnetic moments yet

many-electrons

$$H_e^{\mathrm{NR}} = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_i \frac{Z}{r_i} + \sum_{i>j} \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

one shell, 2nd quantization

$$H_e^{\mathrm{NR}} = \varepsilon_{nl} \sum_{m\sigma} c^\dagger_{m\sigma} c_{m\sigma} + \frac{1}{2} \sum_{\sigma\sigma'} \sum_{m\tilde{m}m'\tilde{m}'} U^l_{mm'\tilde{m}\tilde{m}'} c^\dagger_{m\sigma} c^\dagger_{m'\sigma'} c_{\tilde{m}'\sigma'} c_{\tilde{m}\sigma}$$

kinetic+central

Coulomb

$$U^{iji'j'}_{mm'\tilde{m}\tilde{m}'} = \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 \, \frac{\overline{\psi_{im\sigma}}(\boldsymbol{r}_1)\overline{\psi_{jm'\sigma'}}(\boldsymbol{r}_2)\psi_{j'\tilde{m}'\sigma'}(\boldsymbol{r}_2)\psi_{i'\tilde{m}\sigma}(\boldsymbol{r}_1)}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}$$

many electron atoms

does the atom/ion carry a magnetic moment?

total spin **S** and total angular momentum **L**

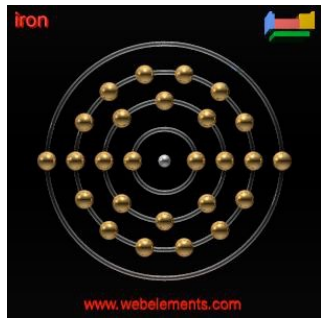
filled shells

S=L=0

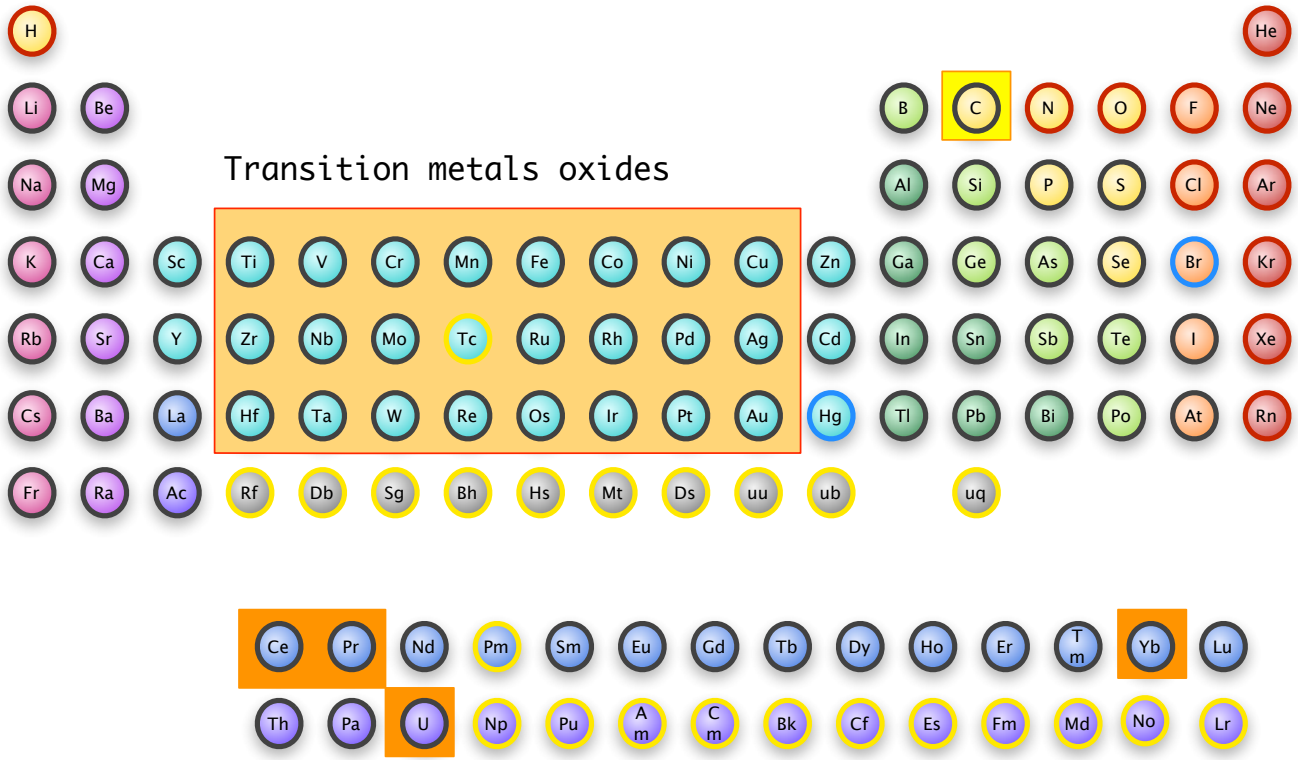
partially filled shell: **magnetic ions**

1. Hund's rule max S

2. Hund's rule max L



strongly correlated systems



here in particular transition-metal oxides
and f electron systems

origin: Coulomb repulsion

direct term: the same for all N electron states

$$U_{\mathrm{avg}} = \frac{1}{(2l+1)^2} \sum_{mm'} U^l_{mm'mm'}$$

exchange term: 1. Hund's rule

$$U_{\mathrm{avg}} - J_{\mathrm{avg}} = \frac{1}{2l(2l+1)} \sum_{mm'} \left(U^l_{mm'mm'} - U^l_{mm'm'm} \right)$$

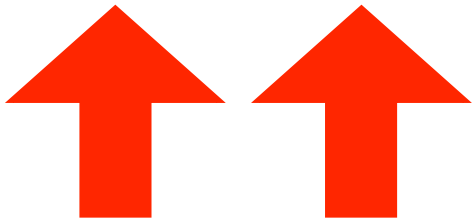
Coulomb exchange

C atom, p shell

$$
\begin{aligned}
J^p_{m,m'} &= U^p_{mm'm'm} \\
&= \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 \, \frac{\overline{\psi_{im\sigma}}(\boldsymbol{r}_1)\overline{\psi_{im'\sigma}}(\boldsymbol{r}_2)\psi_{im\sigma}(\boldsymbol{r}_2)\psi_{im'\sigma}(\boldsymbol{r}_1)}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \\
&= \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 \, \frac{\phi_{imm'\sigma}(\boldsymbol{r}_1)\overline{\phi_{imm'\sigma}}(\boldsymbol{r}_2)}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} = \frac{1}{V}\sum_{\boldsymbol{k}} \frac{4\pi}{k^2} \left|\phi_{imm'\sigma}(\boldsymbol{k})\right|^2 ,
\end{aligned}
$$

positive, hence **always ferromagnetic**

$$
-\frac{1}{2}\sum_{\sigma}\sum_{m\neq m'} J^p_{m,m'} c^\dagger_{m\sigma} c_{m\sigma} c^\dagger_{m'\sigma} c_{m'\sigma} = -\frac{1}{2}\sum_{m\neq m'} 2J^p_{m,m'} \left[S^m_z S^{m'}_z + \frac{1}{4} n_m n'_m \right]
$$



a C atom

[He] $2s^2 2p^2$

incomplete p shell: l=1
total spin and angular momentum

S $1/2 \otimes 1/2 = 0 \oplus 1$

L $1 \otimes 1 = 0 \oplus 1 \oplus 2$

S P D

S=0 ——— S

S=0 ——— D

2. Hund's rule

1. Hund's rule

^3P S=1 ——— P

spin-orbit interaction

if weak, LS coupling approximation

$$H_e^{\mathrm{SO}} \sim \lambda \, \boldsymbol{L} \cdot \boldsymbol{S} = \frac{1}{2} \lambda \, \left(\boldsymbol{J}^2 - \boldsymbol{S}^2 - \boldsymbol{L}^2 \right),$$

$$\lambda \sim \left[2\Theta(1-2n) - 1 \right] \, g\mu_B^2 \, \frac{1}{2S} \left\langle \frac{1}{r} \frac{d}{dr} v_{\mathrm{R}}(r) \right\rangle$$

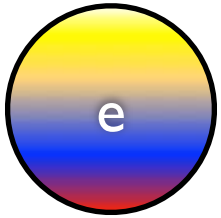
3. Hund's rule

- total angular momentum $J = \begin{cases} |L-S| & \text{for filling } n < 1/2 \\ S & \text{for filling } n = 1/2 \\ L+S & \text{for filling } n > 1/2 \end{cases}$

^{3}P S=1 —— P $^3P_0$ $^{2S+1}L_J$

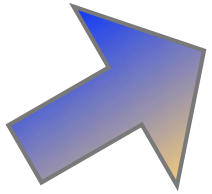
what are local moments ?

emergent entities



integrate out high-energy states (high energy multiplets)

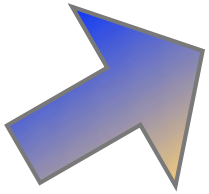
from electrons emerge spins (ground state multiplet)



effective elementary entities

magnetic ions in solids

does the magnetic moment survive?



isolated ion Fe^{3+}

S=5/2

isolated ion Fe^{2+}

S=1/2 L=2 J=5/2

ion in crystals?

electronic Hamiltonian

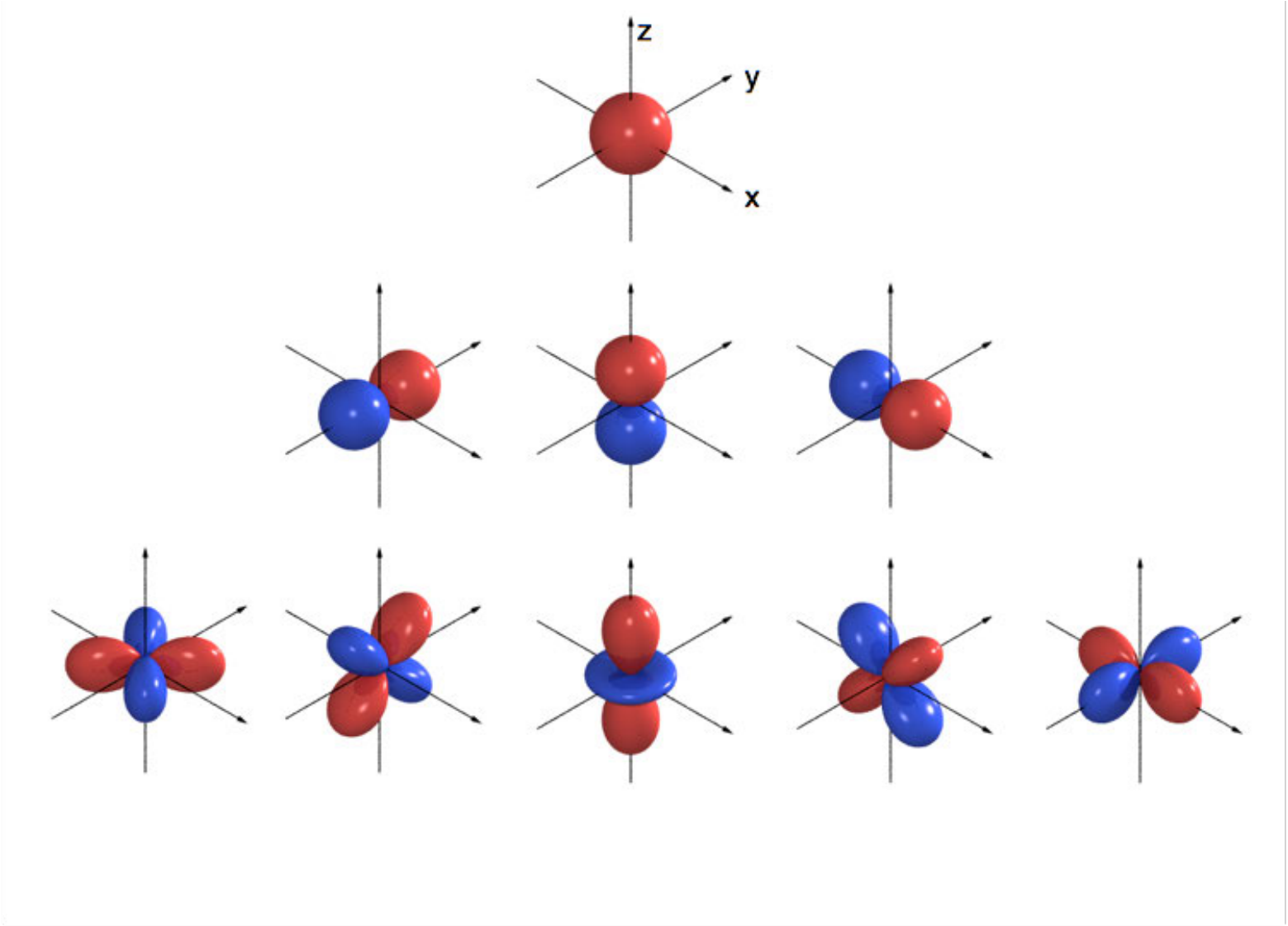
non relativistic electronic Hamiltonian

$$H_e^{\mathrm{NR}} = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_{i'}|} - \sum_{i\alpha} \frac{Z_\alpha}{|\boldsymbol{r}_i - \boldsymbol{R}_\alpha|} + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\boldsymbol{R}_\alpha - \boldsymbol{R}_{\alpha'}|}$$

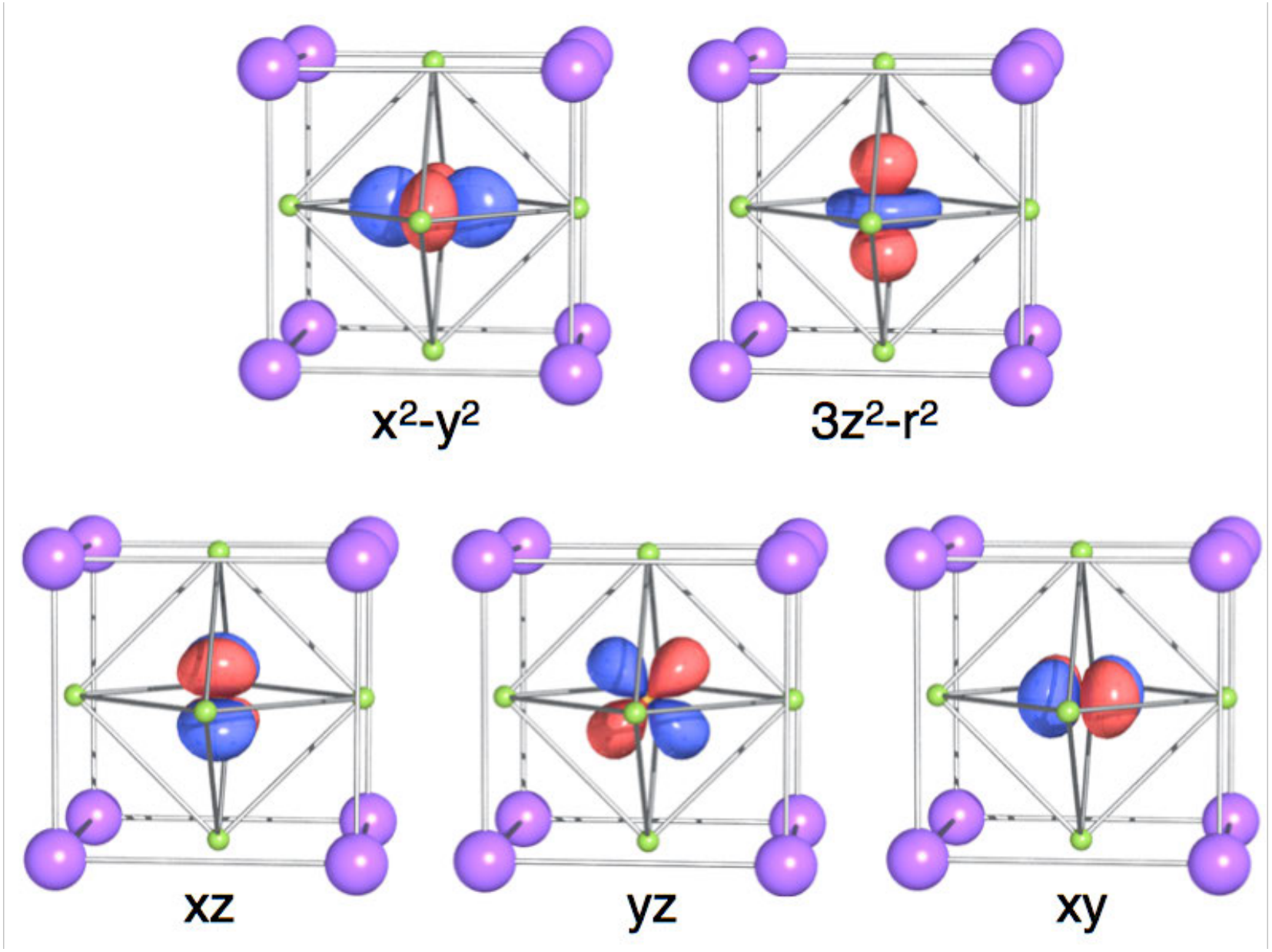
kinetic **Coulomb** **potential** constant

choose a one-electron basis

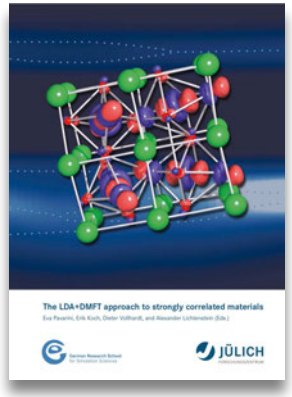
let us chose a one-electron basis



localized Wannier functions



electronic Hamiltonian



$$H_e^{\mathrm{NR}} = -\sum_{ii'\sigma}\sum_{mm'} t^{i,i'}_{m,m'} c^\dagger_{im\sigma} c_{i'm'\sigma}$$

hoppings + crystal field

$$+\frac{1}{2}\sum_{ii'jj'}\sum_{\sigma\sigma'}\sum_{mm'}\sum_{\tilde{m}\tilde{m}'} U^{iji'j'}_{mm'\tilde{m}\tilde{m}'} c^\dagger_{im\sigma} c^\dagger_{jm'\sigma'} c_{j'\tilde{m}'\sigma'} c_{i'\tilde{m}\sigma}$$

Coulomb

crystal field & hopping integrals

$$t^{i,i'}_{m,m'} = -\int d\boldsymbol{r}\, \overline{\psi_{im\sigma}}(\boldsymbol{r}) \left[-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(\boldsymbol{r})\right] \psi_{i'm'\sigma}(\boldsymbol{r})$$

crystal field

i=i’

$$\varepsilon^{i,i}_{m,m'} = t^{i,i}_{m,m'} = -\int d\boldsymbol{r}\, \overline{\psi_{im\sigma}}(\boldsymbol{r}) \left[-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(\boldsymbol{r})\right] \psi_{im'\sigma}(\boldsymbol{r})$$

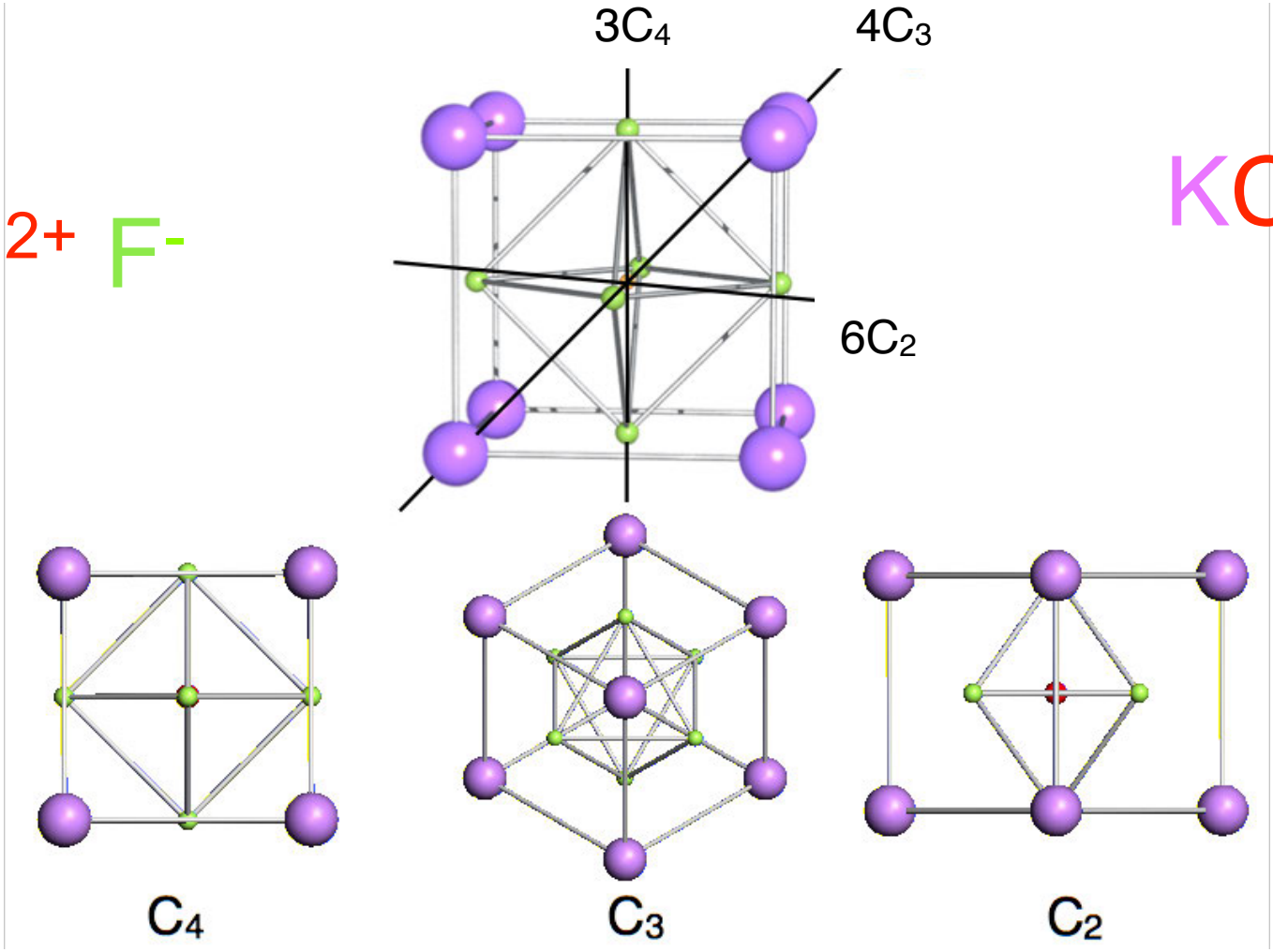
modifies on-site energies

and thus local magnetic moment

perovskite structure ABC_3

K^+ Cu^{2+} F^-

$KCuF_3$



it is the symmetry group of the cube

crystal-field theory

how do *d* levels split at the Cu site?

point charge model

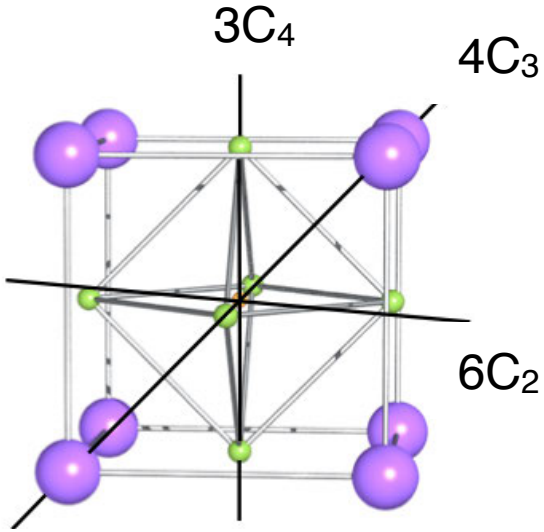
$$v_{\mathrm{R}}(\boldsymbol{r}) = \sum_{\alpha} \frac{q_\alpha}{|\boldsymbol{R}_\alpha - \boldsymbol{r}|} = v_0(r) + \sum_{\alpha \neq 0} \frac{q_\alpha}{|\boldsymbol{R}_\alpha - \boldsymbol{r}|} = v_0(r) + v_c(\boldsymbol{r})$$

crystal field

$KCuF_3$

K^+ Cu^{2+} F^-

q_K q_{Cu} q_F



(in real materials, also covalency effects!)

cubic perovskite

point charge model: F_6 octahedron

$$v_{\mathrm{oct}}(\boldsymbol{r}) = \frac{35}{4}\frac{q_C}{a^5}\left(x^4+y^4+z^4-\frac{3}{5}r^4\right) = D\left(x^4+y^4+z^4-\frac{3}{5}r^4\right).$$

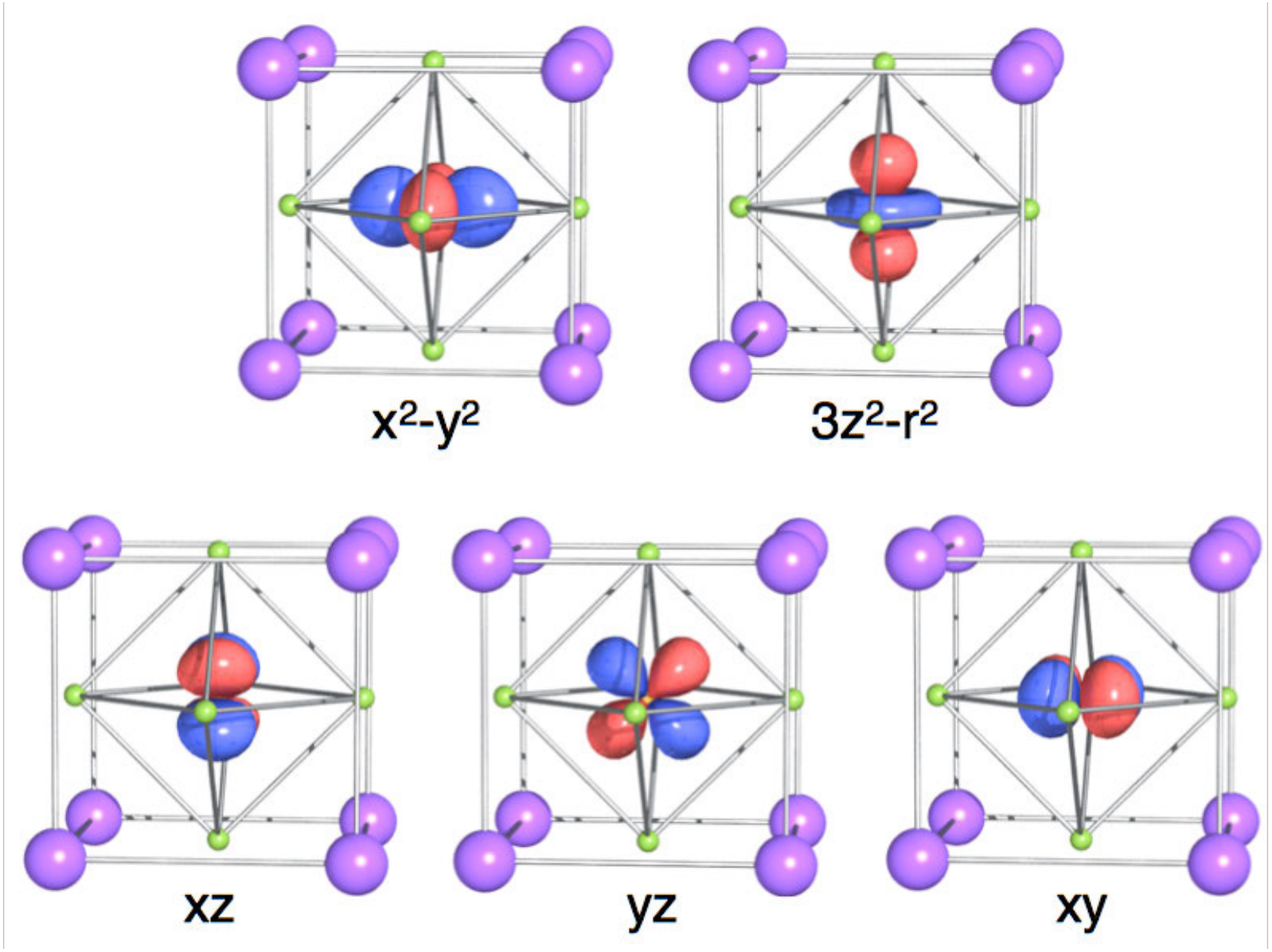
$$H_{\mathrm{CF}} = \begin{array}{c} \begin{array}{ccccc} \text{m=-2} & \text{m=-1} & \text{m=0} & \text{m=1} & \text{m=2} \end{array} \\ \begin{pmatrix} Dq & 0 & 0 & 0 & 5Dq \\ 0 & -4Dq & 0 & 0 & 0 \\ 0 & 0 & 6Dq & 0 & 0 \\ 0 & 0 & 0 & -4Dq & 0 \\ 5Dq & 0 & 0 & 0 & Dq \end{pmatrix} \end{array}.$$

$$\psi_{nlm}(\rho,\theta,\phi) = R_{nl}(\rho)Y_l^m(\theta,\phi)$$

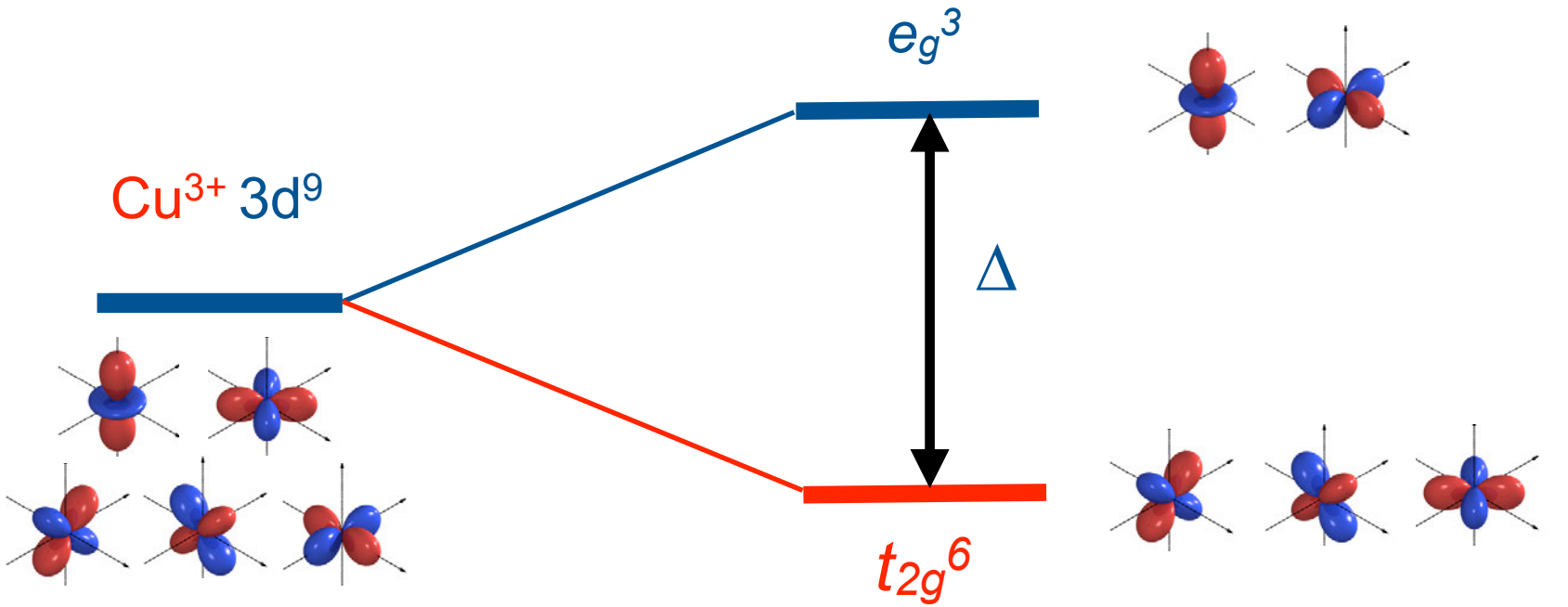
atomic functions

$$Dq = -q_F\langle r^4\rangle/6a^5$$

3d Wannier functions



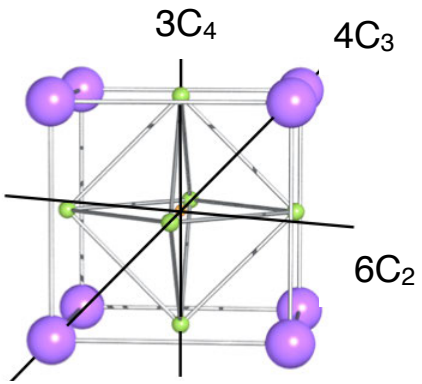
cubic crystal-field



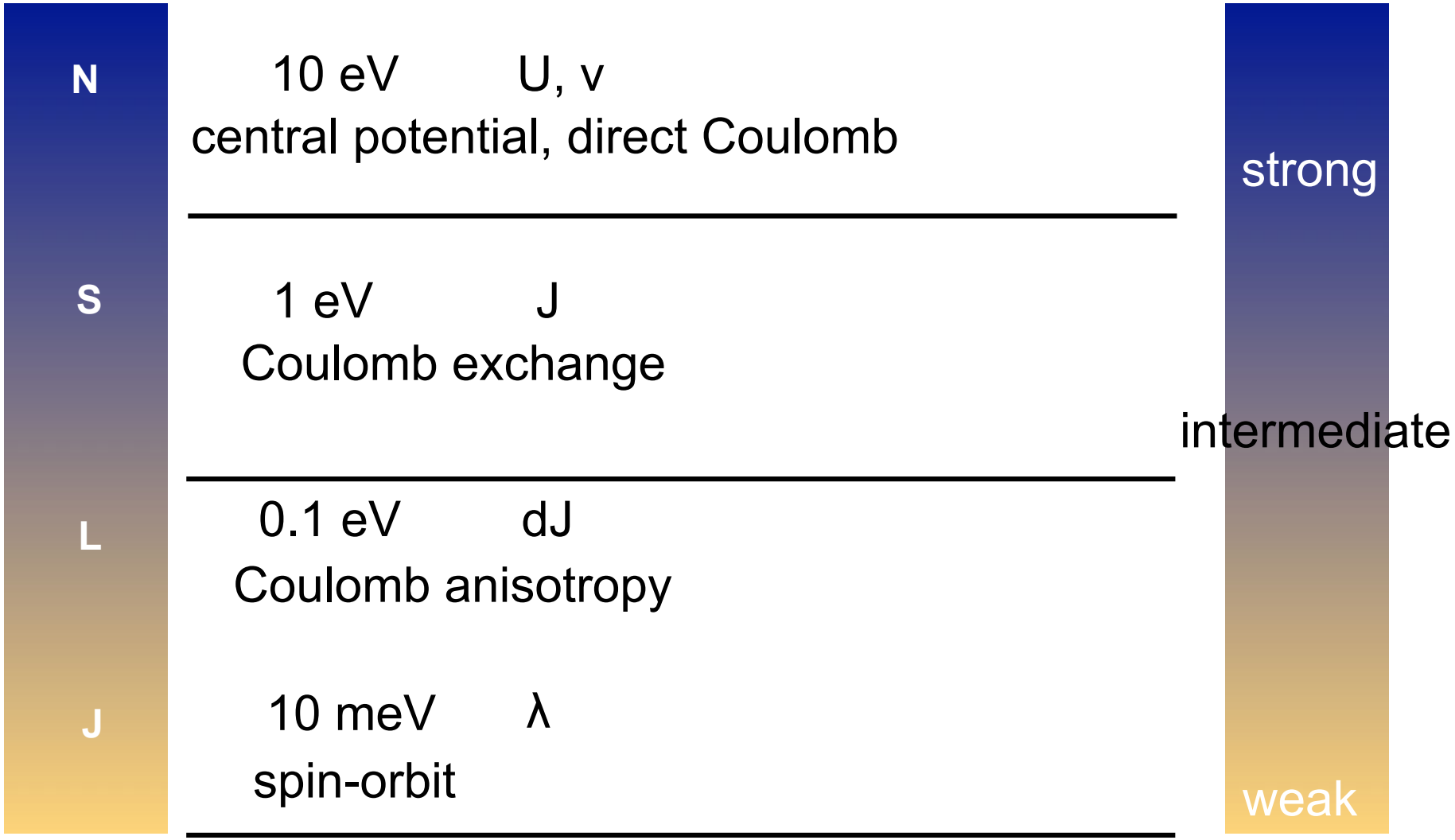
crystal-field states

spherical

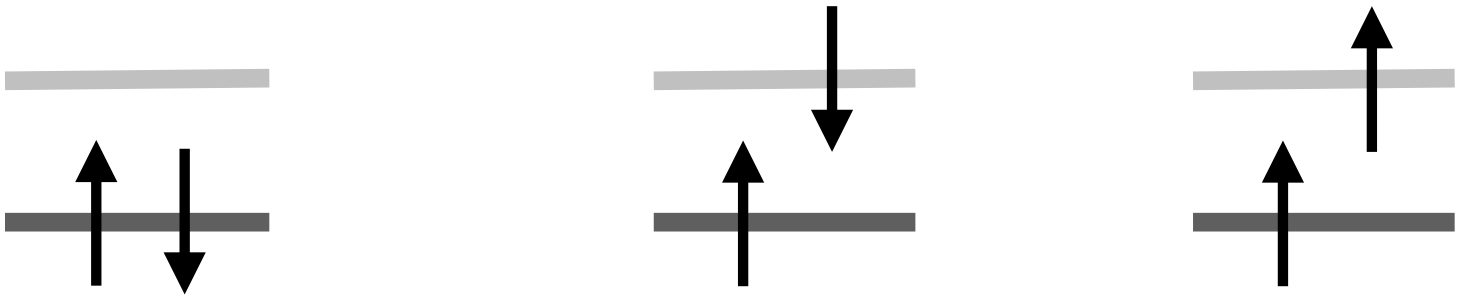
cubic



energy scales



density-density Coulomb

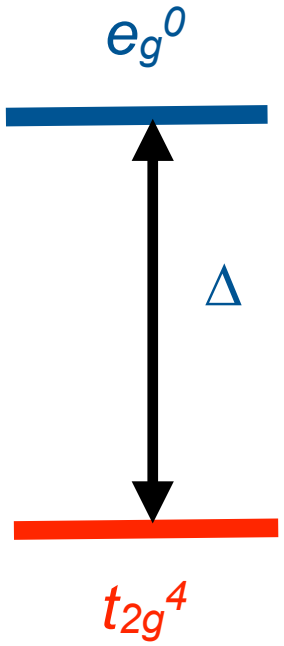


U

U-2J+Δ

U-3J+Δ

strong field

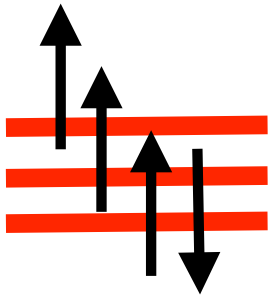


t_{2g}^4

4d, ruthenates

no 1. Hund's rule!

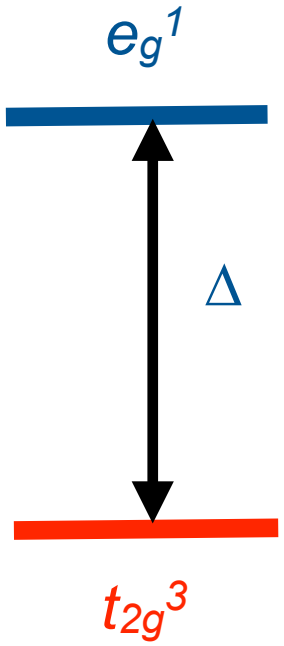
Δ > 3J



S=1

6U-15J

intermediate

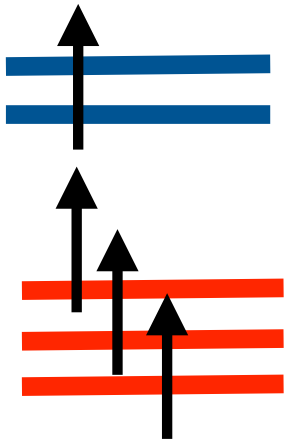


$t_{2g}^3\ e_g^1$

3d, manganites

1. Hund's rule satisfied

however, no 2. Hund's rule!



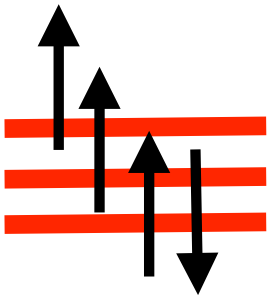
S=2

6U-18J+Δ

does the moment survive?

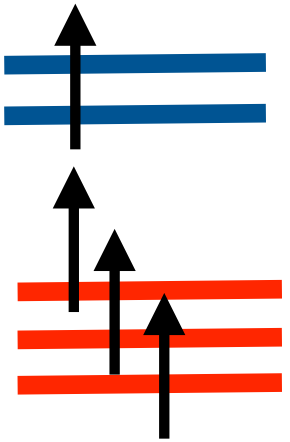
it depends…

Ru^{4+}



t_{2g}^4

S=1



Mn^{3+}

S=2

transition-metal ions

Ion			n	S	L	J	$^{2S+1}L_J$
V^{4+}	Ti^{3+}		$3d^1$	1/2	2	3/2	$^2D_{3/2}$
	V^{3+}		$3d^2$	1	3	2	$^3F_2$
	Cr^{3+}	V^{2+}	$3d^3$	3/2	3	3/2	$^4F_{3/2}$
	Mn^{3+}	Cr^{2+}	$3d^4$	2	2	0	$^5D_0$
	Fe^{3+}	Mn^{2+}	$3d^5$	5/2	0	5/2	$^6S_{5/2}$
		Fe^{2+}	$3d^6$	2	2	4	$^5D_4$
		Co^{2+}	$3d^7$	3/2	3	9/2	$^4F_{9/2}$
		Ni^{2+}	$3d^8$	1	3	4	$^3F_4$
		Cu^{2+}	$3d^9$	1/2	2	5/2	$^2D_{5/2}$

J=S

hopping integrals

hopping integrals

$$H_e^{\mathrm{NR}} = -\sum_{ii'\sigma}\sum_{mm'} t_{m,m'}^{i,i'} c_{im\sigma}^{\dagger} c_{i'm'\sigma} + \frac{1}{2}\sum_{ii'jj'}\sum_{\sigma\sigma'}\sum_{mm'}\sum_{\tilde{m}\tilde{m}'} U_{mm'\tilde{m}\tilde{m}'}^{iji'j'} c_{im\sigma}^{\dagger} c_{jm'\sigma'}^{\dagger} c_{j'\tilde{m}'\sigma'} c_{i'\tilde{m}\sigma}$$

one-electron basis: Wannier functions

crystal field & hopping integrals

$$t_{m,m'}^{i,i'} = -\int d\boldsymbol{r}\, \overline{\psi_{im\sigma}}(\boldsymbol{r}) \left[-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(\boldsymbol{r})\right] \psi_{i'm'\sigma}(\boldsymbol{r})$$

hopping integrals

i≠i′

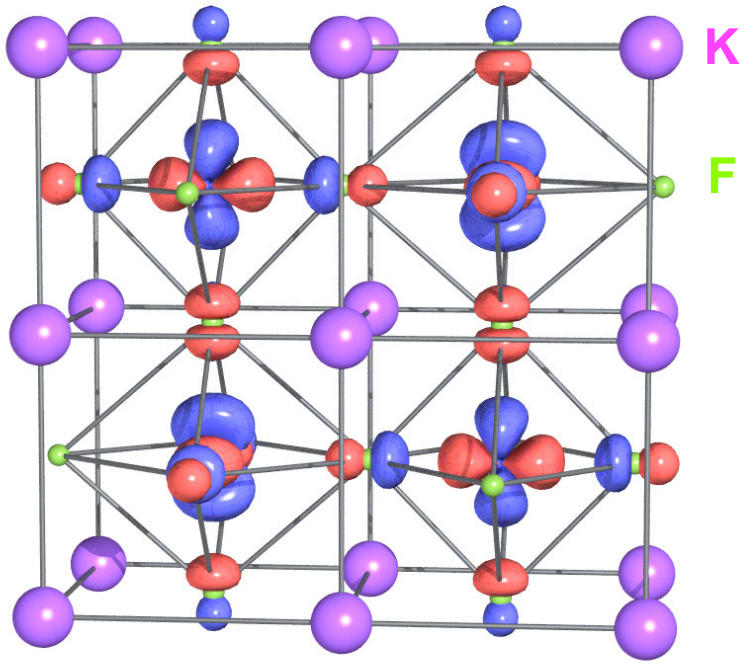
$$t^{i,i'}_{m,m'} = -\int d\boldsymbol{r}\, \overline{\psi_{im\sigma}}(\boldsymbol{r}) \left[-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(\boldsymbol{r})\right] \psi_{i'm'\sigma}(\boldsymbol{r})$$

generates band structure

delocalizes electrons, **suppresses local moment**

an example: $KCuF_3$

atomic orbitals replaced by localized LDA Wannier functions



$K^+ Cu^{2+} F^-$

$K\ 4s^0\ Cu\ 3d^9\ F\ 2p^6$

an example: $KCuF_3$

$$H_e^{\mathrm{NR}} = -\sum_{ii'\sigma}\sum_{mm'} t_{m,m'}^{i,i'} c_{im\sigma}^{\dagger} c_{i'm'\sigma} + \frac{1}{2}\sum_{ii'jj'}\sum_{\sigma\sigma'}\sum_{mm'}\sum_{\tilde{m}\tilde{m}'} U_{mm'\tilde{m}\tilde{m}'}^{iji'j'} c_{im\sigma}^{\dagger} c_{jm'\sigma'}^{\dagger} c_{j'\tilde{m}'\sigma'} c_{i'\tilde{m}\sigma}$$

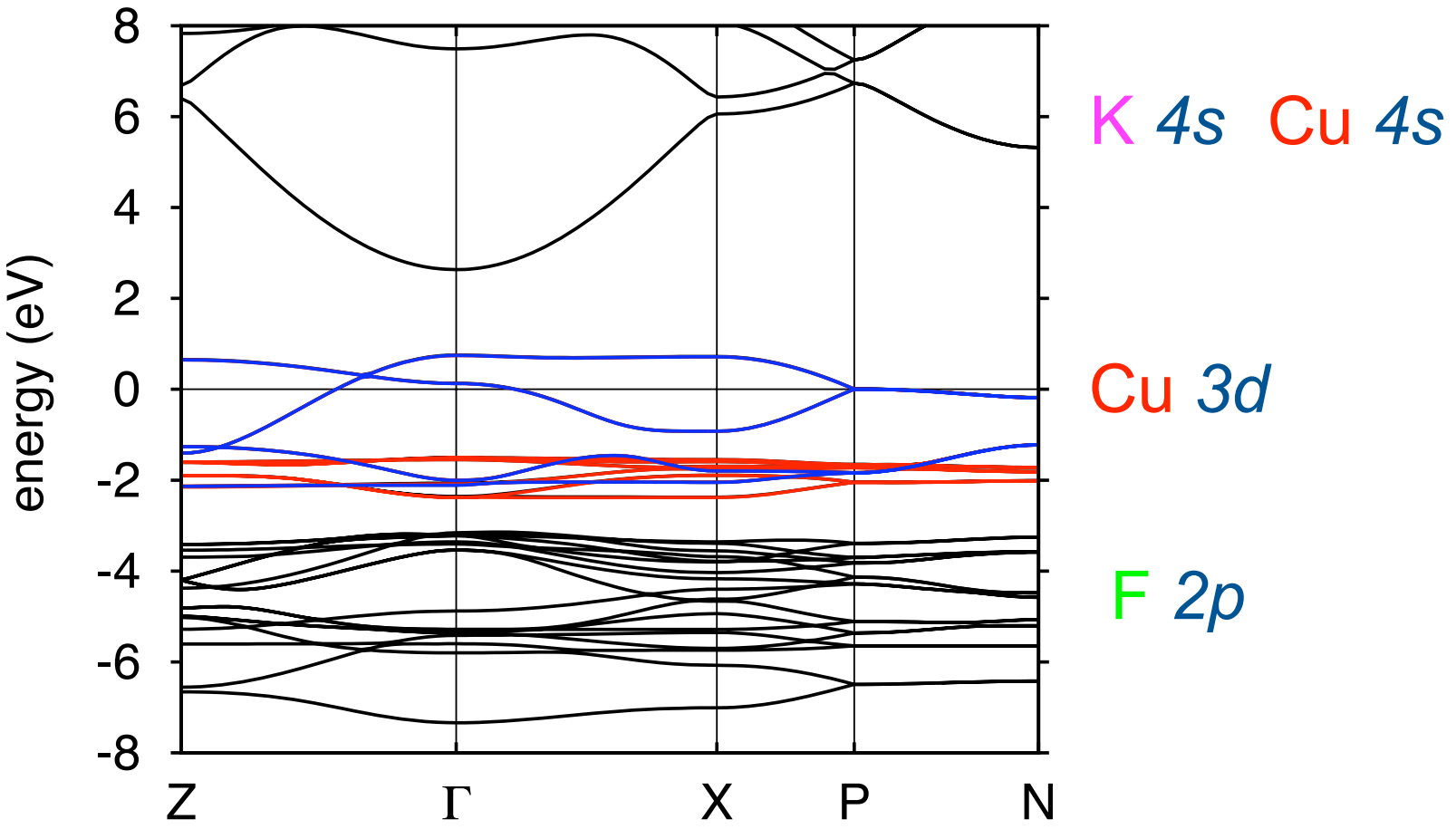
one-electron basis: localized LDA Wannier functions

only Coulomb effects contained in LDA

LDA band structure

partially filled d-like bands, metallic

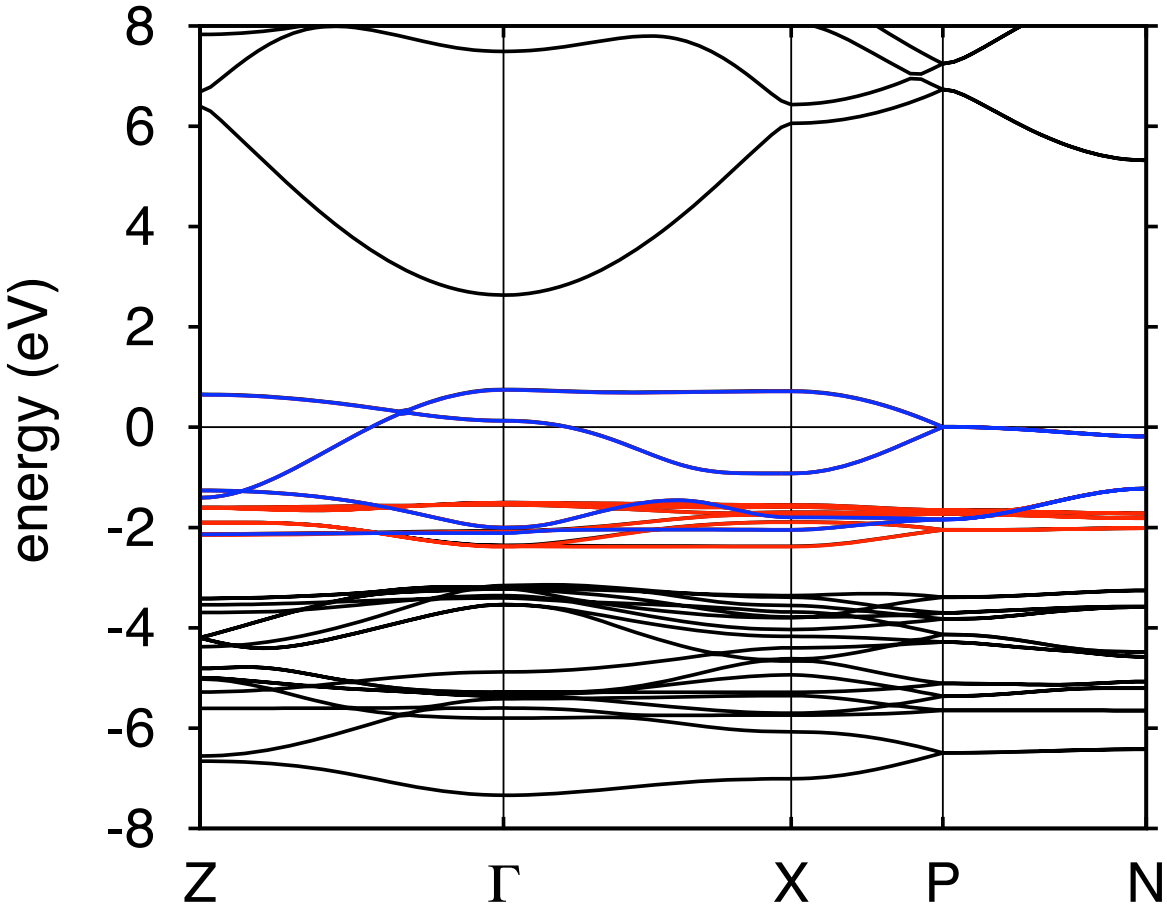
non-magnetic & **no local moments**



(in reality: Mott insulator, local moment, paramagnetic for T>40 K)

does the moment survive?

if *hoppings* very large the do not



how does long-range magnetic order arises?

step 1: from the many-body problem
to the Hubbard model

electronic Hamiltonian

hoppings + crystal field

$$H_e^{\mathrm{NR}} = -\sum_{ii'\sigma}\sum_{mm'} t^{i,i'}_{m,m'} c^\dagger_{im\sigma} c_{i'm'\sigma}$$

$$+\frac{1}{2}\sum_{ii'jj'}\sum_{\sigma\sigma'}\sum_{mm'}\sum_{\tilde{m}\tilde{m}'} U^{iji'j'}_{mm'\tilde{m}\tilde{m}'} c^\dagger_{im\sigma} c^\dagger_{jm'\sigma'} c_{j'\tilde{m}'\sigma'} c_{i'\tilde{m}\sigma}$$

Coulomb

inter-site Coulomb exchange

$$J^{i,i'} = U^{ii'i'i}_{mmmm} = \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 \, \frac{\overline{\psi_{im\sigma}}(\boldsymbol{r}_1)\overline{\psi_{i'm\sigma}}(\boldsymbol{r}_2)\psi_{im\sigma}(\boldsymbol{r}_2)\psi_{i'm\sigma}(\boldsymbol{r}_1)}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|},$$

ferromagnetic!

let us simplify (a lot :)

real Hamiltonian

hoppings + crystal field

$$H_e^{\mathrm{NR}} = -\sum_{ii'\sigma}\sum_{mm'} t_{m,m'}^{i,i'} c_{im\sigma}^{\dagger} c_{i'm'\sigma}$$

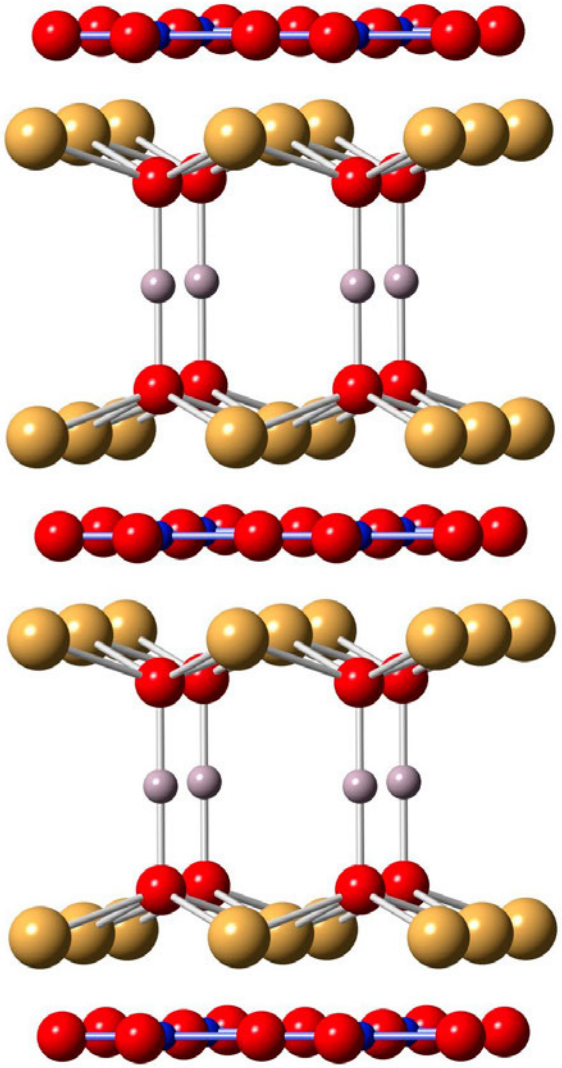
$$+\frac{1}{2}\sum_{ii'jj'}\sum_{\sigma\sigma'}\sum_{mm'}\sum_{\tilde{m}\tilde{m}'} U_{mm'\tilde{m}\tilde{m}'}^{iji'j'} c_{im\sigma}^{\dagger} c_{jm'\sigma'}^{\dagger} c_{j'\tilde{m}'\sigma'} c_{i'\tilde{m}\sigma}$$

Coulomb

one band Hubbard model

$$H = \varepsilon_d \sum_i \sum_\sigma c_{i\sigma}^{\dagger} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c_{i\sigma}^{\dagger} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U$$

high-T_c superconducting cuprates



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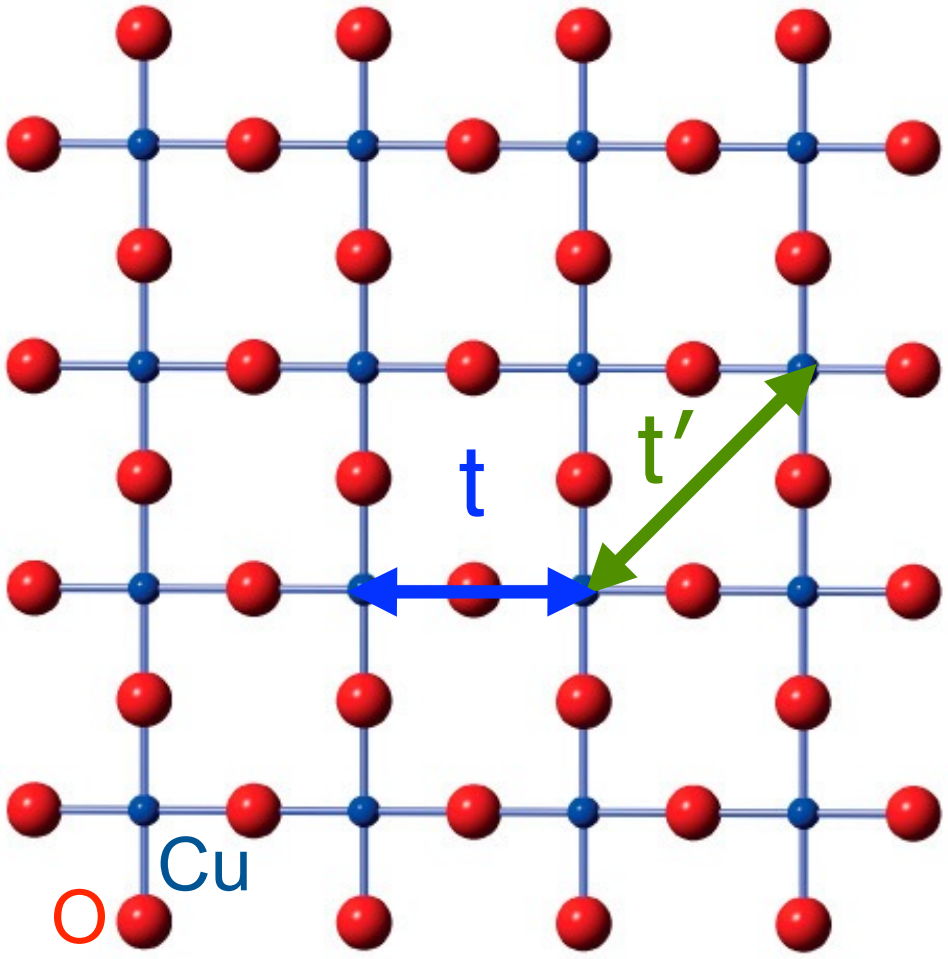


CuO_2 planes

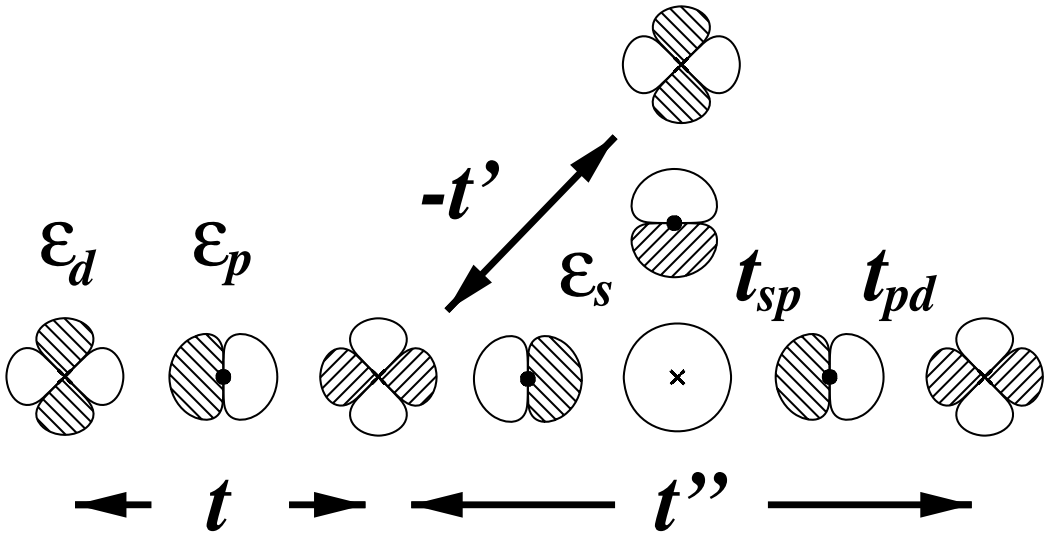
high-T_c superconducting cuprates

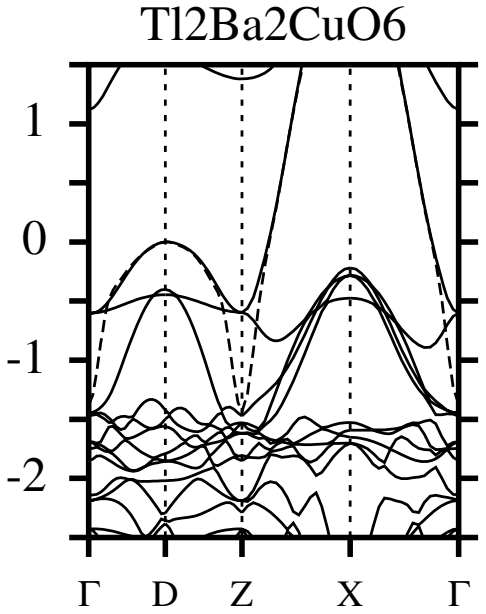
VOLUME 87, NUMBER 4 PHYSICAL REVIEW LETTERS 23 JULY 2001

Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_{c\,\max}$

E. Pavarini, I. Dasgupta,* T. Saha-Dasgupta,† O. Jepsen, and O. K. Andersen
Max-Planck-Institut für Festkörperforschung, D-70506 Stuttgart, Germany
(Received 4 December 2000; published 10 July 2001)

By calculation and analysis of the bare conduction bands in a large number of hole-doped high-temperature superconductors, we have identified the range of the intralayer hopping as the essential, material-dependent parameter. It is controlled by the energy of the axial orbital, a hybrid between Cu $4s$, apical-oxygen $2p_z$, and farther orbitals. Materials with higher $T_{c\,\max}$ have larger hopping ranges and axial orbitals more localized in the CuO_2 layers.





parameters for high-T_c superconductors

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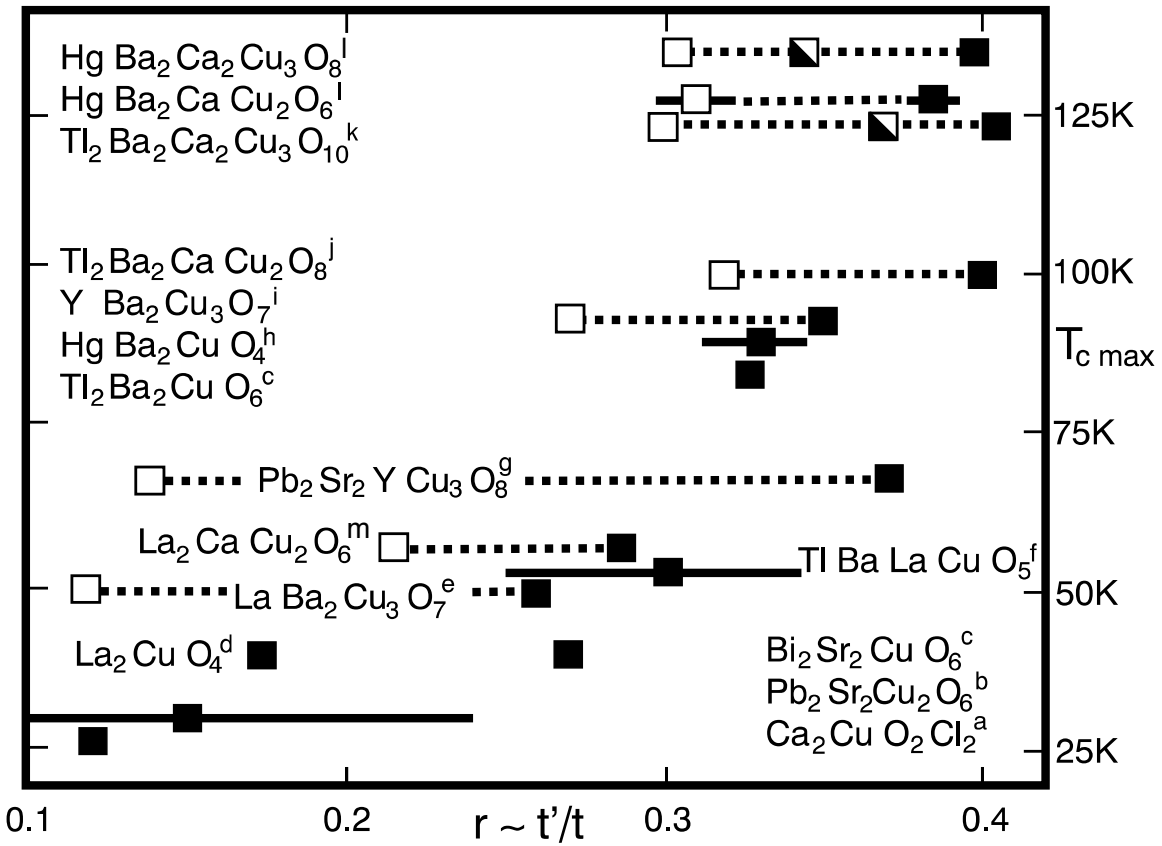


the Hubbard model

the Hubbard model

$$H = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U$$

$$\begin{cases} \varepsilon_d &= -t^{i,i}_{1,1} \\ t &= t^{\langle i,i' \rangle}_{1,1} \\ U &= U^{iiii}_{1111} \end{cases}$$

half filling

t=0: N_s atoms, insulator

U=0: half-filled band, metal

half filling

the *t=0* case: atomic limit

t=0: N_s atoms, insulator

atomic limit (*t=0*) & half filling

$\lvert N,S,S_z\rangle$			N	S	$E(N)$
$\lvert 0,0,0\rangle$	$=$	$\lvert 0\rangle$	0	0	0
$\lvert 1,\frac{1}{2},\uparrow\rangle$	$=$	$c^\dagger_{i\uparrow}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 1,\frac{1}{2},\downarrow\rangle$	$=$	$c^\dagger_{i\downarrow}\lvert 0\rangle$	1	$1/2$	ε_d
$\lvert 2,0,0\rangle$	$=$	$c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}\lvert 0\rangle$	2	0	$2\varepsilon_d+U$

S=1/2

$$H_d + H_U = \varepsilon_d \sum_i n_i + U \sum_i \left[-\left(S^i_z\right)^2 + \frac{n_i^2}{4} \right]$$

emergence of the spin!

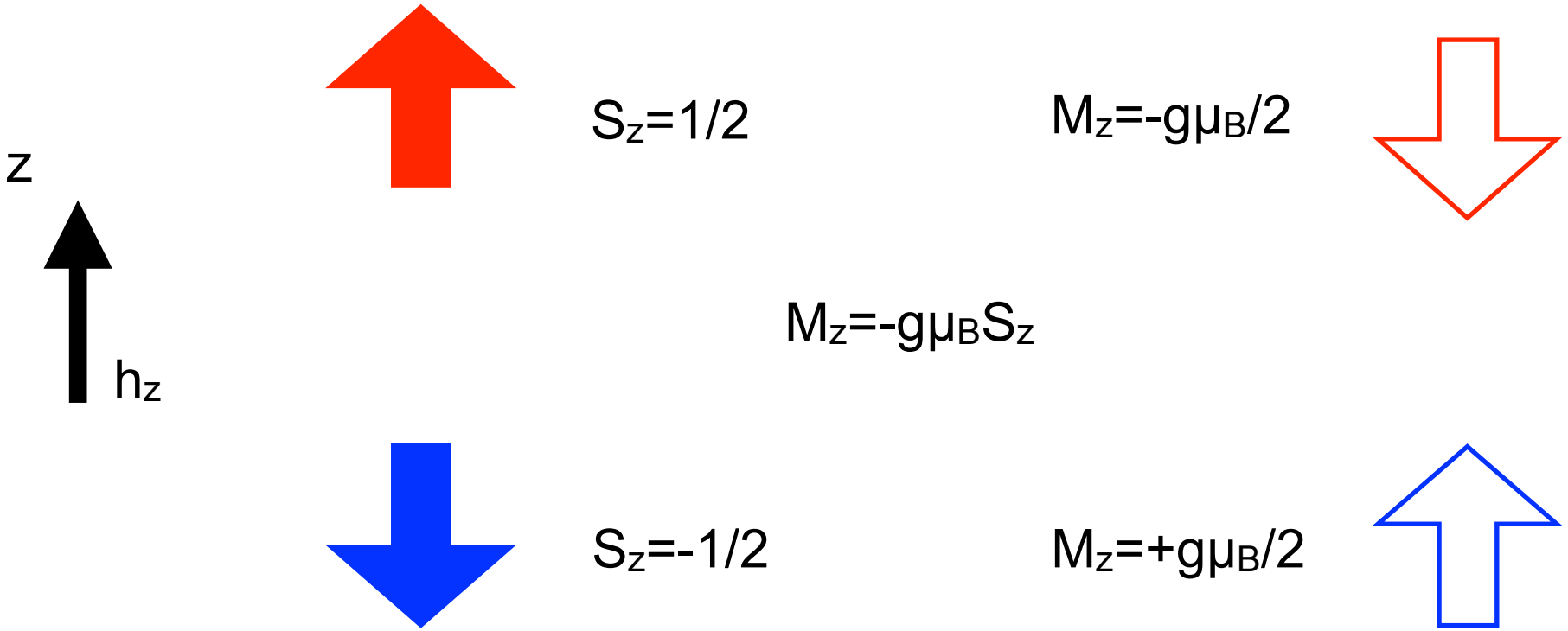
half filling: highly degenerate states, 2^{Ns} degrees of freedom

insulating behavior

magnetic properties isolated S=1/2 ions

Zeeman term

$$H_Z = g\mu_B h_z S_z$$



linear response theory

linear response

$$M_z(\boldsymbol{q};\omega) = \chi_{zz}(\boldsymbol{q};\omega) h_z(\boldsymbol{q};\omega)$$

magnetization

magnetic field

response function

thermodynamic sum rule

$$\chi_{zz}(\mathbf{0};0) = \lim_{h_z \to 0} \frac{\partial M_z}{\partial h_z}$$

magnetization

non interacting ions

uniform magnetic field h_z, Zeeman term

$$M_z = \langle M_z^i \rangle = -g\mu_B \frac{\mathrm{Tr}\left[e^{-g\mu_B h_z \beta S_z^i} S_z^i\right]}{\mathrm{Tr}\left[e^{-g\mu_B h_z \beta S_z^i}\right]} = g\mu_B S \tanh\left(g\mu_B h_z \beta S\right)$$

derivative with respect to h_z

$$\frac{\partial M_z}{\partial h_z} = \left(g\mu_B S\right)^2 \frac{1}{k_B T} \left[1 - \tanh^2\left(g\mu_B h_z \beta S\right)\right]$$

Curie susceptibility

$$\chi_{zz}(\mathbf{0};0) = (g\mu_B S)^2 \frac{1}{k_B T} = \frac{C_{1/2}}{T}$$

Curie constant

$$C_{1/2} = \frac{(g\mu_B)^2 S(S+1)}{3k_B}$$

paramagnet vs disordered system

$$\mathcal{S}_{i,i'} = \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_{i'} \rangle \sim \begin{cases} \langle \boldsymbol{S}_i \rangle \cdot \langle \boldsymbol{S}_{i'} \rangle & \sim 0 \quad i \neq i' \\ \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_i \rangle & = 3/4 \quad i = i' \end{cases}$$

paramagnet

Curie susceptibility

different from

$$\sum_{i' \neq i} \langle S_z^i \cdot S_z^{i'} \rangle \sim 0$$

spin disorder

e.g. spin glass behavior

spin as emergent entity (large U limit)

t=0 Hubbard model

$$\chi_{zz}(\mathbf{0};0) \sim \frac{(g\mu_B)^2}{k_B T}\left\{\frac{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\ \left(S_z^i\right)^2\right]}{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\right]} - \left[\frac{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\ S_z^i\right]}{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\right]}\right]^2\right\}$$

$$= \frac{C_{1/2}}{T}\frac{e^{\beta U/2}}{1+e^{\beta U/2}}$$

$$U = E(N_i+1) + E(N_i-1) - 2E(N_i)$$

infinite U limit: the spin S=1/2

only S=1/2 part of Hilbert space remains

the small *t/U* limit

Mott-insulator spin regime

from electrons emerge localized spins

localized spins interact

perturbation theory

Hubbard model

$$H = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U$$

half filling: N=1 electrons per site

n_D = number of doubly occupied sites

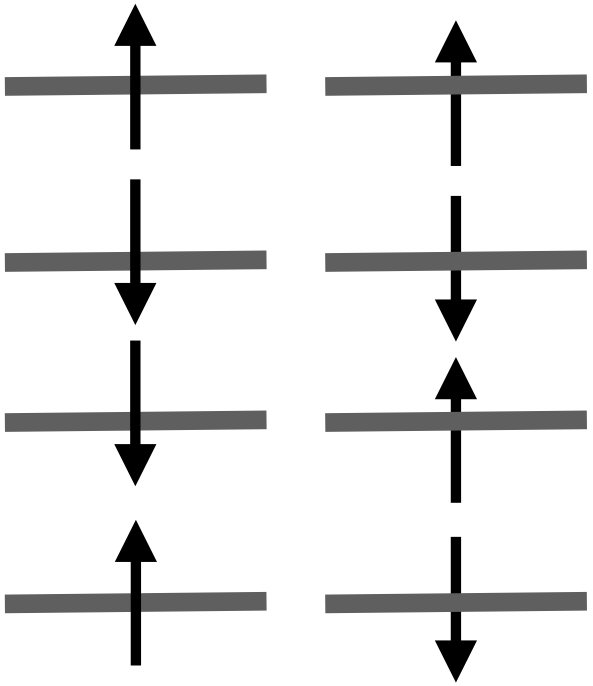
idea: divide Hilbert space into $n_D=0$ and $n_D>0$ sector

next downfold high energy $n_D>0$ sector

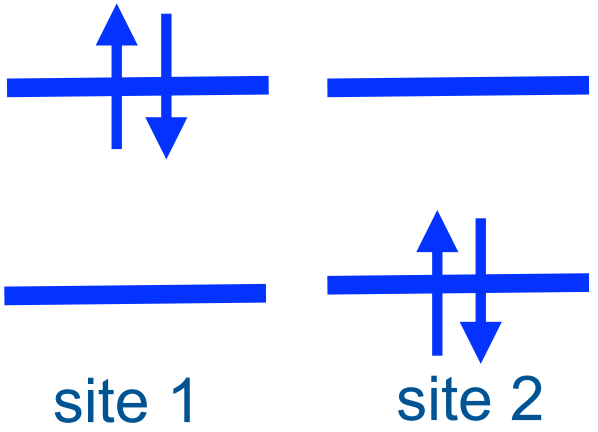
two sites

N=1 per site; $N_{tot}=2$

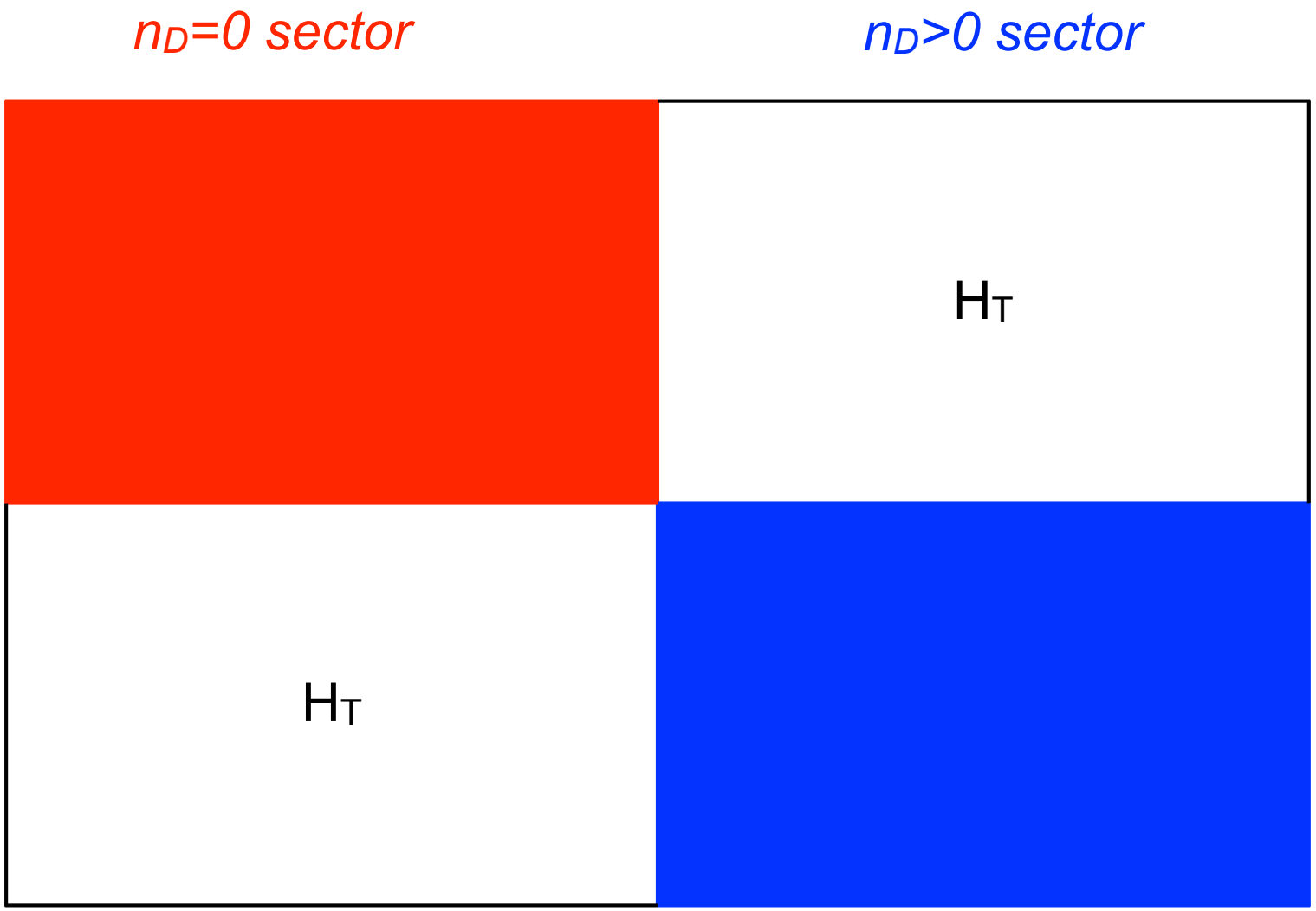
n_D=0 sector



n_D=1 sector



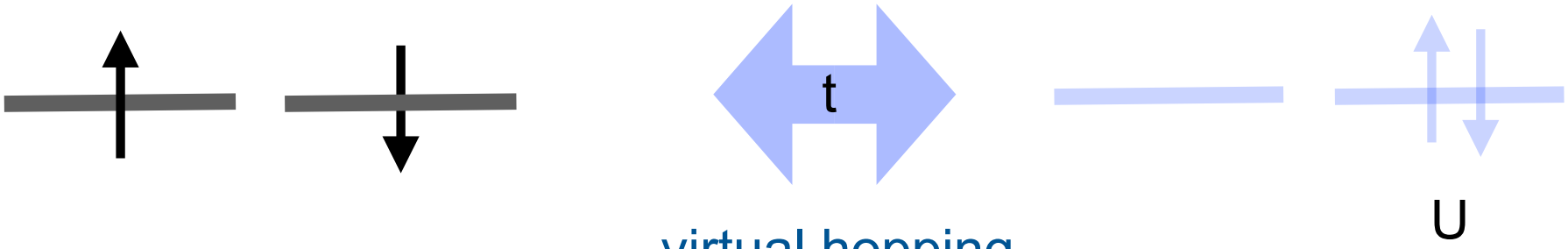
Hilbert space



next downfold high energy $n_D>0$ sector

low energy model

eliminate states with a doubly occupied site



virtual hopping

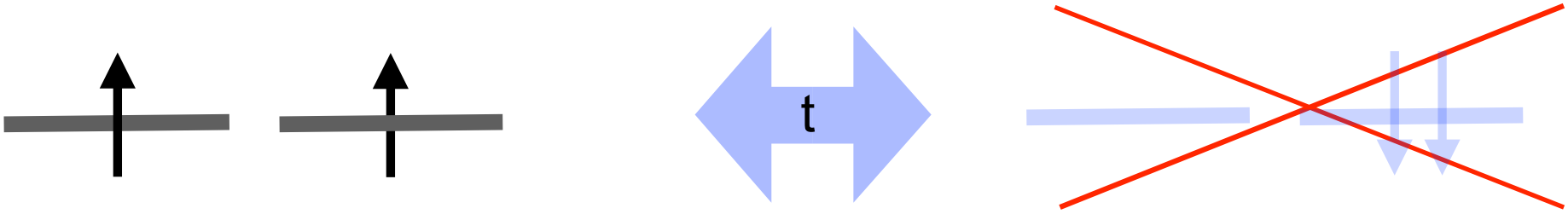
energy gain

$$\Delta E_{\uparrow\downarrow} \sim -\sum_I \langle\uparrow,\downarrow|H_T|I\rangle\langle I\left|\frac{1}{E(2)+E(0)-2E(1)}\right|I\rangle\langle I|H_T|\uparrow,\downarrow\rangle \sim -\frac{2t^2}{U}.$$

=t =1/U =t

low energy model

energy gain only for antiferromagnetic arrangement



$$\frac{1}{2}\Gamma \sim (\Delta E_{\uparrow\uparrow} - \Delta E_{\uparrow\downarrow}) = \frac{1}{2}\frac{4t^2}{U}$$

Pauli principle

$$H_S = \frac{1}{2}\Gamma \sum_{\langle ii' \rangle} \left[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i'} - \frac{1}{4} n_i n_{i'} \right]$$

a canonical transformation

Hubbard model

$$H = -t \sum_{\langle ii' \rangle} \sum_{\sigma} c^{\dagger}_{i\sigma} c_{i'\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} = H_T + H_U$$

here for simplicity $\varepsilon_d = 0$

half filling: N=1 per site

PHYSICAL REVIEW B VOLUME 37, NUMBER 16 1 JUNE 1988

t/U expansion for the Hubbard model

A. H. MacDonald, S. M. Girvin, and D. Yoshioka*
Department of Physics, Indiana University, Bloomington, Indiana 47405
(Received 8 January 1988)

a canonical transformation

$$H_T = -t \sum_{\langle ii' \rangle} \sum_{\sigma} c^{\dagger}_{i\sigma} c_{i'\sigma} = H_T^0 + H_T^+ + H_T^-$$

$$H_T^0 = -t \sum_{\langle ii' \rangle} \sum_{\sigma} n_{i-\sigma} c^{\dagger}_{i\sigma} c_{i'\sigma} n_{i'-\sigma} - t \sum_{\langle ii' \rangle} \sum_{\sigma} (1 - n_{i-\sigma})\, c^{\dagger}_{i\sigma} c_{i'\sigma}\, (1 - n_{i'-\sigma}),$$

no change in n_D

$$H_T^+ = -t \sum_{\langle ii' \rangle} \sum_{\sigma} n_{i-\sigma} c^{\dagger}_{i\sigma} c_{i'\sigma}\, (1 - n_{i'-\sigma}),$$

from n_D to n_D+1

$$H_T^- = \left(H_T^+\right)^{\dagger}$$

from n_D to n_D-1

n_D = number of doubly occupied states

a canonical transformation

$$H = -t \sum_{\langle ii' \rangle} \sum_{\sigma} c^{\dagger}_{i\sigma} c_{i'\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} = H_T + H_U$$

$$S = -\frac{i}{U} \left(H_T^+ - H_T^- \right)$$

$$H_S = e^{iS} H e^{-iS} = H + [iS, H] + \frac{1}{2} [iS, [iS, H]] + \ldots .$$

$[H_T^{\pm}, H_U] = \mp U H_T^{\pm}$ cancels $H_T^+ + H_T^-$

in $$H_T = -t \sum_{\langle ii' \rangle} \sum_{\sigma} c^{\dagger}_{i\sigma} c_{i'\sigma} = H_T^0 + H_T^+ + H_T^-,$$

half filling

thus

$$H_S = H_U + H_T^0 + \frac{1}{U}\left\{\left[H_T^+, H_T^-\right] + \left[H_T^0, H_T^-\right] + \left[H_T^+, H_T^0\right]\right\} + O(U^{-2})$$

these are zero at half filling

(no hopping possible without changing n_D)

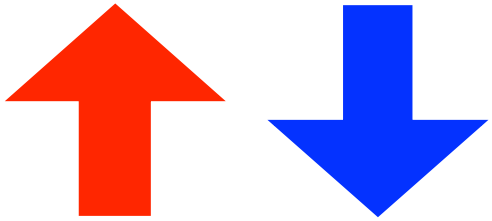
the remaining term is

$$H_S^{(2)} = \frac{1}{2}\frac{4t^2}{U}\sum_{ii'}\left[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i'} - \frac{1}{4}n_i n_{i'}\right].$$

example of kinetic exchange

interacting spins

$$H_S = \frac{1}{2}\Gamma \sum_{\langle ii' \rangle} \left[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i'} - \frac{1}{4} n_i n_{i'} \right]$$



from Hubbard model

to **antiferromagnetic** Heisenberg model

(remember, Coulomb exchange ferromagnetic)

interacting local moments

$$H = \frac{1}{2}\Gamma \sum_{ii'} \left[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i'} - \frac{1}{4} n_i n_{i'} \right]$$

Weiss mean-field approach

$$H = g\mu_B \sum_i \left[\boldsymbol{S}_i \cdot (\boldsymbol{h} + \boldsymbol{h}_i^m) + \text{const} \right]$$

$$\boldsymbol{h}_i^m = n_{\langle ii' \rangle} \Gamma \langle \boldsymbol{S}_{i'} \rangle / g\mu_B$$

antiferromagnetic case

bipartite lattice

sublattice A and sublattice B

& Zeeman term

$$\begin{cases} M_z^A/M_0 &= B_{1/2}\left[M_0(h_z+\Delta h_z^A)\beta\right] \\ M_z^B/M_0 &= B_{1/2}\left[M_0(h_z+\Delta h_z^B)\beta\right] \end{cases}$$

$$\begin{cases} \Delta h_z^A = & -(M_z^B/M_0)\, S^2 \Gamma n_{\langle ii'\rangle}/M_0 \\ \Delta h_z^B = & -(M_z^A/M_0)\, S^2 \Gamma n_{\langle ii'\rangle}/M_0 \end{cases}$$

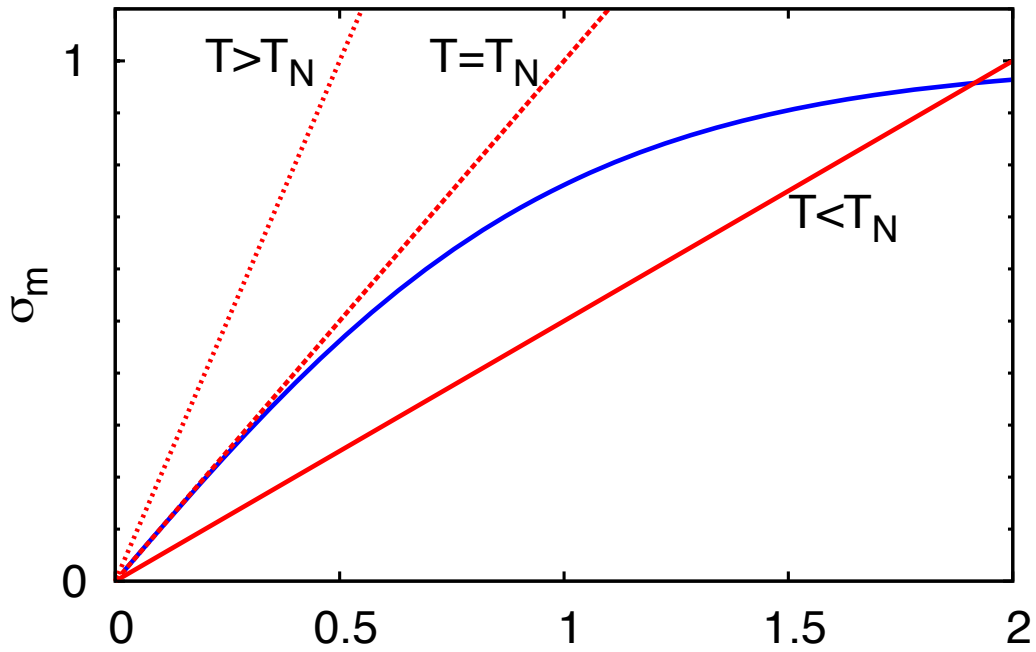
self-consistent equation

order parameter

$$\sigma_m = (M_z^B - M_z^A)/2M_0 = B_{1/2}\left[\sigma_m S^2 \Gamma n_{\langle ii' \rangle} \beta\right]$$

$$\sigma_m = B_{1/2}\left[\frac{T_{\mathrm{N}}}{T}\sigma_m\right]$$

T_N: Neel temperature



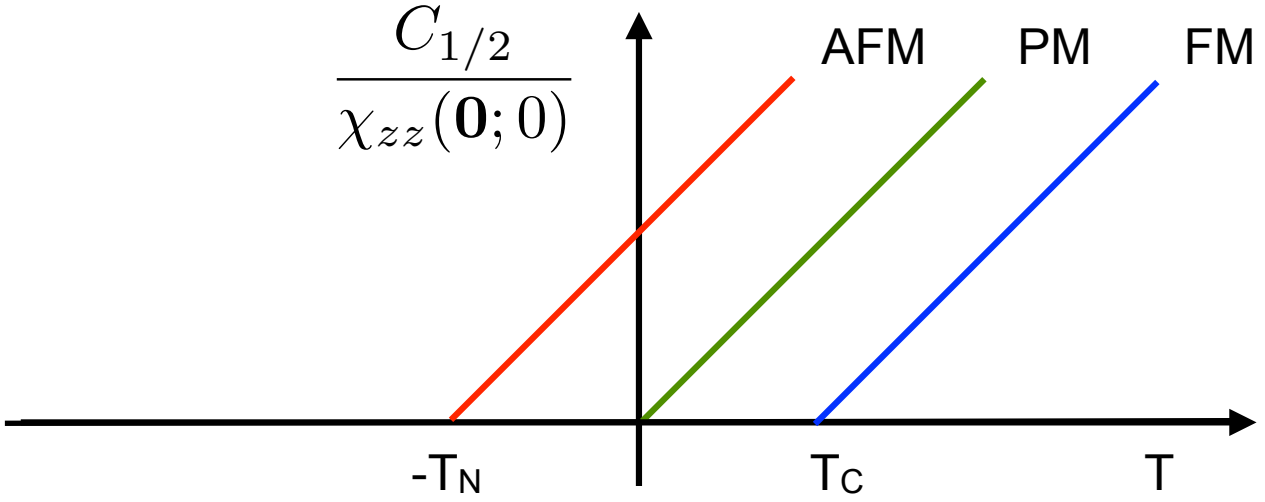
uniform response function

$$\chi_{zz}(\mathbf{0};0) = \frac{C_{1/2}(1-\sigma_m^2)}{T + (1-\sigma_m^2)T_{\mathrm{N}}}$$

Curie-Weiss high-temperature behavior

$$\chi_{zz}(\mathbf{0};0) \sim \frac{C_{1/2}}{T + T_{\mathrm{N}}}$$

no divergence!



finite q

$$\langle M_z^{ji} \rangle \quad = \quad -\sigma_m M_0 \cos(\boldsymbol{q} \cdot \boldsymbol{R}_j) = -g\mu_B \, m \, \cos(\boldsymbol{q} \cdot \boldsymbol{R}_j)$$

relation between critical temperature and couplings

$$k_B T_{\boldsymbol{q}} = \frac{S(S+1)}{3} \Gamma_{\boldsymbol{q}}, \quad \Gamma_{\boldsymbol{q}} = -\sum_{ij \neq 0} \Gamma^{00,ij} e^{i\boldsymbol{q} \cdot (\boldsymbol{T}_i + \boldsymbol{R}_j)}$$

$$\chi_{zz}(\boldsymbol{q}; 0) = \frac{C_{1/2}(1-\sigma_m^2)}{T - (1-\sigma_m^2) T_{\boldsymbol{q}}}$$

divergence at critical temperature

effective magnetic moment

generalization to materials

$$C_{1/2} \to C_{\rm eff} = \mu_{\rm eff}^2/3k_B$$

depends on: Hund's rules, crystal field etc..

effective moment

$$3k_B T \chi_{zz}(\boldsymbol{q};0) \to \mu_{\rm eff}$$

very large temperature limit

half filling

the *U=0* case: band limit

U=0: half-filled band, metal

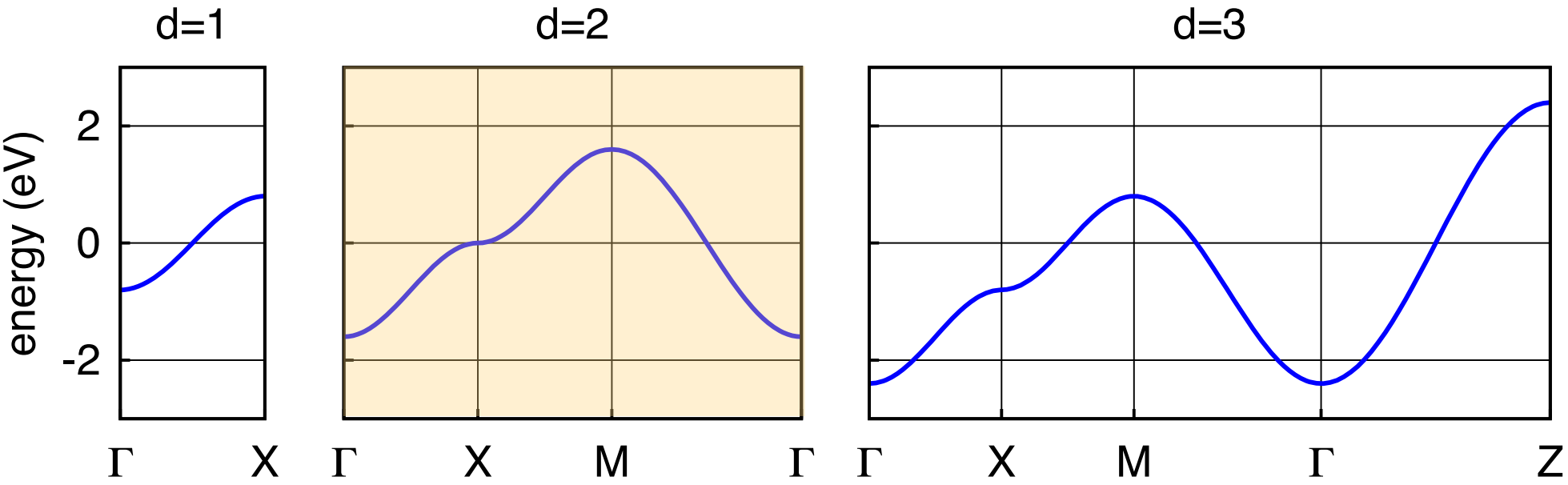
no localized spins

the *U=0* limit

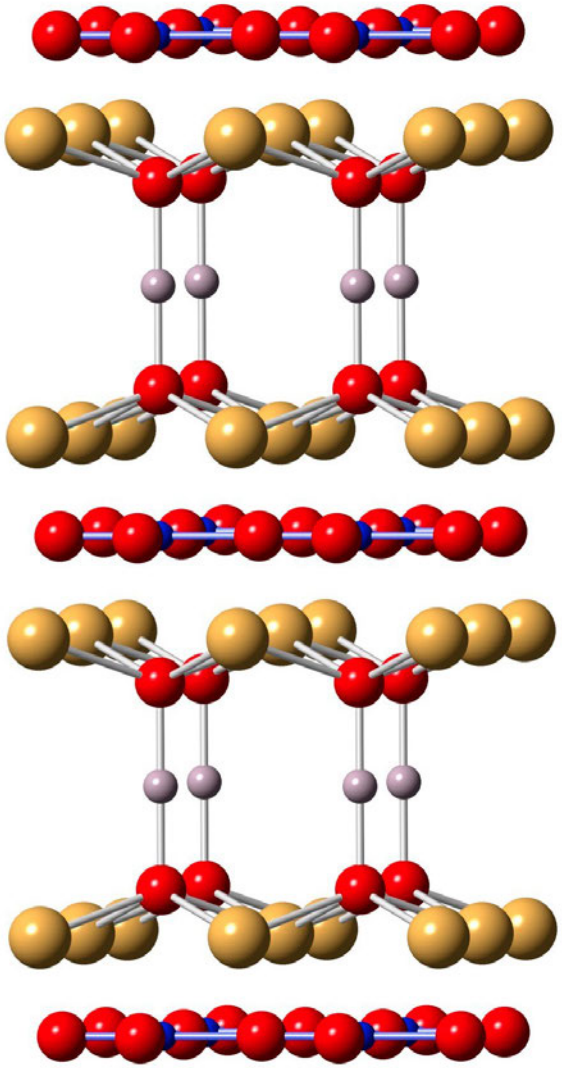
$$H_d + H_T = \sum_{\boldsymbol{k}} \sum_{\sigma} [\varepsilon_d + \varepsilon_{\boldsymbol{k}}] c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$$

hypercubic lattice

$$\varepsilon_{\boldsymbol{k}} = -2t \sum_{\nu=1}^{d} \cos(k_{r_\nu} a)$$



high-T_c superconducting cuprates



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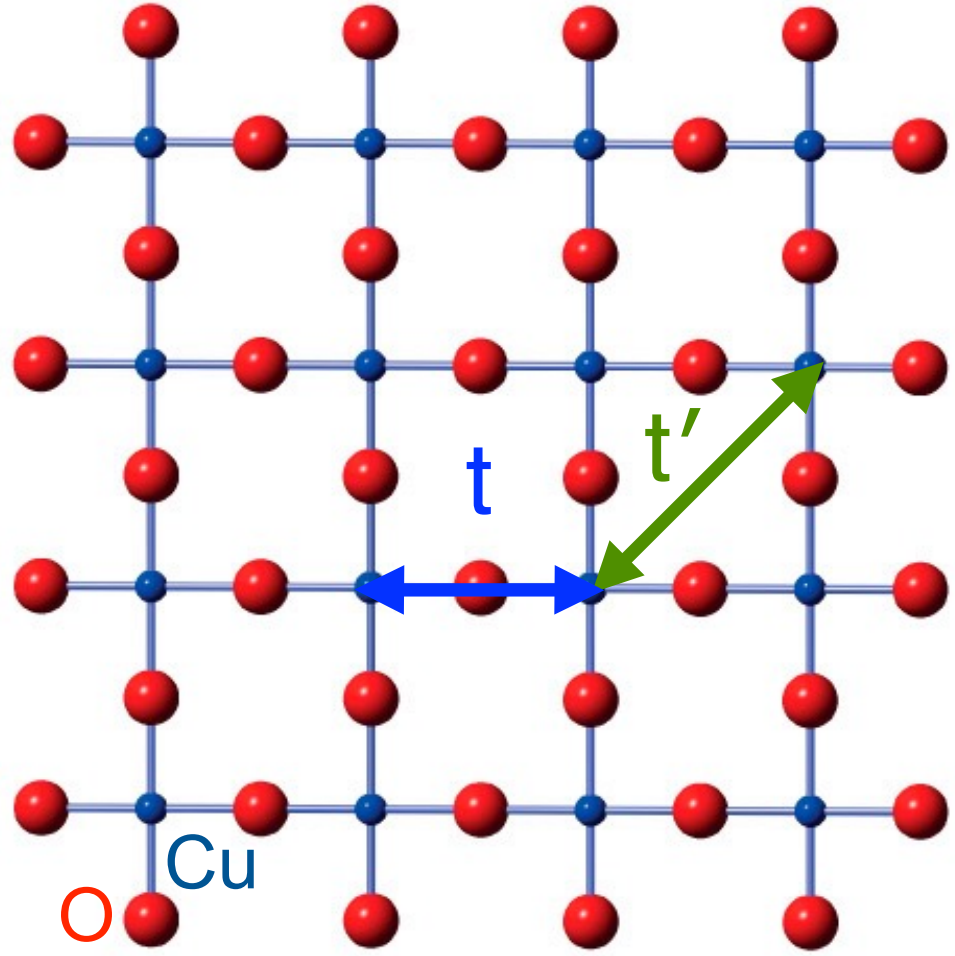
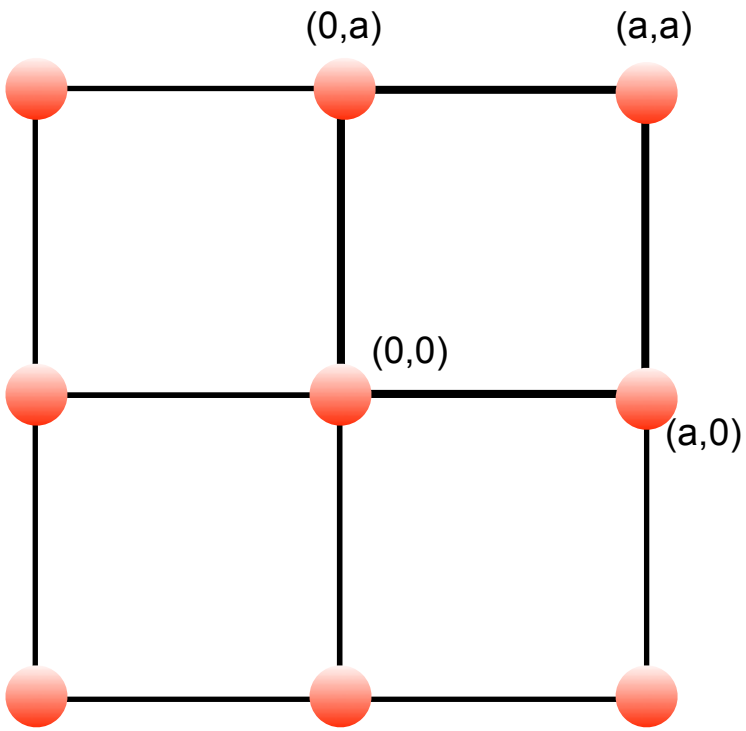


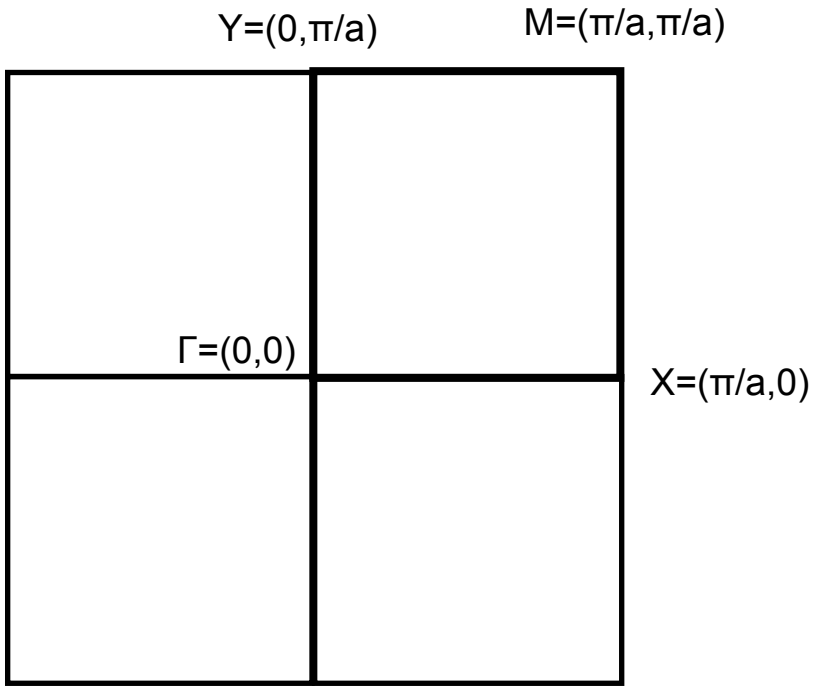
CuO_2 planes

unit cell and Brillouin zone

unit cell



Brillouin zone



high-T_c superconducting cuprates

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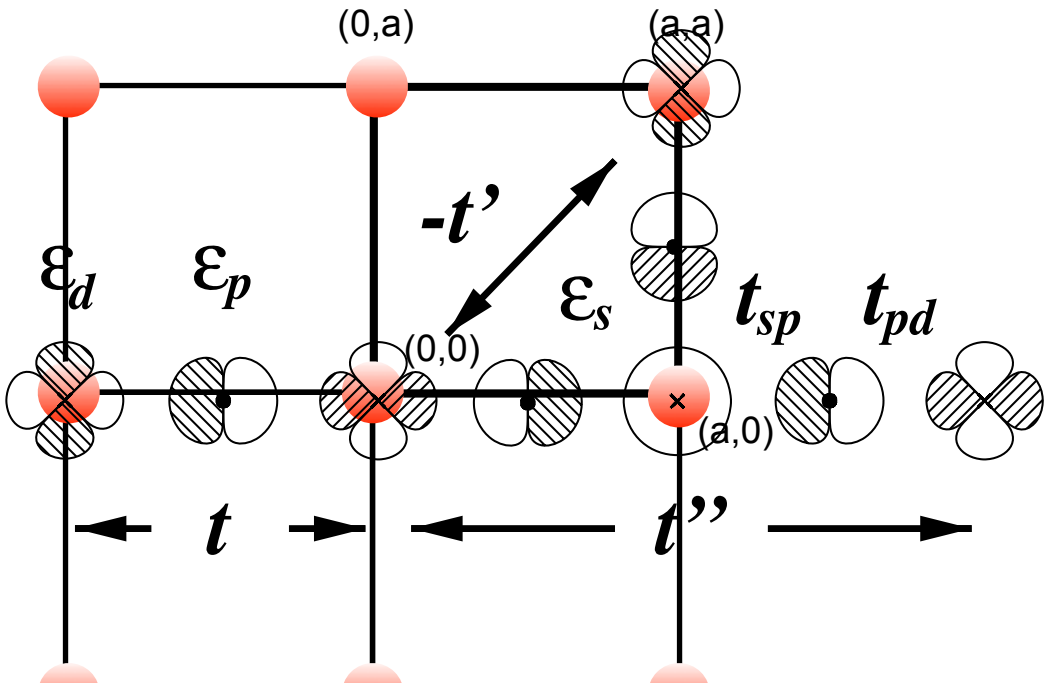
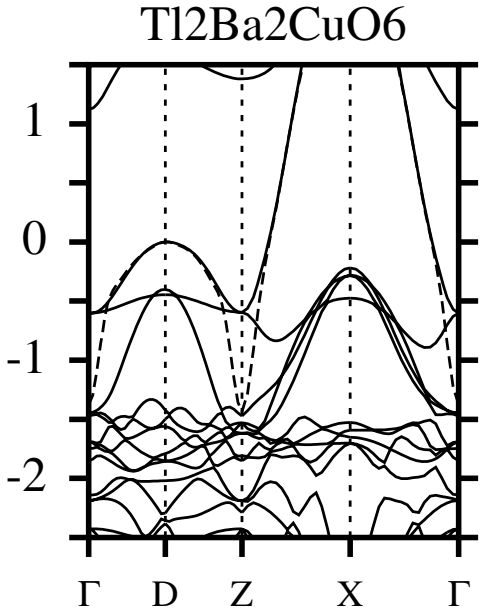


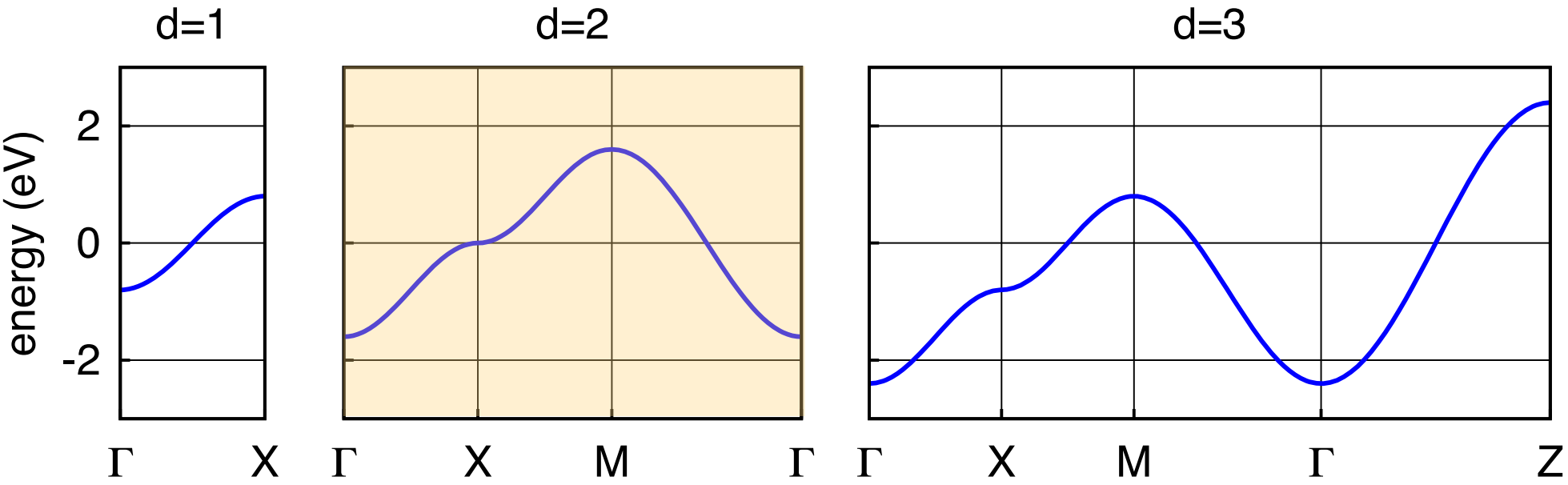


the *U=0* limit, *t'=0*

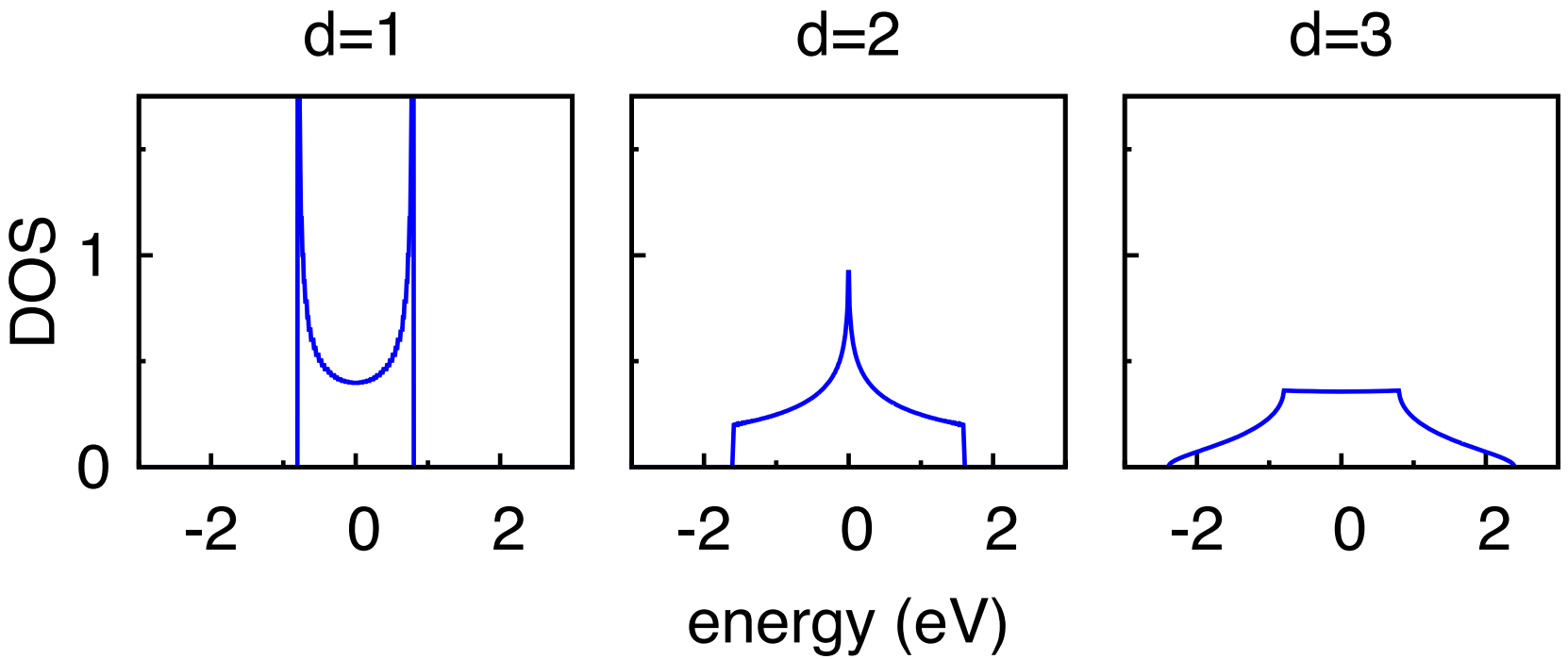
$$H_d + H_T = \sum_{\boldsymbol{k}} \sum_{\sigma} [\varepsilon_d + \varepsilon_{\boldsymbol{k}}] c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$$

hypercubic lattice

$$\varepsilon_{\boldsymbol{k}} = -2t \sum_{\nu=1}^{d} \cos(k_{r_\nu} a)$$

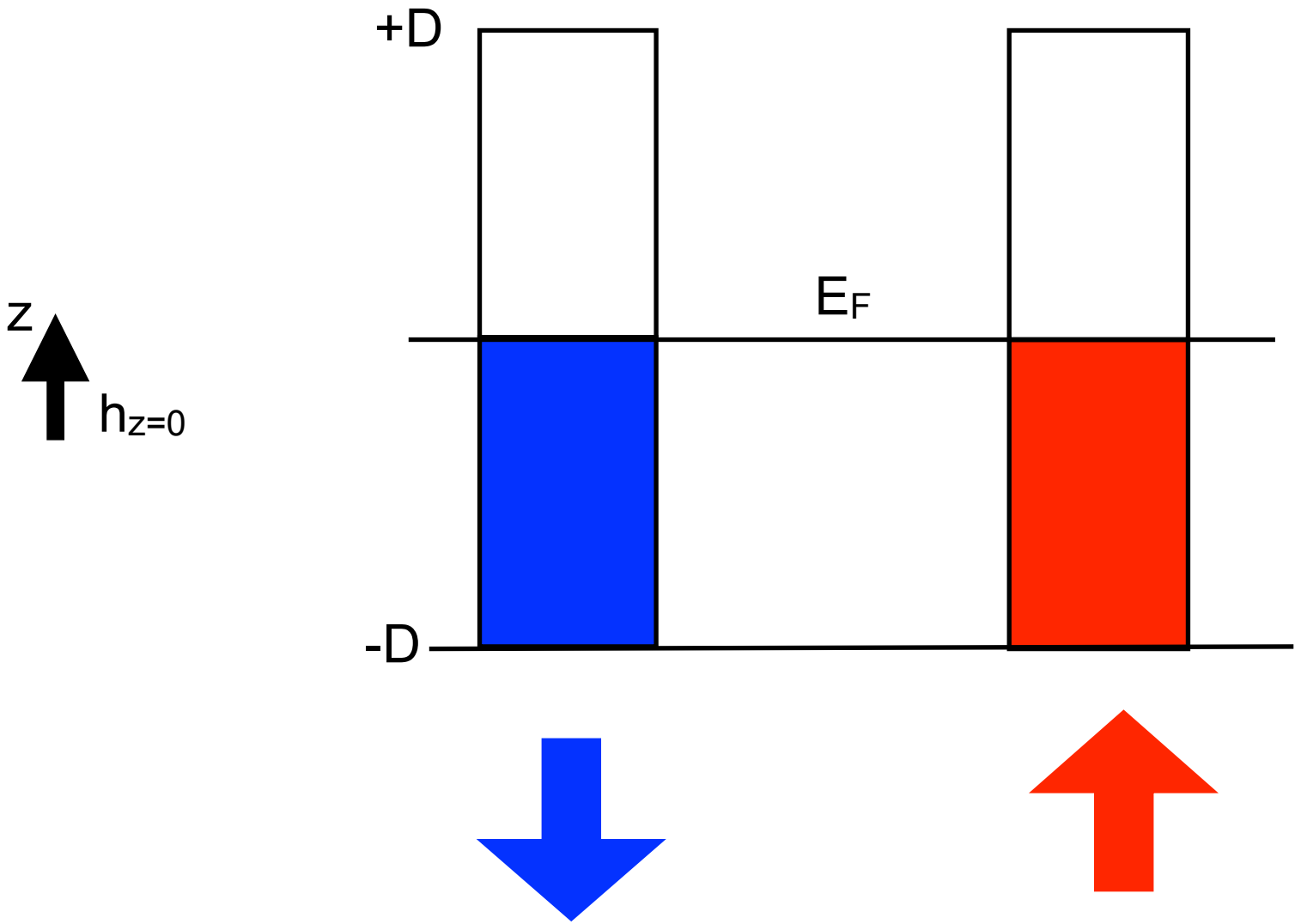


density of states, *t'=0*



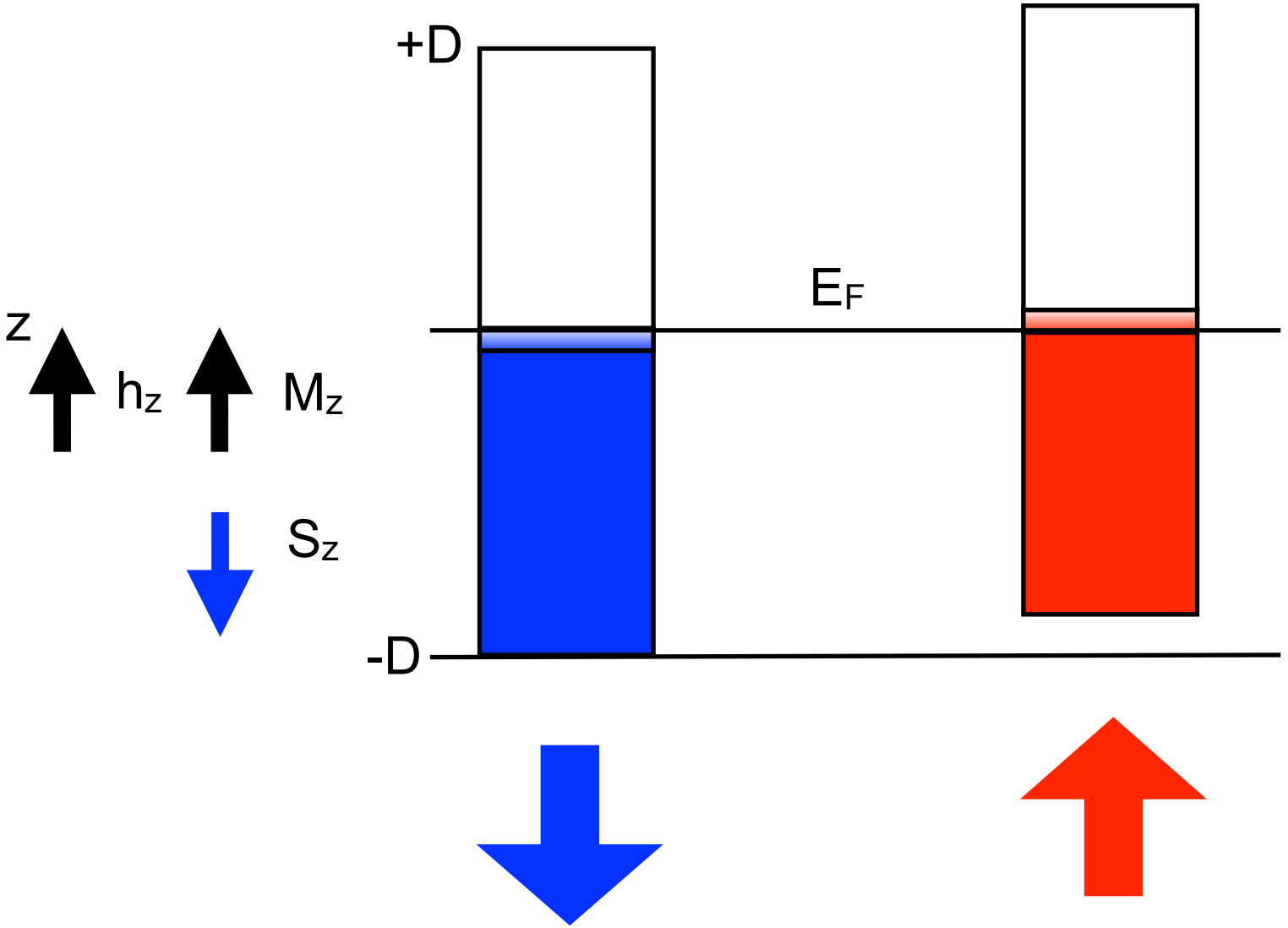
Pauli paramagnetism

$$\varepsilon_{\boldsymbol{k}\uparrow} = \varepsilon_{\boldsymbol{k}\downarrow}$$



Pauli paramagnetism

$$\varepsilon_{\boldsymbol{k}} \to \varepsilon_{\boldsymbol{k}\sigma} = \varepsilon_{\boldsymbol{k}} + \frac{1}{2}\sigma g \mu_B h_z$$



Pauli paramagnetism

$$M_z = -\frac{1}{2}(g\mu_B)\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}}\left[n_{\boldsymbol{k}\uparrow} - n_{\boldsymbol{k}\downarrow}\right] \sim \frac{1}{4}\left(g\mu_B\right)^2 \rho(\varepsilon_F) h_z$$

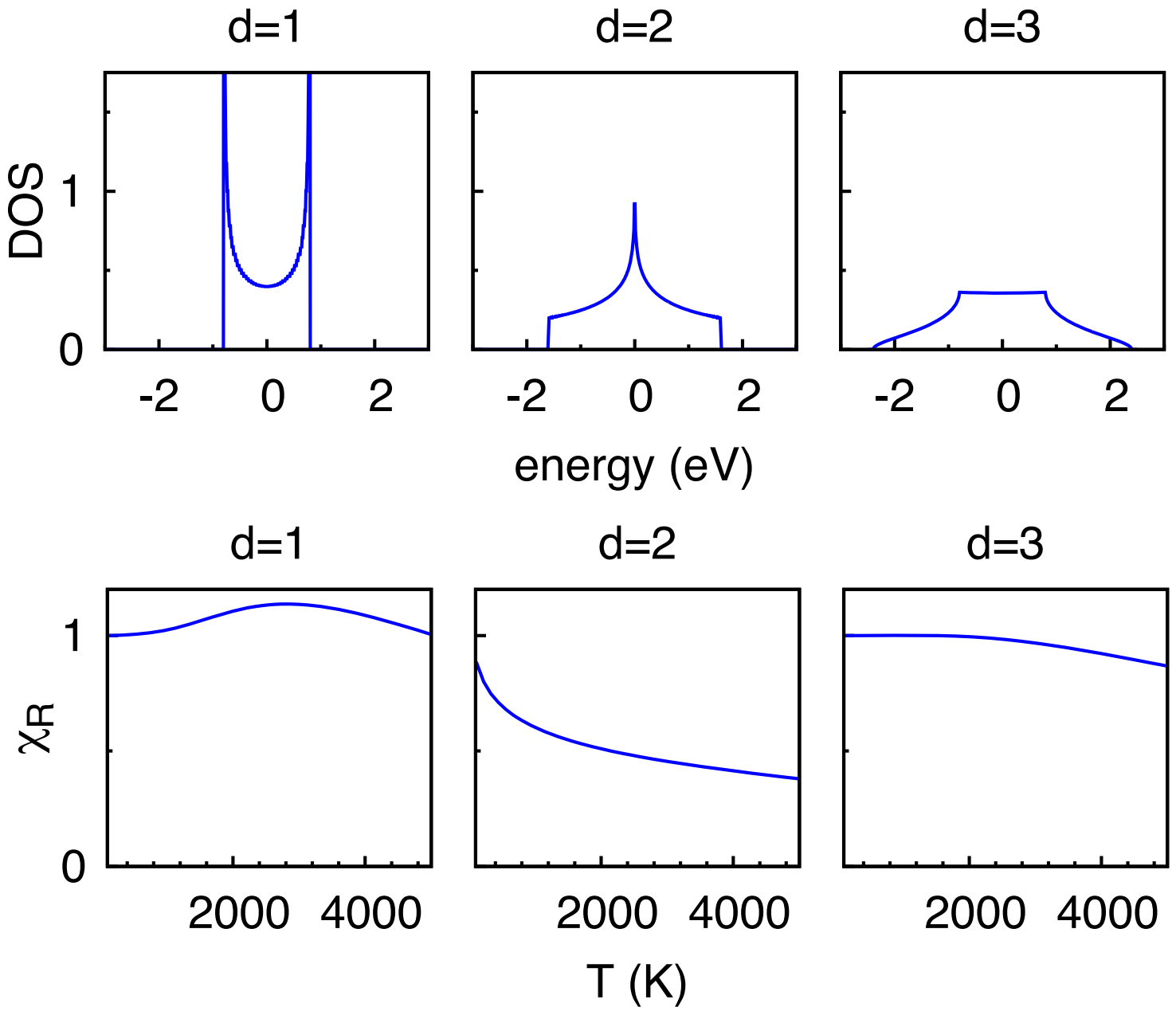
zero temperature

$$\chi^P(0) = \frac{1}{4}\left(g\mu_B\right)^2 \rho(\varepsilon_F)$$

finite temperature

$$\chi^P(T) = \frac{1}{4}\left(g\mu_B\right)^2 \int d\varepsilon \rho(\varepsilon) \left(-\frac{dn(\varepsilon)}{d\varepsilon}\right)$$

finite temperature, *t'=0*

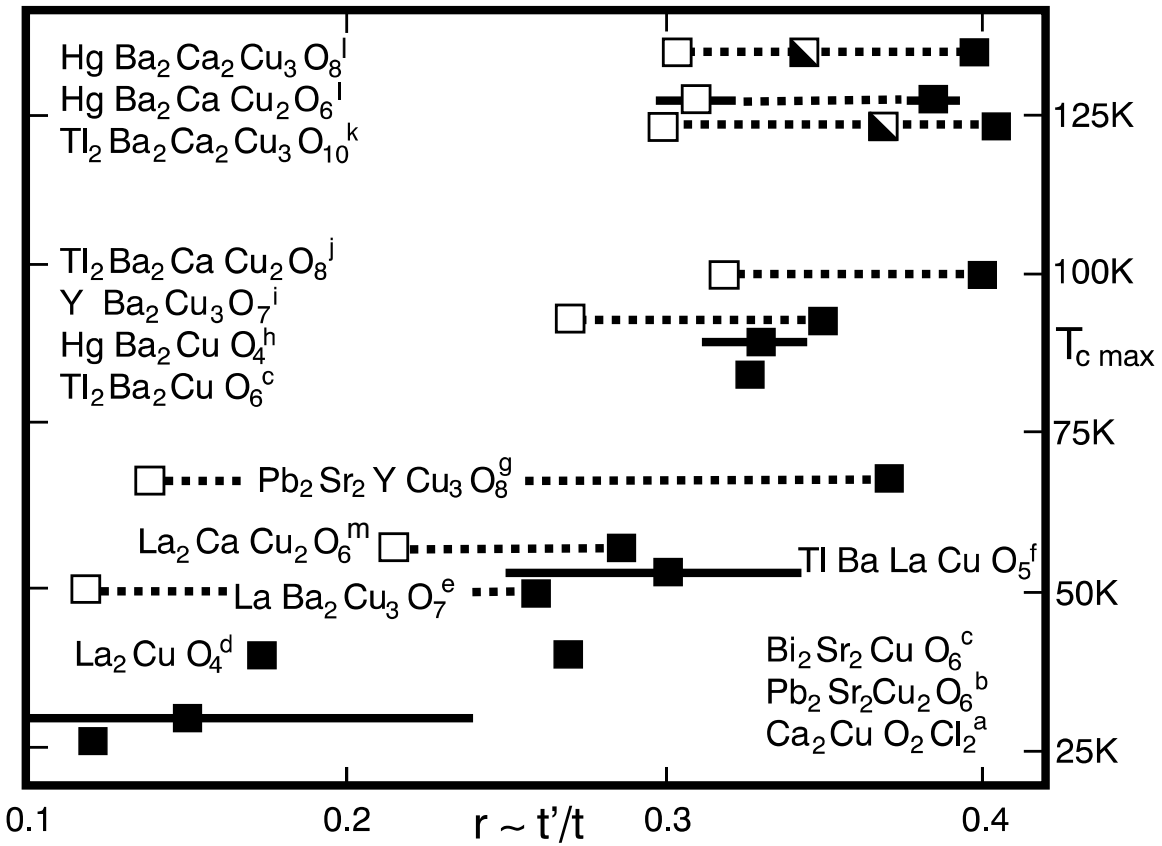


parameters for high-T_c superconductors

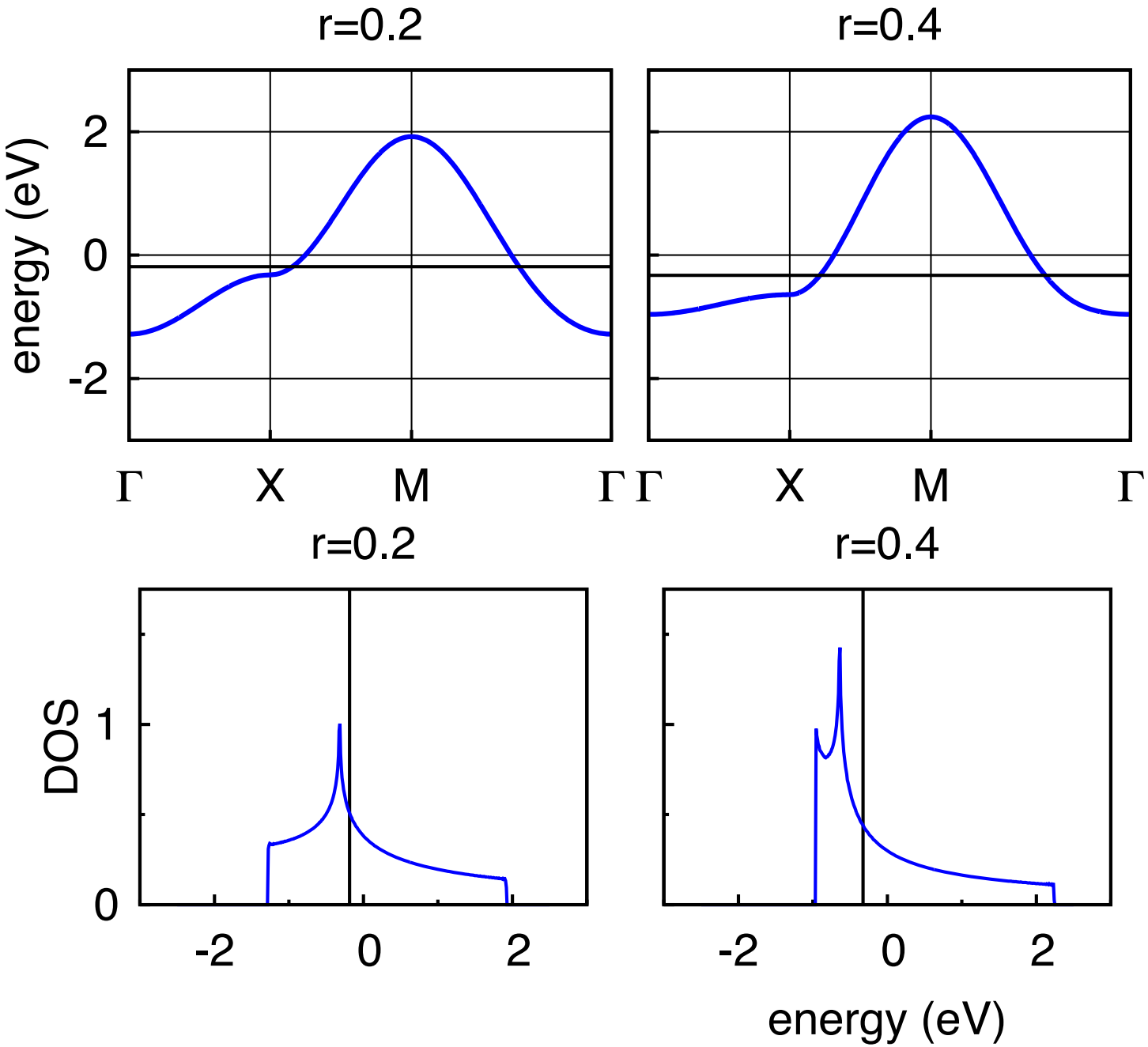
VOLUME 87, NUMBER 4 PHYSICAL REVIEW LETTERS 23 JULY 2001

Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_{c\,\max}$

E. Pavarini, I. Dasgupta,* T. Saha-Dasgupta,† O. Jepsen, and O. K. Andersen
Max-Planck-Institut für Festkörperforschung, D-70506 Stuttgart, Germany



density of states, *t'* finite



linear response theory

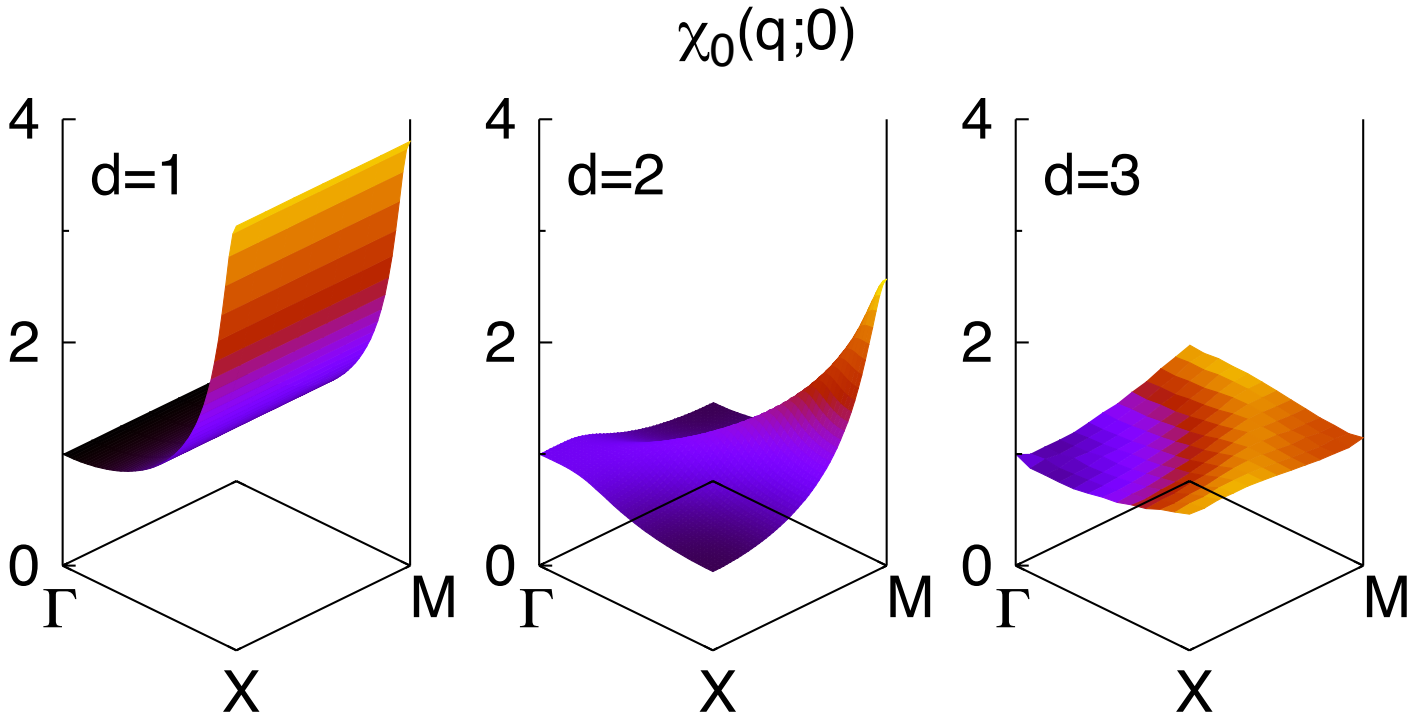
Pauli susceptibility: uniform and static

$$M_z(\boldsymbol{q};\omega) = \chi_{zz}(\boldsymbol{q};\omega) h_z(\boldsymbol{q};\omega)$$

non-interacting susceptibility, t'=0

$$\varepsilon_{\boldsymbol{k}} = -2t[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]$$

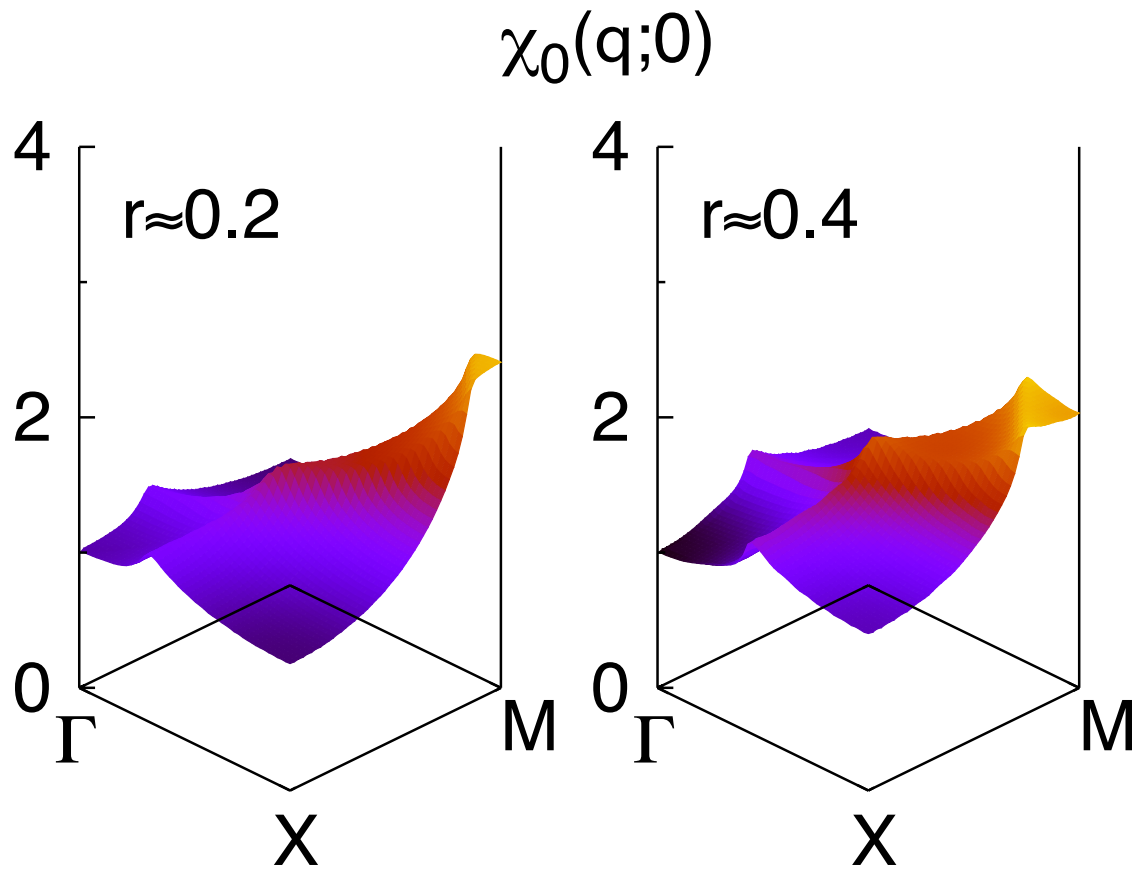
finite temperature ~ 350 K



2-dimensional case: M point!

non-interacting susceptibility, t' finite

$r \sim t'/t$



$$\varepsilon_{\boldsymbol{k}} = -2t[\cos(k_x a) + \cos(k_y a)] + 4t' \cos(k_x a)\ \cos(k_y a)$$

the large *t/U* limit

Fermi-liquid regime

quasi-electrons with heavy masses

Fermi liquid

in *some* limit an interacting electron system can be described via independent quasi-electrons

weakly interacting: small U/t ratio

one-to-one correspondence between electrons & quasiparticles

$$\frac{m^*}{m} = 1 + \frac{1}{3}F_1^s > 1, \qquad F_1^s > 0$$

enhanced masses

$$\frac{\chi}{\chi^P} = \frac{m^*}{m}\frac{1}{1+F_0^a} > 1, \qquad F_0^a < 0$$

enhanced Pauli susceptibility

F_0^a and F_1^s: Landau parameters

Stoner instabilities: Hartree Fock

$$
\begin{aligned}
H_U &= U \sum_i n_{i\uparrow} n_{i\downarrow} \rightarrow H_U^{\mathrm{HF}} \\
H_U^{\mathrm{HF}} &= U \sum_i \left[n_{i\uparrow} \langle n_{i\downarrow} \rangle + \langle n_{i\uparrow} \rangle n_{i\downarrow} - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \right].
\end{aligned}
$$

ferromagnetic instability?

$$
\langle n_{i\sigma} \rangle = n_\sigma = \frac{n}{2} + \sigma m
$$

$$
\varepsilon^U_{\boldsymbol{k}\sigma} = \varepsilon_{\boldsymbol{k}} + n_{-\sigma} U = \varepsilon_{\boldsymbol{k}} + \frac{n}{2} U - \sigma m U
$$

effective total magnetic field

$$\varepsilon_{\boldsymbol{k}\sigma} = \varepsilon^{U}_{\boldsymbol{k}\sigma} + \frac{1}{2} g \mu_B h_z \sigma$$

Zeeman

$$H_U^{\mathrm{HF}} = U \sum_i \left[-2 m S_z^i + m^2 + \frac{n^2}{4} \right]$$

HF

Stoner instabilities

linear response

$$M_z \sim \chi^P(0)\left[h_z - \frac{2}{g\mu_B}Um\right] = \chi^P(0)\left[h_z + 2(g\mu_B)^{-2}UM_z\right]$$

self-consistent solution for M_z

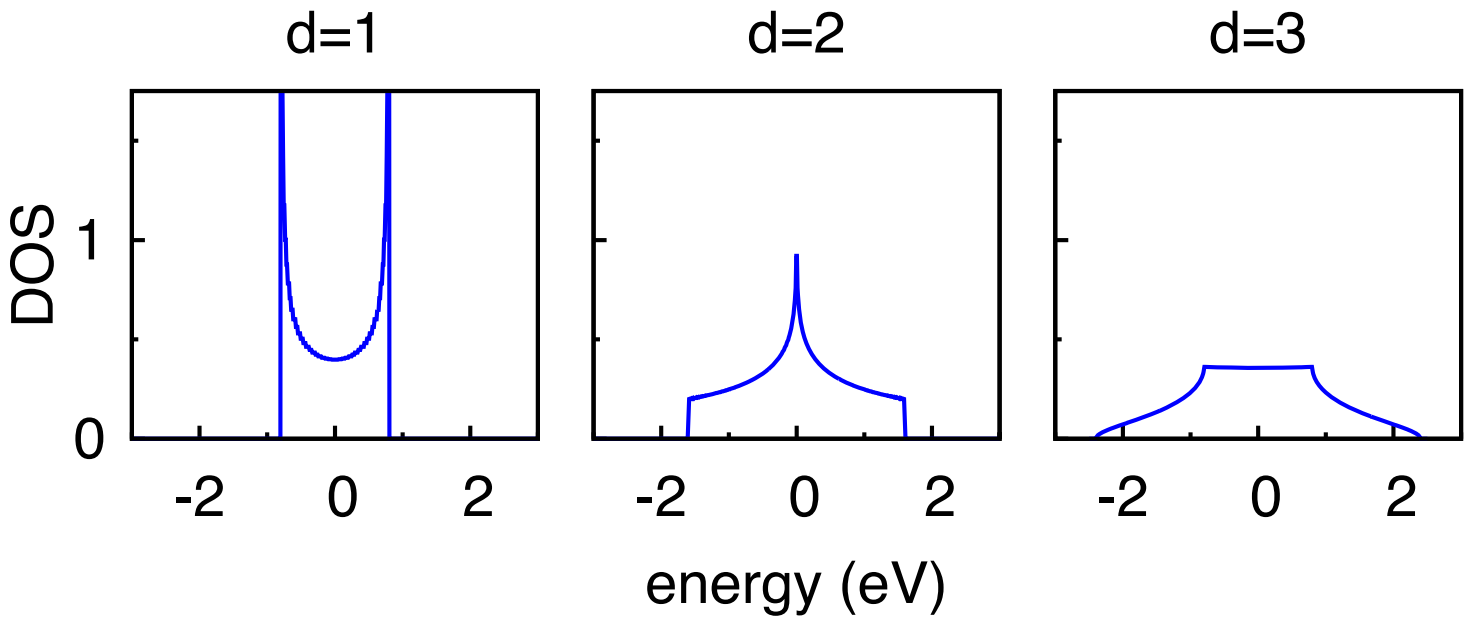
$$\chi^S(\mathbf{0};0) = \frac{\chi^P(0)}{1 - 2\left(g\mu_B\right)^{-2}U\chi^P(0)}$$

RPA susceptibility

$$U_c = 2/\rho(\varepsilon_F)$$

critical U

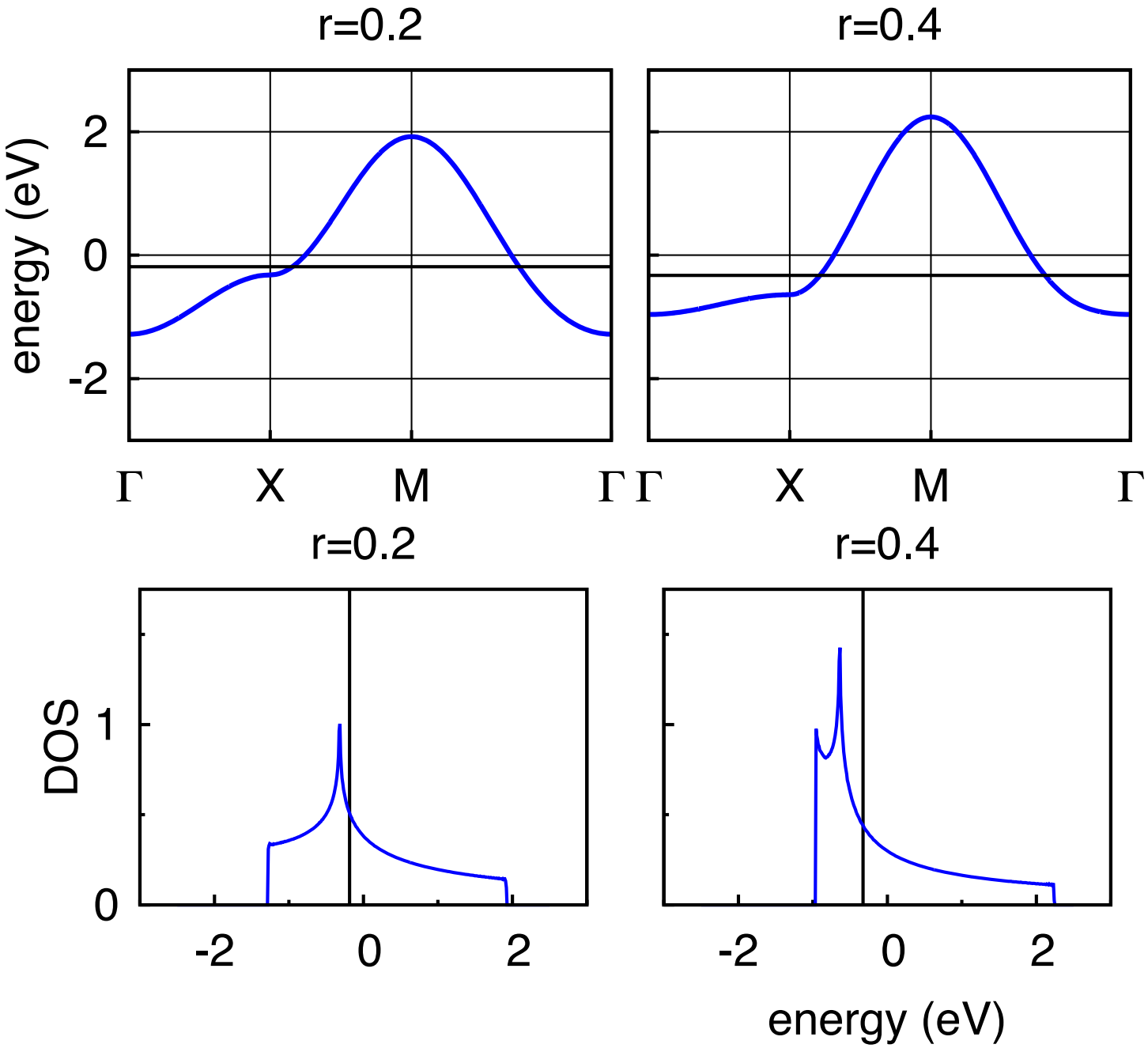
2-dimensional case



logarithmic singularity

any U>0 triggers the instability

band and density of states

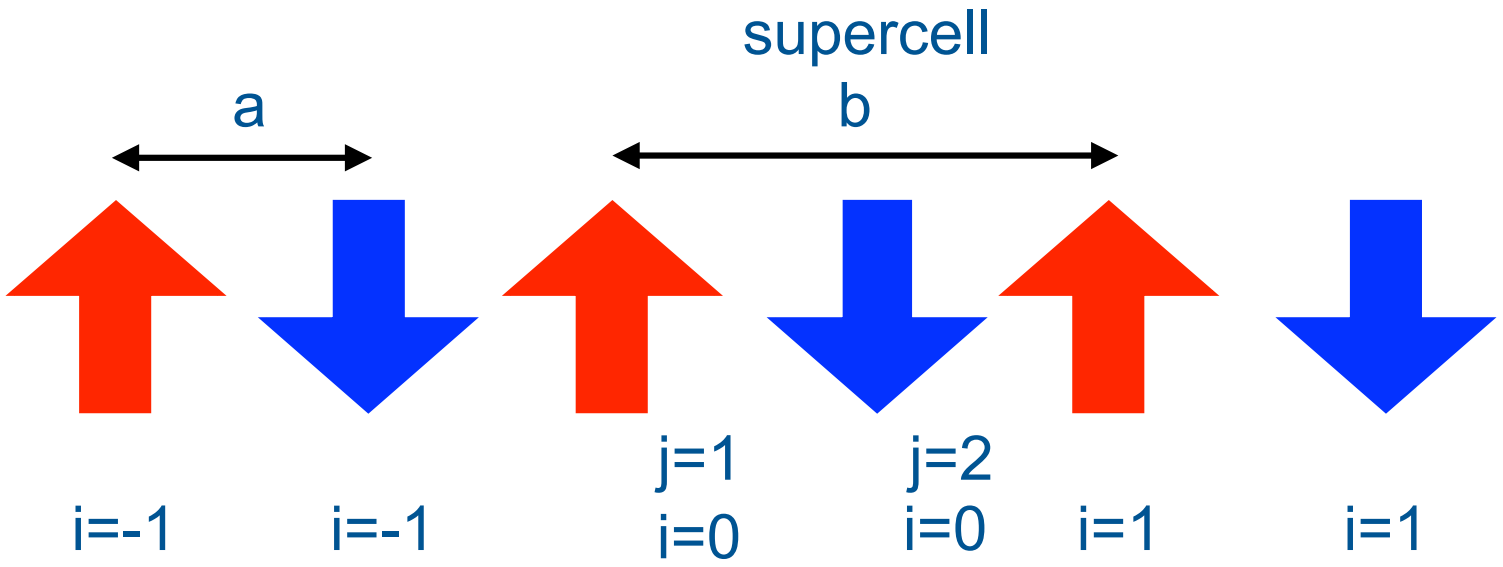


Stoner instabilities with finite q

oscillating magnetic
field and spin polarization

$$S_z^i(\boldsymbol{q}) = \sum_j e^{i\boldsymbol{q}\cdot\boldsymbol{R}_j} S_z^{ji}$$

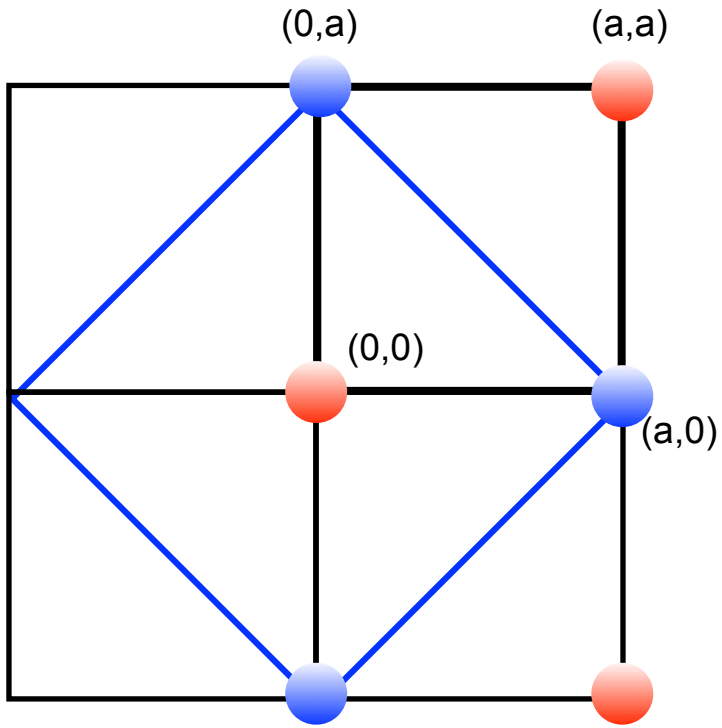
$$\langle S_z^{ji} \rangle = m\cos(\boldsymbol{q}\cdot\boldsymbol{R}_j)$$

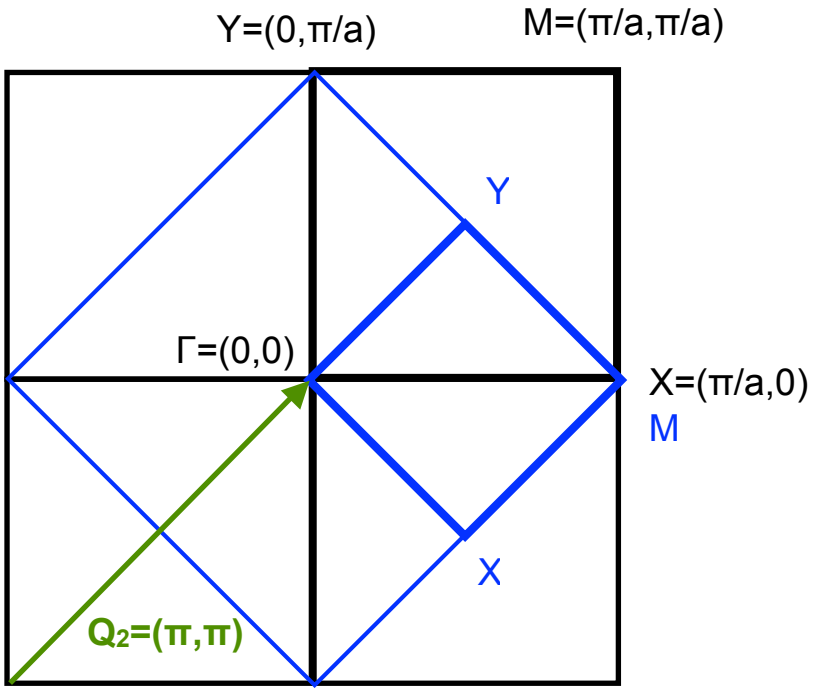


linear chain, **q**=(π/a,0,0)

antiferromagnetism

two dimensional case





Stoner instabilities with finite q

$$H_U^{\mathrm{HF}} + H_Z = \sum_i \left[\frac{g\mu_B}{2} \left(h_z - \frac{2}{g\mu_B} mU \right) \left[S_z^i(\boldsymbol{q}) + S_z^i(-\boldsymbol{q}) \right] + m^2 + \frac{n^2}{4} \right]$$

sums over supercell sites!

$$\chi^S(\boldsymbol{q};0) = \frac{1}{2}(g\mu_B)^2 \frac{\chi_0(\boldsymbol{q};0)}{[1 - U\chi_0(\boldsymbol{q};0)]},$$

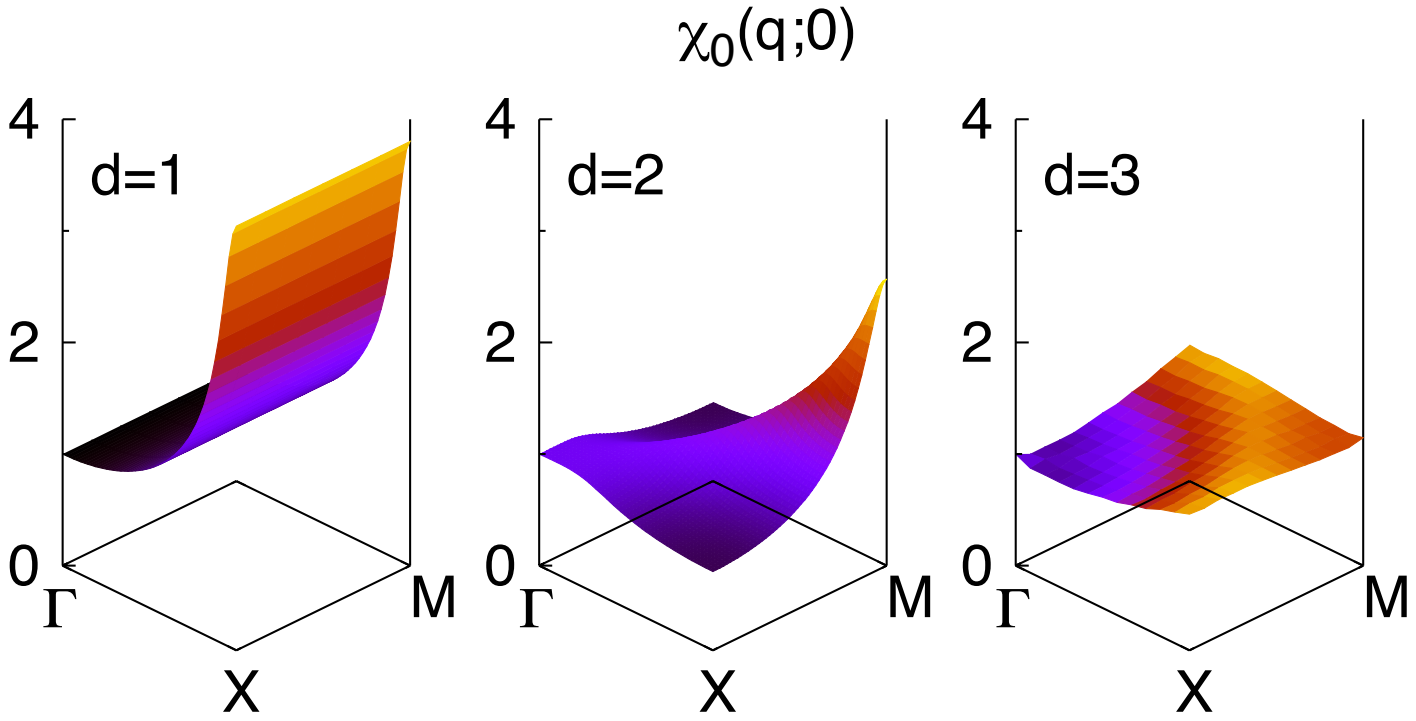
$$\chi_0(\boldsymbol{q};0) = -\frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \frac{n_{\boldsymbol{k}+\boldsymbol{q}} - n_{\boldsymbol{k}}}{\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}}}$$

$$\chi_0(\mathbf{0};0) = 2\,(g\mu_B)^{-2}\,\chi^P(0) \sim \frac{1}{2}\rho(\varepsilon_F)$$

Stoner instabilities with finite q

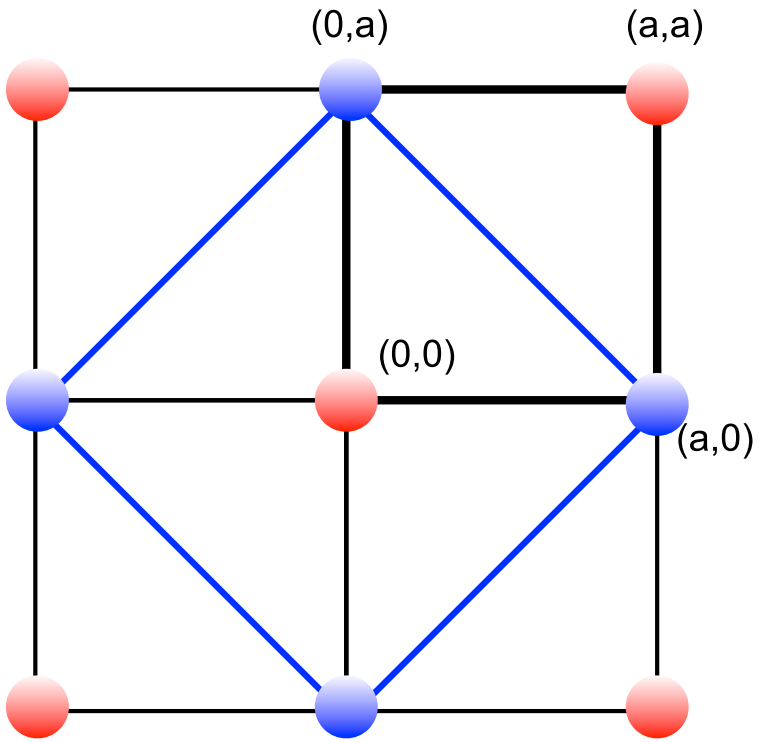
$$\varepsilon_{\boldsymbol{k}} = -2t[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]$$

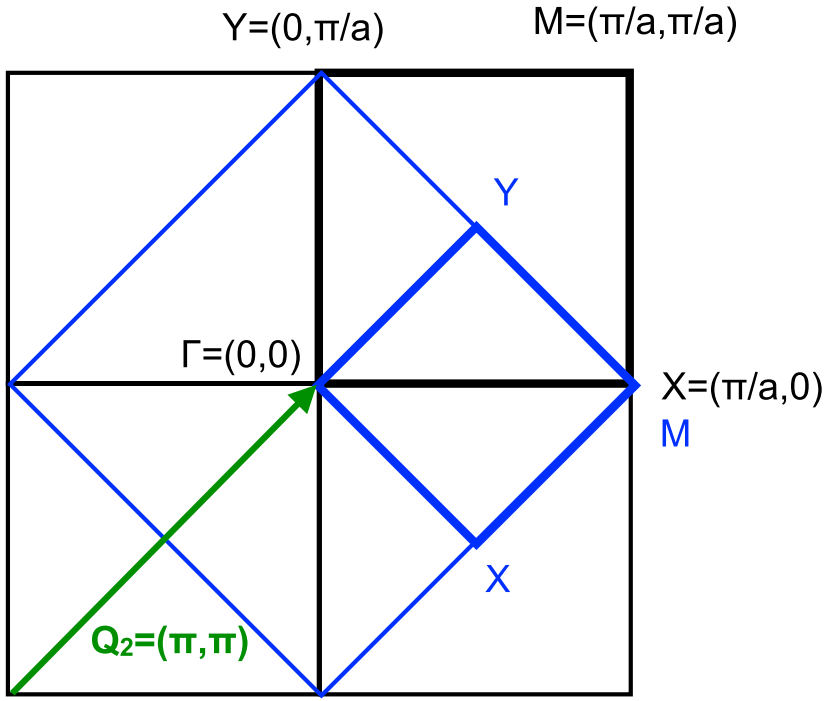
finite temperature ~ 350 K



2-dimensional case: M point!

two-dimensional case





perfect nesting

$$\varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_i} = -\varepsilon_{\boldsymbol{k}}$$

$$\chi_0(\boldsymbol{Q}_i;0) \propto \frac{1}{4}\int_{-\infty}^{\varepsilon_F=0} d\varepsilon \rho(\varepsilon)\frac{1}{\varepsilon} \to \infty.$$

2-dimensional case: Q_2=M point

2-dimensional case: divergence also at Γ point

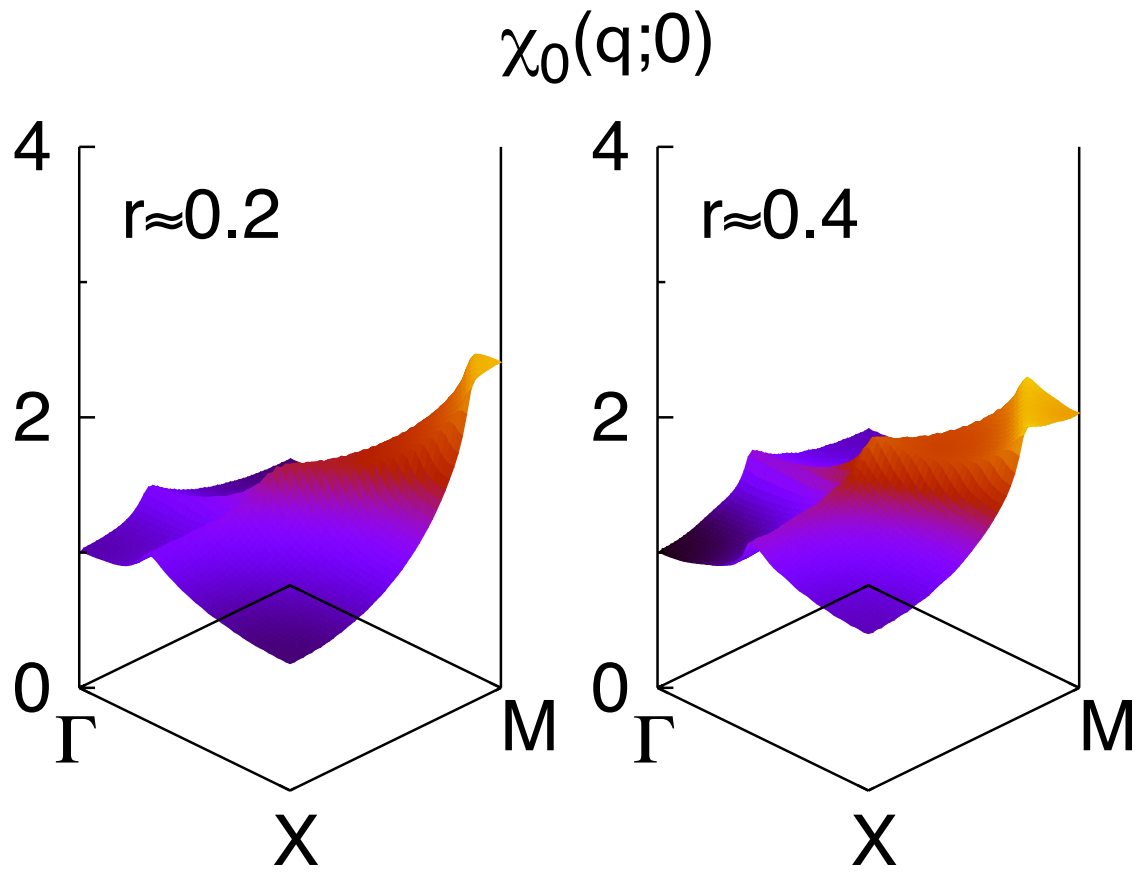
however, finite T: Q_2 singularity most important one

what about t' ?

$$\varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_2} = -\varepsilon_{\boldsymbol{k}} + 8t' \cos(k_x a)\ \cos(k_y a)$$

two-dimensional case

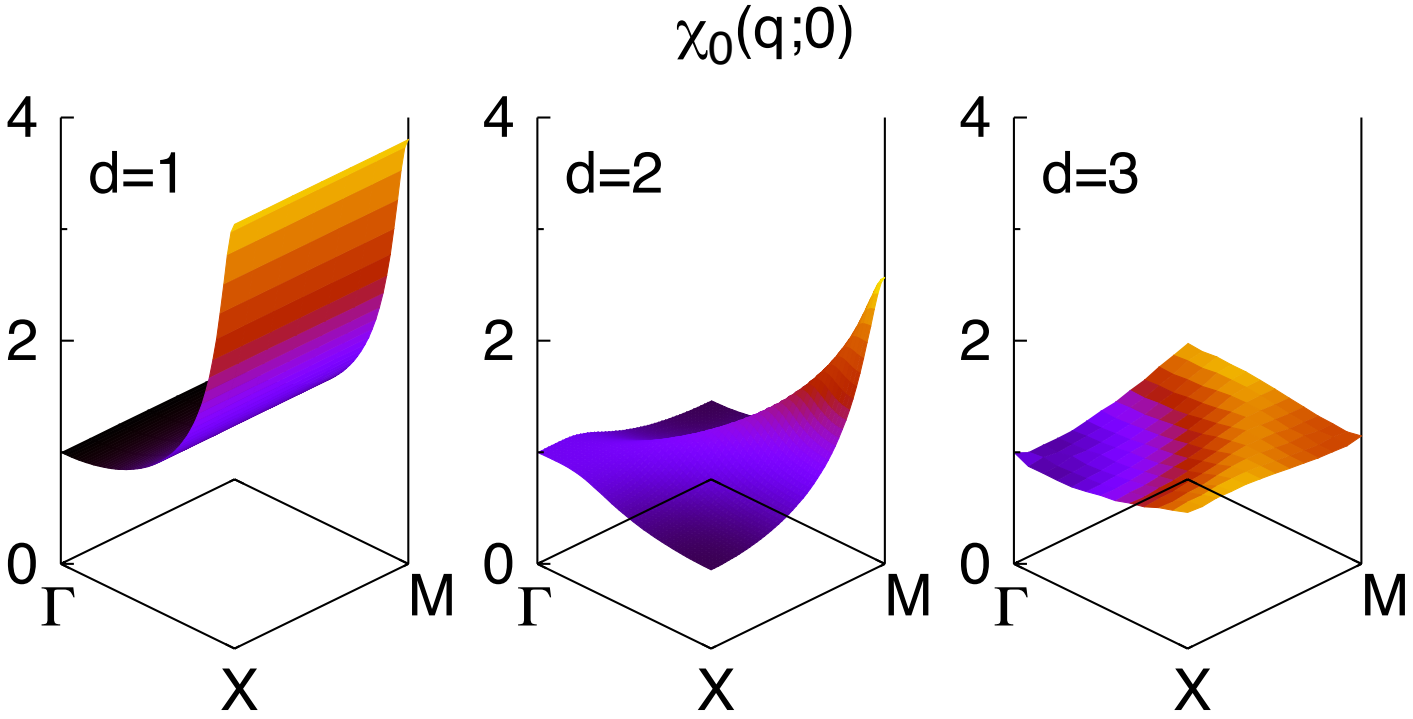
$r \sim t'/t$



$$\varepsilon_{\boldsymbol{k}} = -2t[\cos(k_x a) + \cos(k_y a)] + 4t' \cos(k_x a)\ \cos(k_y a)$$

remarks

- in general several instabilities possible (different **q**)
- which one dominates: check finite temperature susceptibility!
- instabilities possible at any doping
- **q** can also be incommensurate with lattice



Mott insulators:
large U limit in Hartree Fock

local moment regime and HF

paramagnetic & ferromagnetic case

Bloch function

$$\Psi_{\boldsymbol{k}\sigma}(\boldsymbol{r}) = \frac{1}{\sqrt{N_s}} \sum_i e^{i\boldsymbol{k}\cdot\boldsymbol{T}_i} \; \Psi_{i\sigma}(\boldsymbol{r})$$

spin scattering function

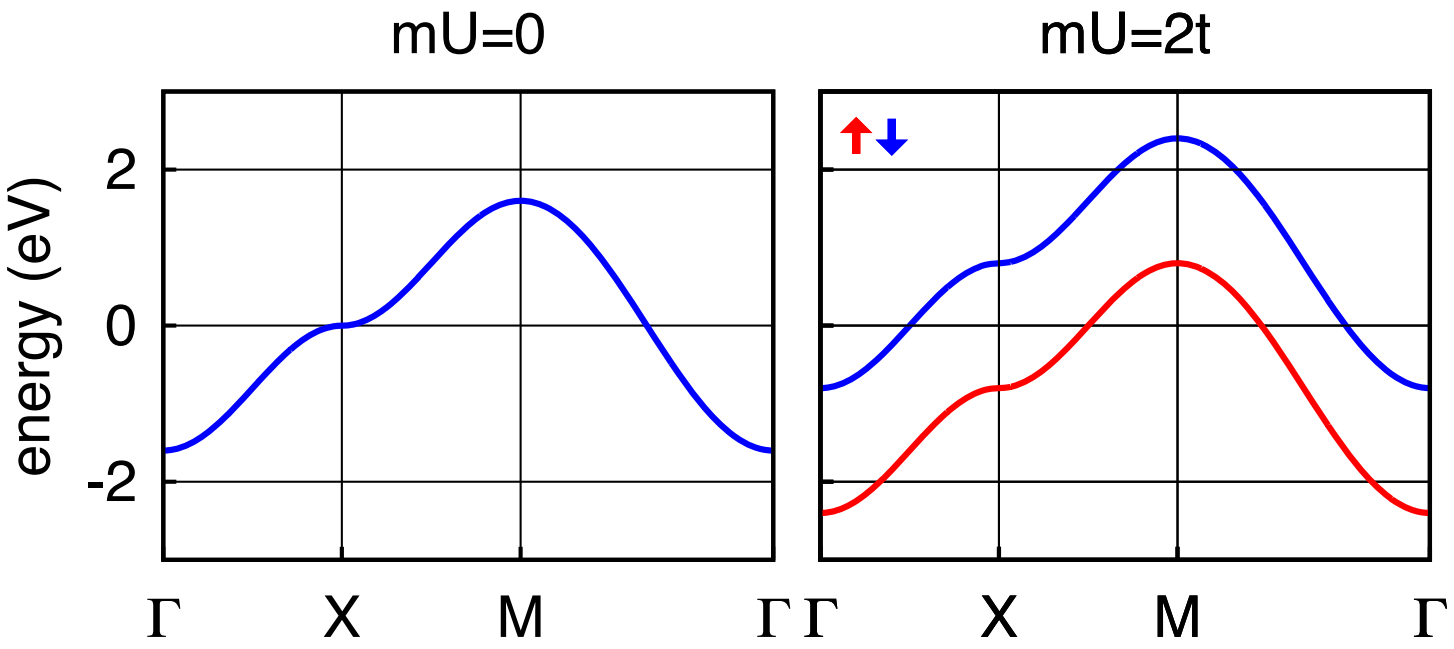
$$S_z(\boldsymbol{k},\boldsymbol{k}') = \frac{1}{N_s} \sum_i e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{T}_i} \; \underbrace{\frac{1}{2} \sum_\sigma \sigma c^\dagger_{i\sigma} c_{i\sigma}}_{S^i_z}$$

ferromagnetic case

Hartree-Fock Hamiltonian and bands

$$H = \sum_{\sigma} \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + U \sum_{\boldsymbol{k}} \left[-2m\, S_z(\boldsymbol{k}, \boldsymbol{k}) + m^2 + \frac{n^2}{4} \right]$$

diagonal in ***k***



Hartree-Fock bands

very large mU case, half filling

spin down band empty, m=1/2

total energy

$$E_{\mathrm{F}} = \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \left[\varepsilon_{\boldsymbol{k}\sigma} - \mu \right] = \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \left[\varepsilon_{\boldsymbol{k}} - \frac{1}{2} U \right] = -\frac{1}{2} U$$

no t^2/U term!

antiferromagnetic case

two sublattices with opposite magnetization +m and -m

$$H_U^{\mathrm{HF}} = \sum_{i\in A}\left[-2mS_z^i + m^2 + \frac{n^2}{4}\right] + \sum_{i\in B}\left[+2mS_z^i + m^2 + \frac{n^2}{4}\right]$$

Bloch function

original lattice

Bloch functions

two sublattices A and B

$$\Psi_{\boldsymbol{k}\sigma}(\boldsymbol{r}) = \frac{1}{\sqrt{2}}\left[\Psi^A_{\boldsymbol{k}\sigma}(\boldsymbol{r}) + \Psi^B_{\boldsymbol{k}\sigma}(\boldsymbol{r})\right]$$

$$\Psi^\alpha_{\boldsymbol{k}\sigma}(\boldsymbol{r}) = \frac{1}{\sqrt{N_{s_\alpha}}}\sum_{i_\alpha} e^{i\boldsymbol{T}_i^\alpha\cdot\boldsymbol{k}}\,\Psi_{i_\alpha\sigma}(\boldsymbol{r})$$

antiferromagnetic case

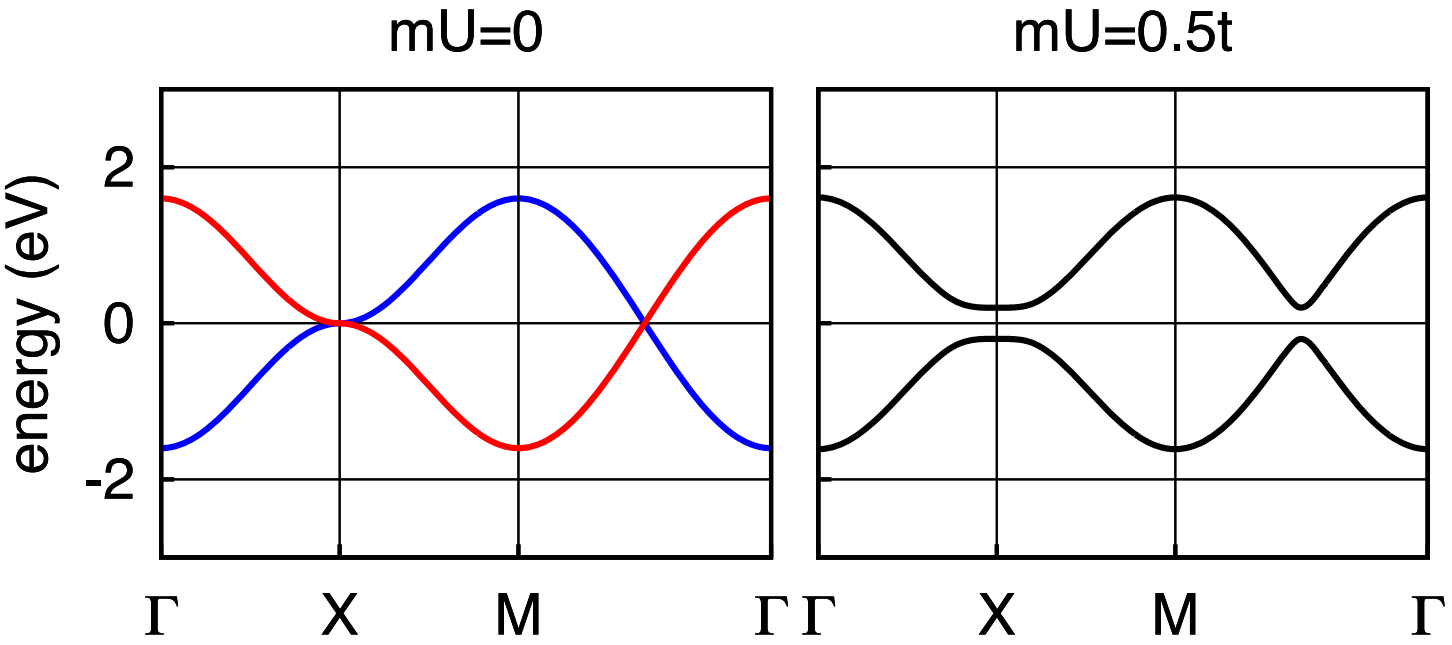
$$
\begin{aligned}
H &= \sum_{\boldsymbol{k}} \sum_{\sigma} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k}} \sum_{\sigma} \varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_2} n_{\boldsymbol{k}+\boldsymbol{Q}_2\sigma} \\
&+ U \sum_{\boldsymbol{k}} \left[-2m\, S_z(\boldsymbol{k}, \boldsymbol{k}+\boldsymbol{Q}_2) + 2m^2 + 2\frac{n^2}{4} \right]
\end{aligned}
$$

scattering function couples ***k*** and ***k*+*Q*$_2$**

$$
\varepsilon_{\boldsymbol{k}\pm} - \mu = \frac{1}{2}(\varepsilon_{\boldsymbol{k}} + \varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_2}) \pm \frac{1}{2}\sqrt{(\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_2})^2 + 4(mU)^2}
$$

HF bands

antiferromagnetic case



gap: mU

$$\varepsilon_{\boldsymbol{k}\pm} - \mu = \frac{1}{2}(\varepsilon_{\boldsymbol{k}} + \varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_2}) \pm \frac{1}{2}\sqrt{(\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{Q}_2})^2 + 4(mU)^2}$$

HF bands

antiferromagnetic case

very large U case

half-filling, m=1/2

$$\varepsilon_{\boldsymbol{k}-} - \mu \sim -\frac{1}{2}U - \frac{\varepsilon_{\boldsymbol{k}}^2}{U} = -\frac{1}{2}U - \frac{4t^2}{U}\left(\frac{\varepsilon_{\boldsymbol{k}}}{2t}\right)^2$$

total energy

$$E_{\mathrm{AF}} = -\frac{1}{2}U - \frac{4t^2}{U}\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}}\left(\frac{\varepsilon_{\boldsymbol{k}}}{2t}\right)^2 \sim -\frac{1}{2}U - \frac{4t^2}{U}$$

energy difference

$$\Delta E^{\mathrm{HF}} = E^{\mathrm{HF}}_{\uparrow\uparrow} - E^{\mathrm{HF}}_{\uparrow\downarrow} = \frac{2}{n_{\langle ii' \rangle}} \left[E_{\mathrm{F}} - E_{\mathrm{AF}} \right] \sim \frac{1}{2} \frac{4t^2}{U} \sim \frac{1}{2} \Gamma$$

in this example for this quantity we obtain
the same result as in exact solution!

however, this is not the triplet-singlet splitting

$$\Delta E = E_{S=1} - E_{S=0} = \Gamma$$

Hartree-Fock problems

Slater vs Mott insulator

insulator with much smaller U than exact solution

gap in single HF calculation ~U

HF does not give correct spin excitation spectrum

NB. HF is used in the LDA+*U* approach

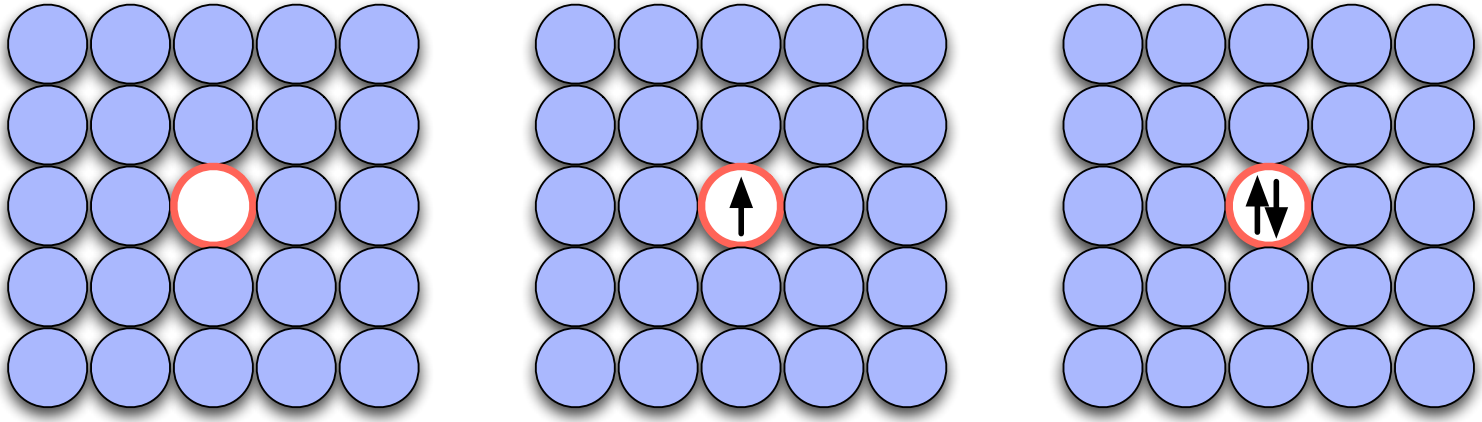
Mott insulators:
the dynamical mean-field approach

… should describe at least Mott physics ..
… should be flexible, work for all models of Hubbard type ..

NB: flexible alone is not enough
e.g.: very flexible: HF, or LDA; however, no Mott transition

DMFT

stat-of-the art approach for Hubbard-like models



$$G_0{}^{-1} - G^{-1} = \Sigma(\omega)$$

dynamics captured — self-energy local

exact in infinite dimensions

Metzner and Vollhardt, PRL **62**, 324 (1989); Georges and Kotliar, PRB **45,** 6479 (1992)

connections

lattice model

$$H = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U$$

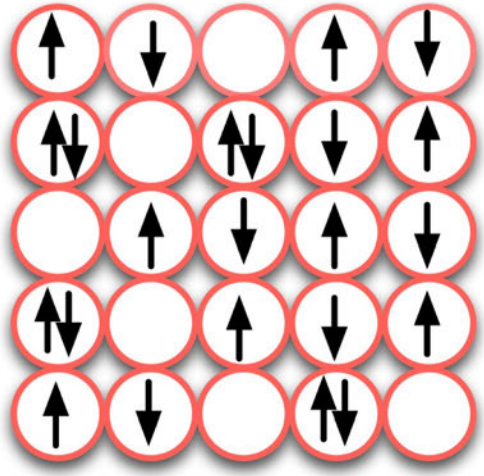
impurity model (Anderson model)

$$H_{\mathrm{A}} = \sum_\sigma \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_\sigma \varepsilon_f n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow}$$

$$+ \sum_\sigma \sum_{\boldsymbol{k}} \left[V_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{f\sigma} + h.c. \right]$$

self-consistency loop

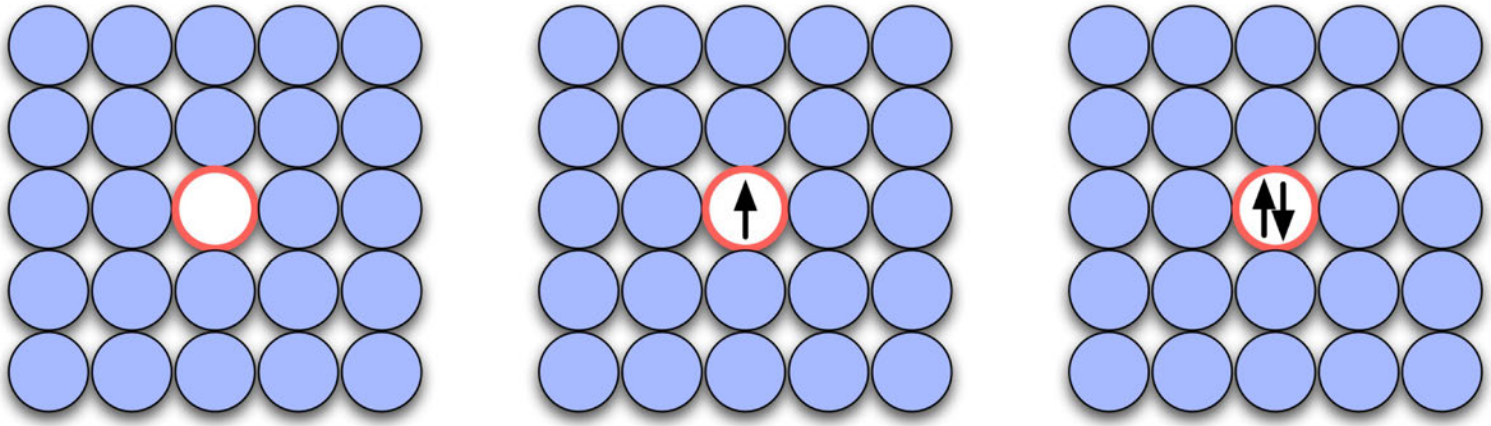
dynamical mean-field theory



$G^{i,j}$

H^{LDA}

$U^{i,i}$

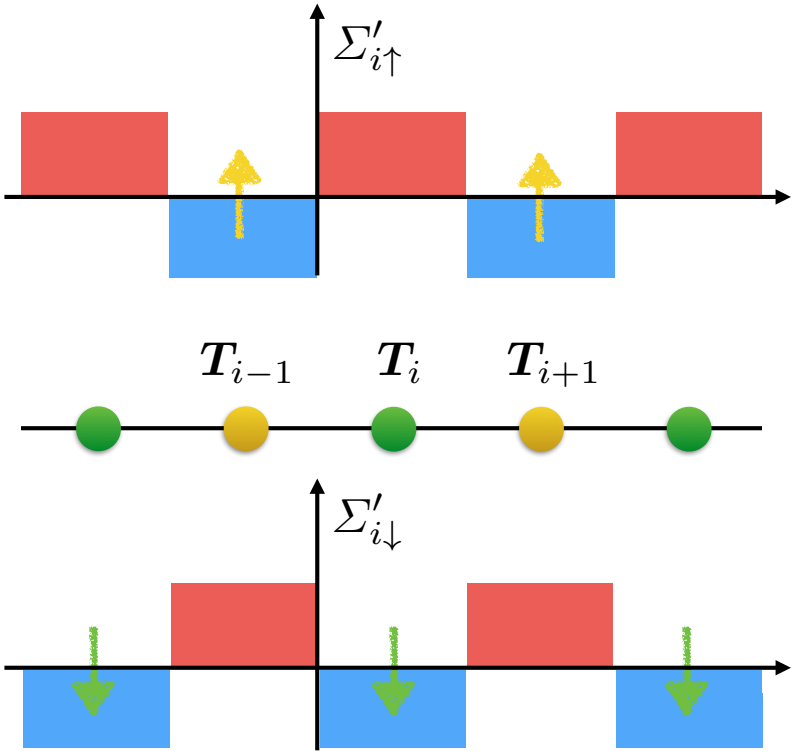


$$\mathcal{G}^{-1} = G^{-1} + \Sigma$$

$$G = G^{i,i}$$

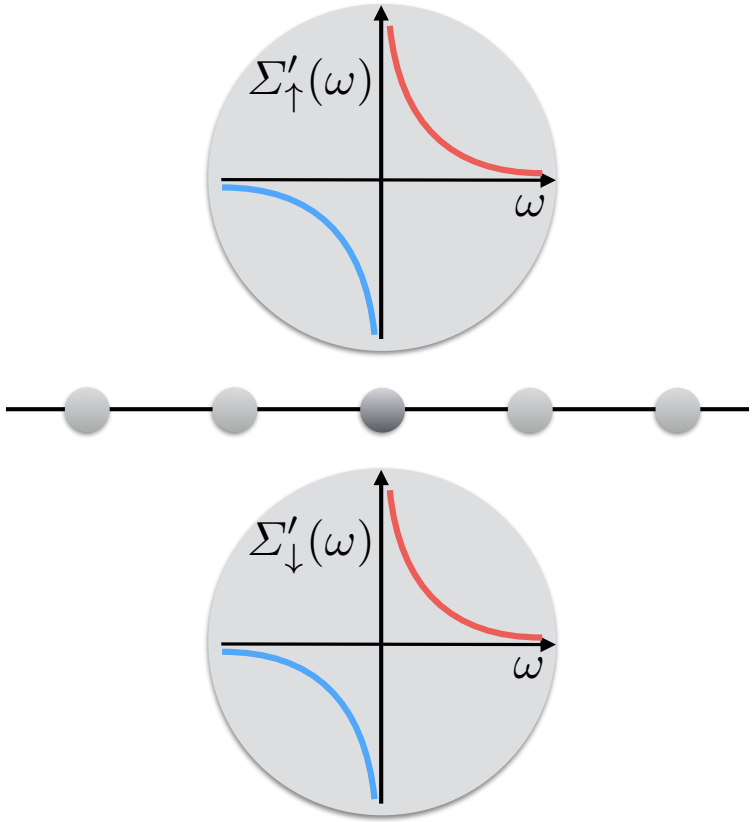
Mott transition: Hartree-Fock vs DMFT

Hartree-Fock



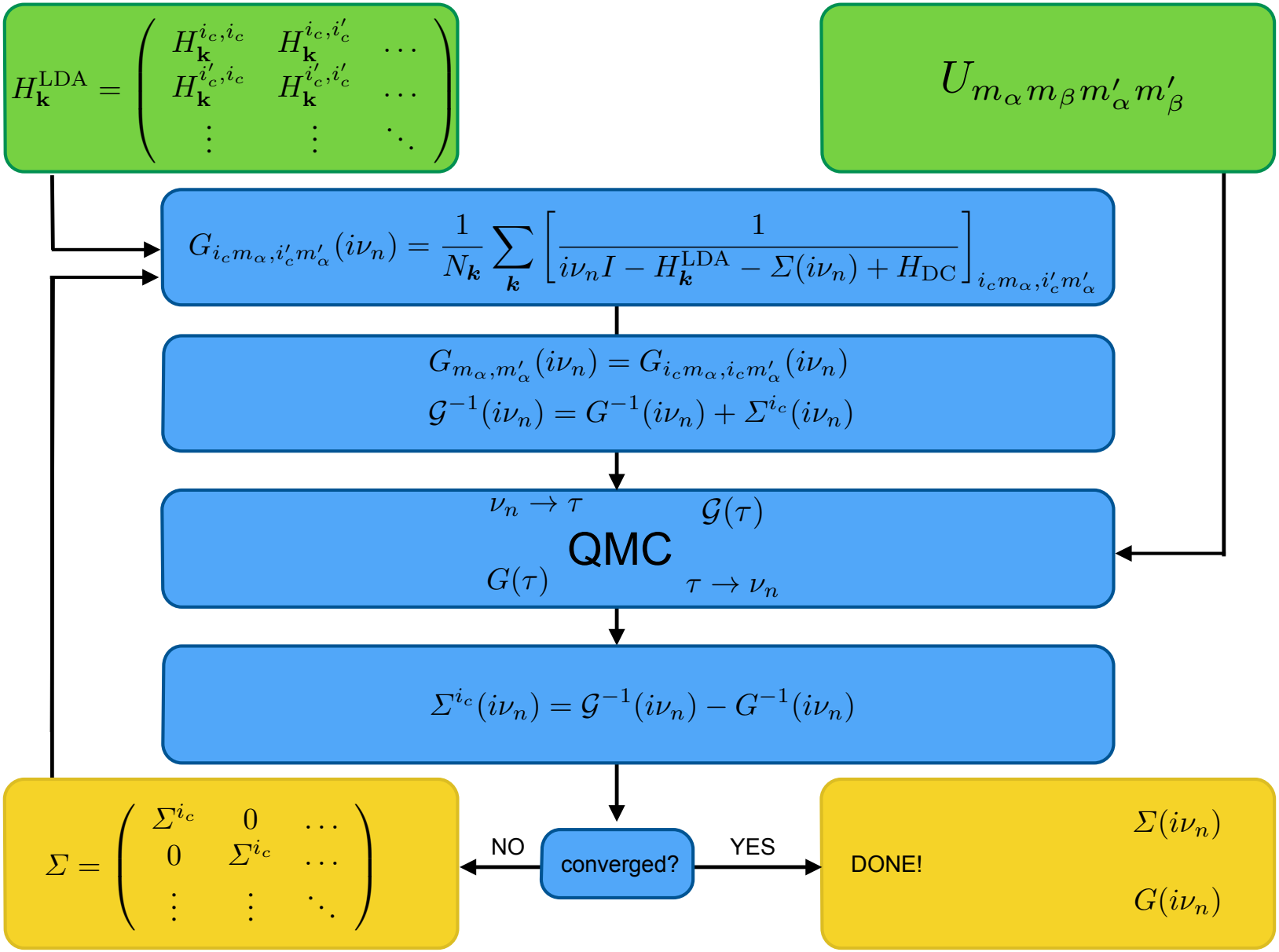
LDA+U

DMFT



LDA+DMFT

LDA+DMFT


$H_{\mathbf{k}}^{\mathrm{LDA}} = \begin{pmatrix} H_{\mathbf{k}}^{i_c,i_c} & H_{\mathbf{k}}^{i_c,i'_c} & \cdots \\ H_{\mathbf{k}}^{i'_c,i_c} & H_{\mathbf{k}}^{i'_c,i'_c} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$
$U_{m_\alpha m_\beta m'_\alpha m'_\beta}$
$G_{i_c m_\alpha, i'_c m'_\alpha}(i\nu_n) = \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \left[\frac{1}{i\nu_n I - H_{\boldsymbol{k}}^{\mathrm{LDA}} - \Sigma(i\nu_n) + H_{\mathrm{DC}}} \right]_{i_c m_\alpha, i'_c m'_\alpha}$
$G_{m_\alpha, m'_\alpha}(i\nu_n) = G_{i_c m_\alpha, i_c m'_\alpha}(i\nu_n)$
$\mathcal{G}^{-1}(i\nu_n) = G^{-1}(i\nu_n) + \Sigma^{i_c}(i\nu_n)$
$\nu_n \to \tau$
$\mathcal{G}(\tau)$
QMC
$G(\tau)$
$\tau \to \nu_n$
$\Sigma^{i_c}(i\nu_n) = \mathcal{G}^{-1}(i\nu_n) - G^{-1}(i\nu_n)$
$\Sigma = \begin{pmatrix} \Sigma^{i_c} & 0 & \cdots \\ 0 & \Sigma^{i_c} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$
NO
converged?
YES
DONE!
$\Sigma(i\nu_n)$
$G(i\nu_n)$

LDA+DMFT with Wannier functions

$$H = -\sum_{ii'}\sum_{mm'}\sum_{\sigma} t^{ii'}_{mm'} c^{\dagger}_{im\sigma} c_{i'm'\sigma}$$

self-energy matrix spin-orbital space

$$+ U \sum_{im} n_{im\uparrow} n_{im\downarrow}$$

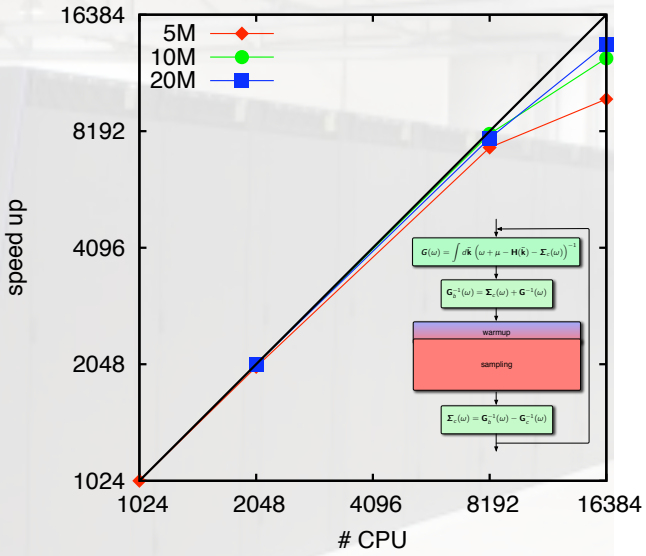
$$+ \frac{1}{2} \sum_{im \neq m' \sigma\sigma'} (U - 2J - J\delta_{\sigma\sigma'}) n_{im\sigma} n_{im'\sigma'}$$

$$- J \sum_{m \neq m'} (c^{\dagger}_{m\uparrow} c^{\dagger}_{m'\downarrow} c_{m'\uparrow} c_{m\downarrow} + c^{\dagger}_{m\uparrow} c^{\dagger}_{m\downarrow} c_{m'\uparrow} c_{m'\downarrow})$$

DMFT and cDMFT

quantum impurity solvers:

general HF QMC
general CT-INT QMC
general CT-HYB QMC

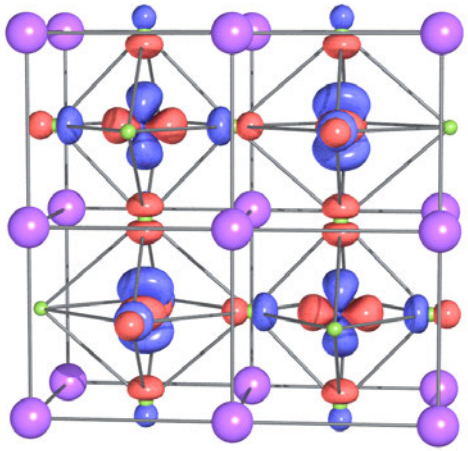


- A. Flesch, E. Gorelov, E. Koch and E. Pavarini
  Multiplet effects in orbital and spin ordering phenomena: A hybridization-expansion quantum impurity solver study
  Phys. Rev. B **87**, 195141 (2013)

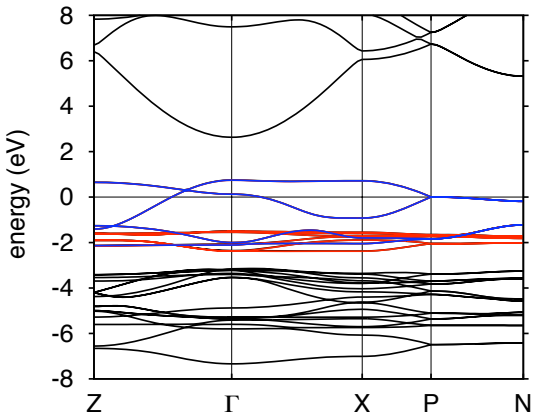
JÜLICH
FORSCHUNGSZENTRUM

an example: $KCuF_3$

insulator, **paramagnetic** for *T>40 K*



LDA



K *4s*

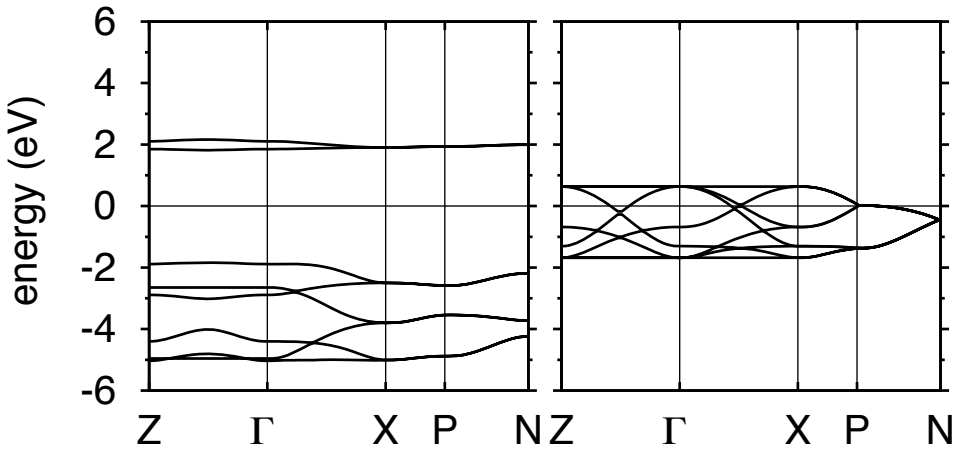
Cu *4s*

Cu *3d*

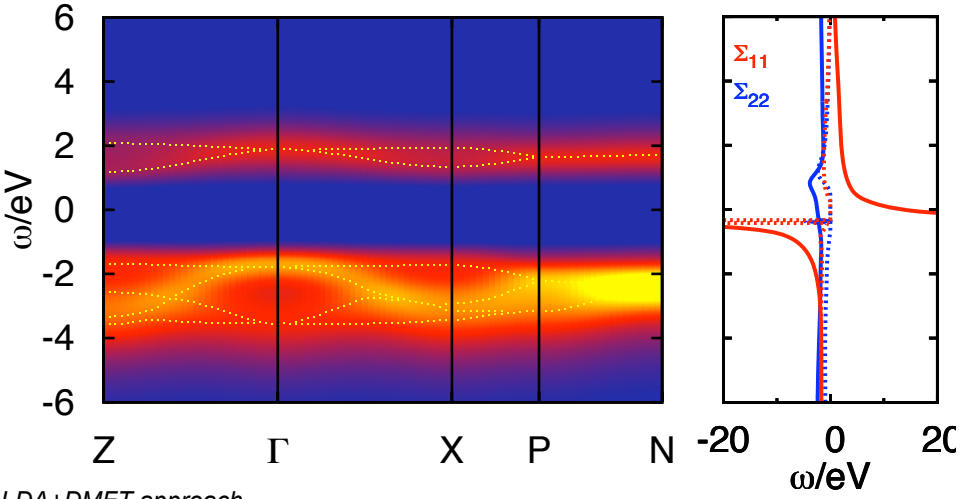
F *2p*

AF-magnetic **LDA+U**

non-magnetic **LDA**



paramagnetic **LDA+DMFT**



E. Pavarini, *Electronic structure calculations with LDA+DMFT*
in Many-Electron Approaches in Physics, Chemistry and Mathematics
Eds. V. Bach and L. Delle Site, Springer (2014)
arXiv:1411.6906

E. Pavarini, *The LDA+DMFT approach,*
in The LDA+DMFT method,
Eds. E.Pavarini, E. Koch, D. Vollhardt. A.I. Lichtenstein, Forschungszentrum Juelich Verlag (2011)
www.cond-mat.de/correl11

early successes: details matter

mechanism of Mott transition in the series explained

VOLUME 92, NUMBER 17 PHYSICAL REVIEW LETTERS week ending 30 APRIL 2004

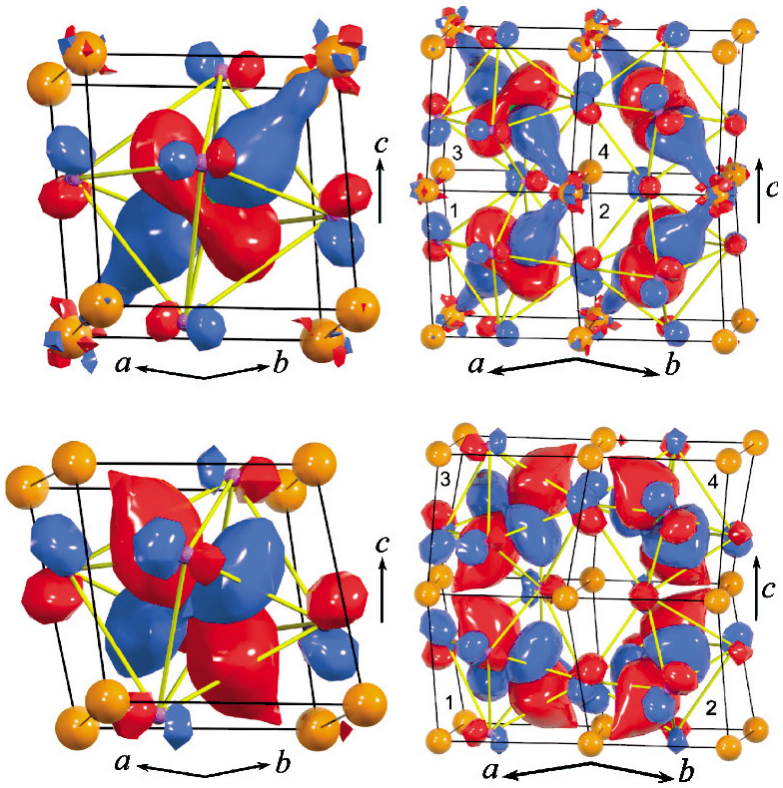
Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic $3d^1$ Perovskites

E. Pavarini,[1] S. Biermann,[2] A. Poteryaev,[3] A. I. Lichtenstein,[3] A. Georges,[2] and O. K. Andersen[4]

t_{2g}^1

Δ=200-300 meV

LDA+DMFT 770 K



a small crystal field plays a key role

spectral functions

(one-electron Green function)

VOLUME 92, NUMBER 17 PHYSICAL REVIEW LETTERS week ending 30 APRIL 2004

Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic $3d^1$ Perovskites

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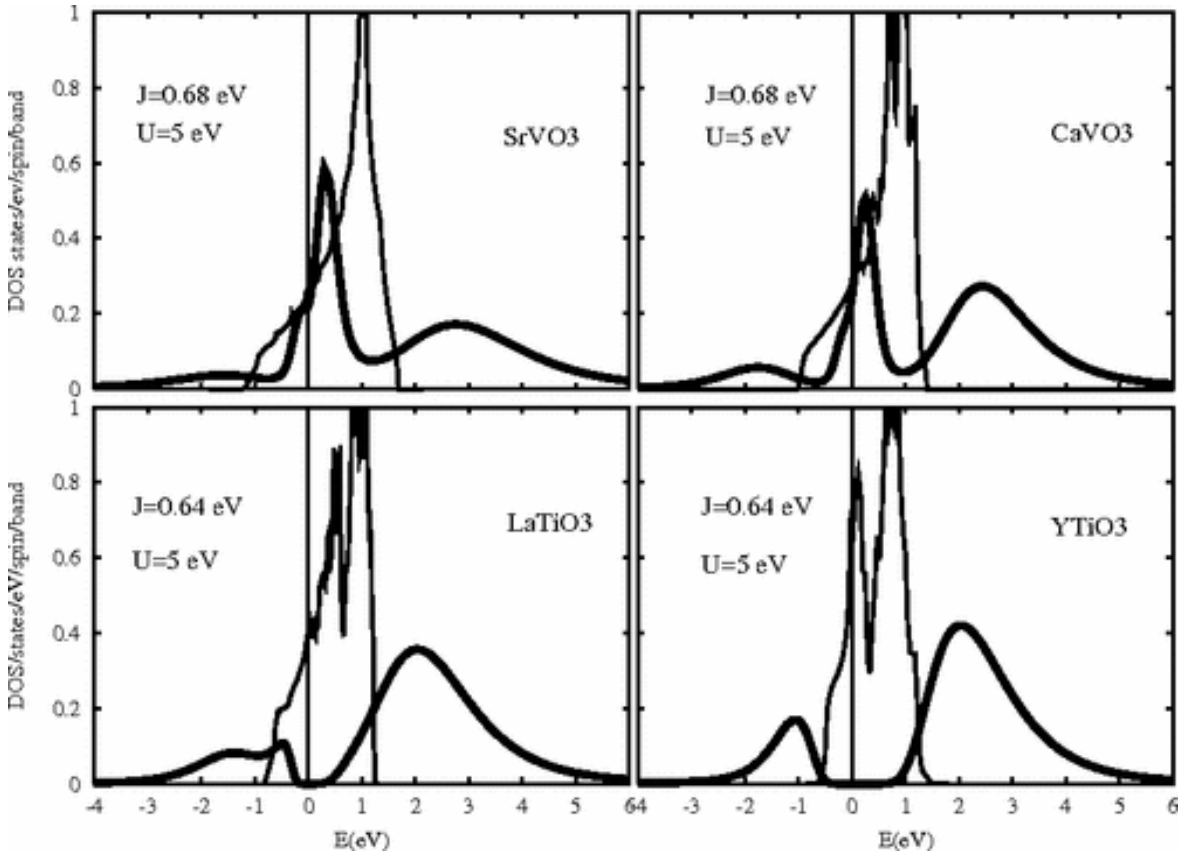


what about linear response functions?

Green Function

k-dependent Dyson equation matrix

$$G(\boldsymbol{k}; i\nu_n) = G_0(\boldsymbol{k}; i\nu_n) + G_0(\boldsymbol{k}; i\nu_n)\Sigma(\boldsymbol{k}; i\nu_n)G(\boldsymbol{k}; i\nu_n)$$

local self-energy approximation

$$\Sigma(\boldsymbol{k}; i\nu_n) \to \Sigma(i\nu_n)$$

local Dyson equation

$$G(i\nu_n) = G_0(i\nu_n) + G_0(i\nu_n)\Sigma(i\nu_n)G(i\nu_n)$$

Susceptibility

q-dependent Bethe-Salpeter equation matrix

$$\chi(\boldsymbol{q}; i\omega_m) = \chi_0(\boldsymbol{q}; i\omega_m) + \chi_0(\boldsymbol{q}; i\omega_m)\Gamma(\boldsymbol{q}; i\omega_m)\chi(\boldsymbol{q}; i\omega_m)$$

local vertex approximation

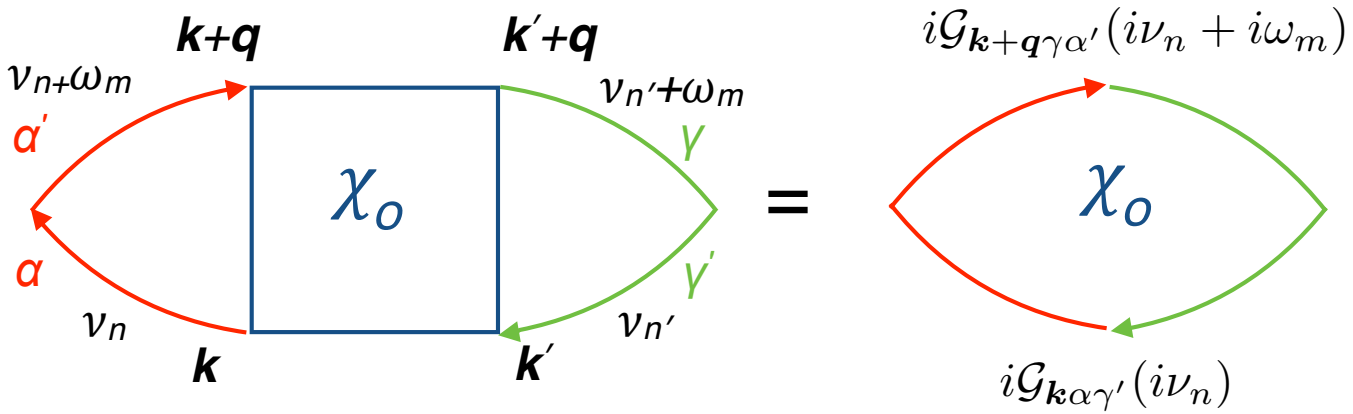
$$\Gamma(\boldsymbol{q}; i\omega_m) \to \Gamma(i\omega_m)$$

local Bethe-Salpeter equation

$$\chi(i\omega_m) = \chi_0(i\omega_m) + \chi_0(i\omega_m)\Gamma(i\omega_m)\chi(i\omega_m)$$

non-interacting case

Wick's theorem holds



$$[\chi_0(\boldsymbol{q}; i\omega_m)]_{\boldsymbol{k}L_\alpha, \boldsymbol{k}'L_\gamma} = -\beta N_{\boldsymbol{k}} \mathcal{G}_{\boldsymbol{k}\alpha\gamma'}(i\nu_n) \mathcal{G}_{\boldsymbol{k}'+\boldsymbol{q}\alpha'\gamma}(i\nu_{n'} + i\omega_m) \delta_{n,n'} \delta_{\boldsymbol{k},\boldsymbol{k}'}$$

generalized susceptibility in LDA+DMFT

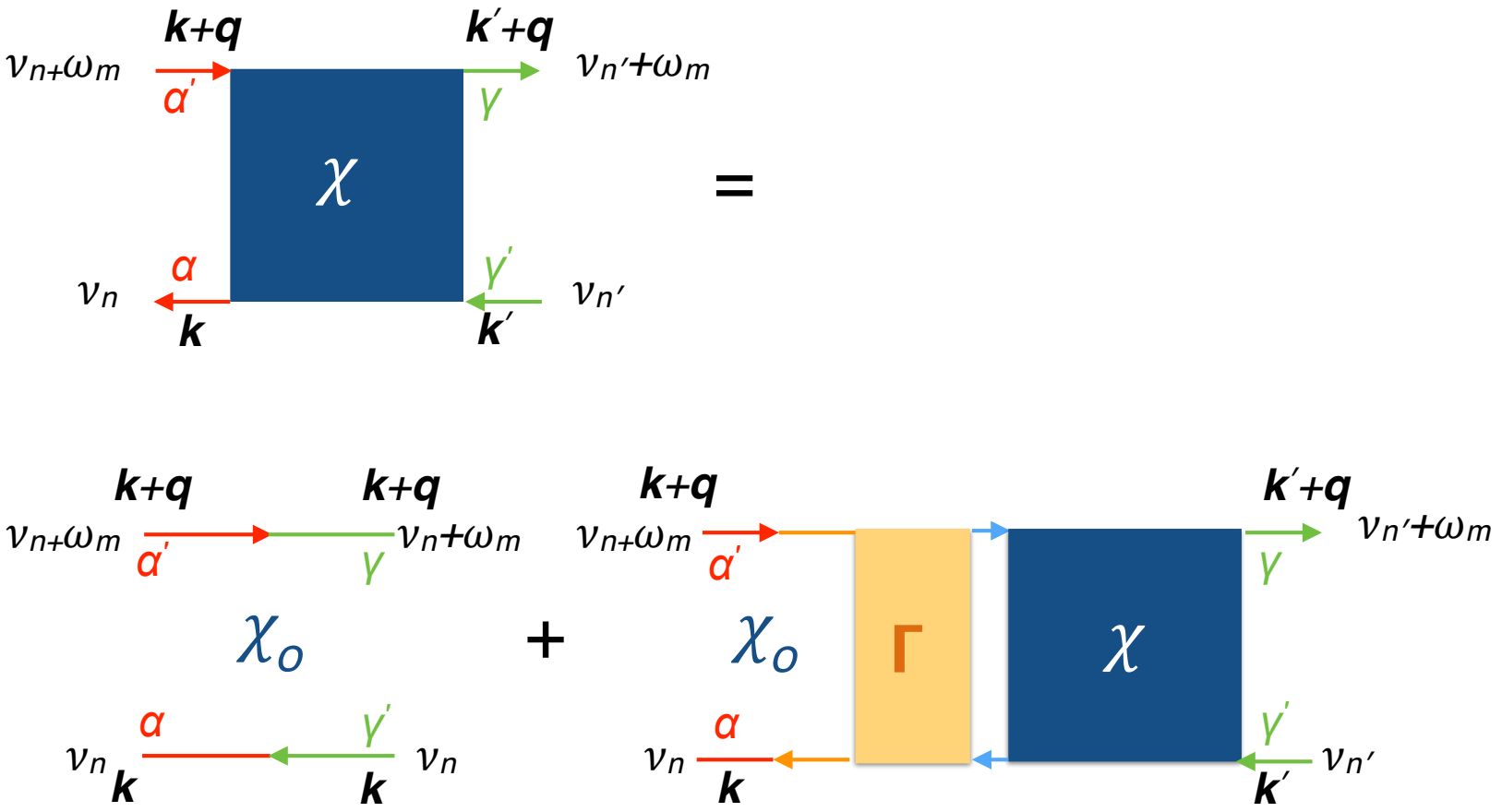
replace non-interacting *G* with G^{DMFT}

G^{DMFT} is the Green function obtained via DMFT

$$[\chi_0(\boldsymbol{q}; i\omega_m)]_{L_\alpha, L_\gamma} = -\beta\delta_{nn'} \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} G^{\mathrm{DMFT}}_{\alpha\gamma'}(\boldsymbol{k}; i\nu_n) G^{\mathrm{DMFT}}_{\alpha'\gamma}(\boldsymbol{k}+\boldsymbol{q}; i\nu_n + i\omega_m)$$

this term is relatively easy to calculate

Bethe-Salpeter equation



local-vertex approximation

vertex in BS equation local in infinite dimensions

approximation for real materials

$$[\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma} = [\chi_0(\boldsymbol{q};\omega_m) + \chi_0(\boldsymbol{q};i\omega_m)\Gamma(i\omega_m)\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma}$$

define local susceptibilities

$$[\chi_0(i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}} = \frac{1}{N_{\boldsymbol{q}}}\sum_{\boldsymbol{q}}[\chi_0(\boldsymbol{q};i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}} \ ,$$

$$[\chi(i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}} = \frac{1}{N_{\boldsymbol{q}}}\sum_{\boldsymbol{q}}[\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}}$$

local-vertex approximation

assume that local BS equation
is also valid for the local susceptibility

$$\left[\Gamma(i\omega_m)\right]_{L_\alpha,L_\gamma} = \left[\chi_0^{-1}(i\omega_m)\right]_{L_\alpha,L_\gamma} - \left[\chi^{-1}(i\omega_m)\right]_{L_\alpha,L_\gamma}$$

local susceptibility: from **quantum impurity solver**

insert vertex in BS equation

$$\left[\chi(\boldsymbol{q};i\omega_m)\right]_{L_\alpha,L_\gamma} = \left[\chi_0(\boldsymbol{q};\omega_m) + \chi_0(\boldsymbol{q};i\omega_m)\Gamma(i\omega_m)\chi(\boldsymbol{q};i\omega_m)\right]_{L_\alpha,L_\gamma}$$

q-dependence here from non-interacting part

Hubbard Model in Infinite Dimensions: A Quantum Monte Carlo Study

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Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221

(Received 5 December 1991)

An essentially exact solution of the infinite-dimensional Hubbard model is made possible by a new self-consistent Monte Carlo procedure. Near half filling antiferromagnetism and a pseudogap in the single-particle density of states are found for sufficiently large values of the intrasite Coulomb interaction. At half filling the antiferromagnetic transition temperature obtains its largest value when the intrasite Coulomb interaction $U \approx 3$.

PACS numbers: 75.10.Jm, 71.10.+x, 75.10.Lp, 75.30.Kz

Hirsch-Fye QMC

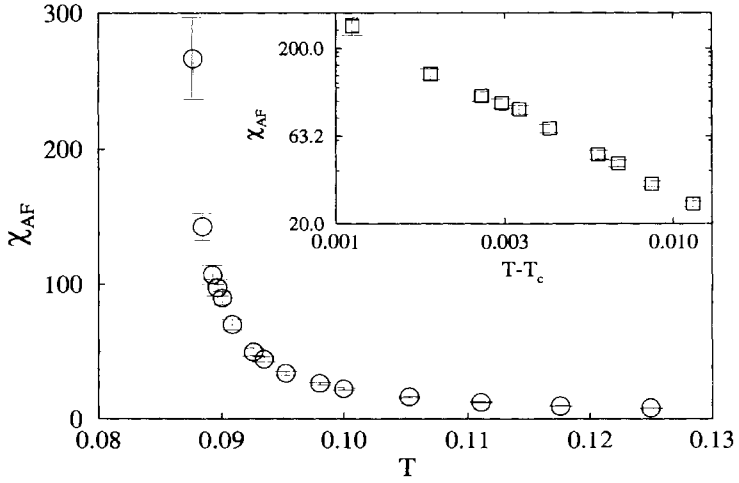
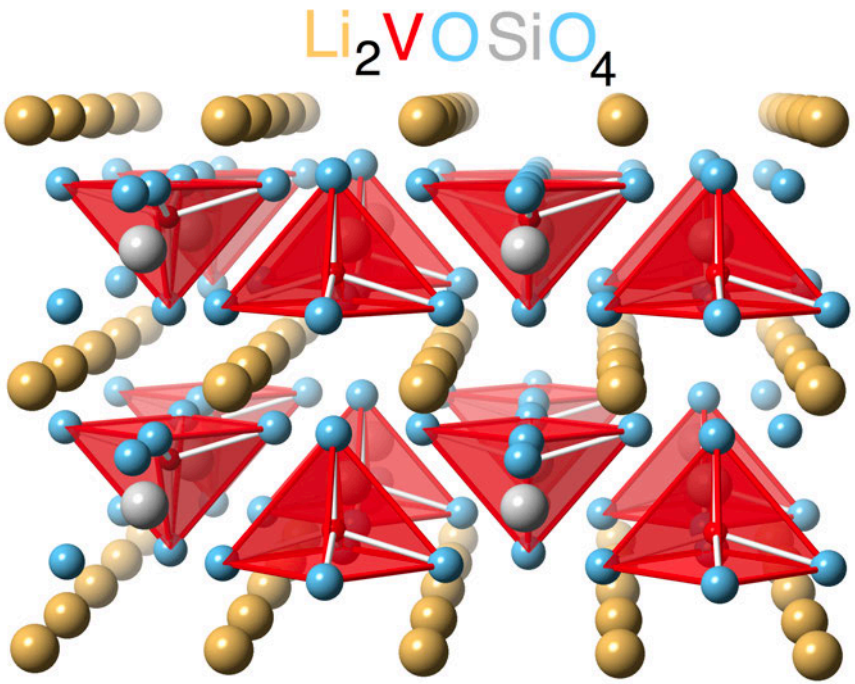
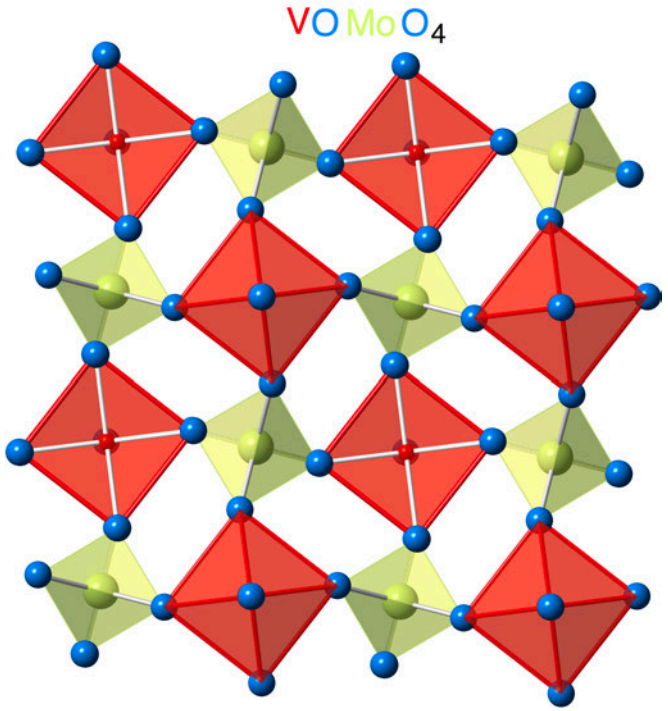


FIG. 3. Antiferromagnetic susceptibility $\chi_{AF}(T)$ vs temperature T when $U=1.5$ and $\epsilon=0.0$. The logarithmic scaling behavior is shown in the inset. The data close to the transition fit the form $\chi_{AF} \propto |T-T_c|^{\nu}$ with $T_c=0.0866\pm0.0003$ and $\nu=-0.99\pm0.05$. The points at $U=0$ reflect exactly known limits.

Li_2VOSiO_4 vs $VOMoO_4$

poster Amin Kiani

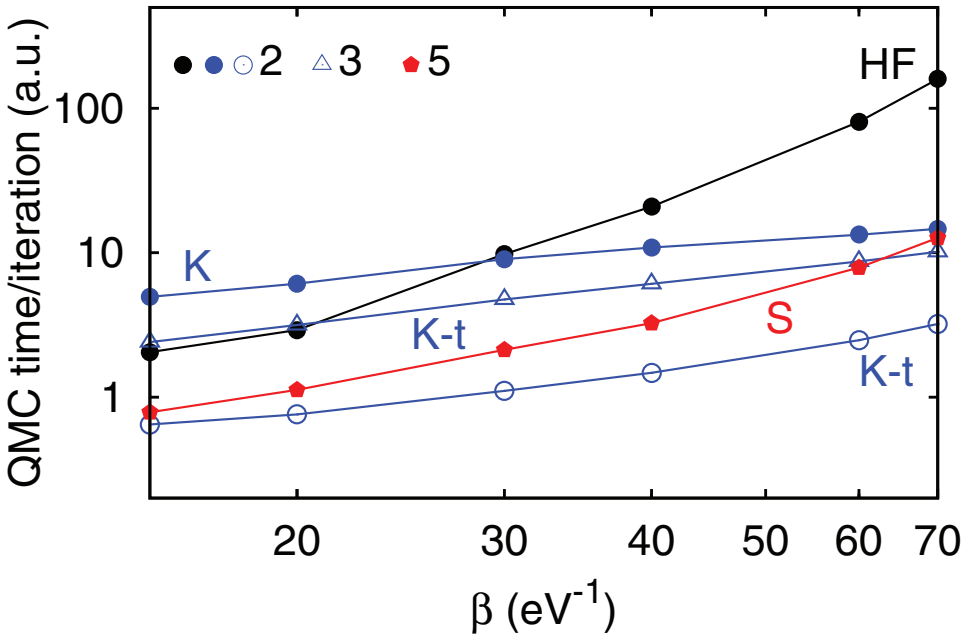




CT-QMC solver

(performance of our general code on BlueGene)

poster Julian Musshoff



can include:

full self-energy matrix in spin-orbital space

full Coulomb matrix

spin-orbit

Phys. Rev. B **87**, 195141

t_{2g} full self-energy matrix

full Coulomb matrix

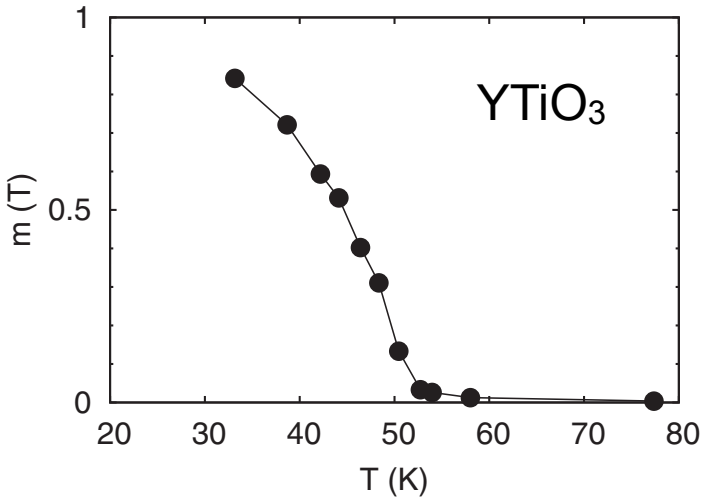


FIG. 3. Ferromagnetic spin polarization as a function of temperature in $YTiO_3$. The plot shows a transition at the critical temperature $T_C \sim 50$ K, slightly overestimating the experimental value $T_C \sim 30$ K, as one might expect from a mean-field calculations.

Mott-insulator, approximate solution

X_0 term

in the *t=0* limit

$$G(i\nu_n) = \frac{1}{i\nu_n + \mu - \Sigma(i\nu_n)}$$

$$\Sigma(i\nu_n) = \mu + \frac{U^2}{4}\frac{1}{i\nu_n}$$

what about the small *t/U* limit?

let us consider an approximate form for the self-energy

$$\Sigma(i\nu_n) = \mu + \frac{r_U U^2}{4}\frac{1}{i\nu_n}$$

X_0 term

(replace susceptibility tensors with physical susceptibilities)

X_0 term

perform Matsubara sums

$$\chi^0_{zz}(\boldsymbol{q};0) = (g\mu_B)^2 \frac{1}{4} \sum_\sigma \frac{1}{\beta^2} \sum_n \chi^{\sigma\sigma}_{n,n}(0)$$

$$= (g\mu_B)^2 \frac{1}{2} \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \Big[\underbrace{-I^{++}_{\boldsymbol{k},\boldsymbol{q}} - I^{--}_{\boldsymbol{k},\boldsymbol{q}}}_{A_{\boldsymbol{k},\boldsymbol{q}}} + \underbrace{I^{+-}_{\boldsymbol{k},\boldsymbol{q}} + I^{-+}_{\boldsymbol{k},\boldsymbol{q}}}_{B_{\boldsymbol{k},\boldsymbol{q}}}, \Big]$$

"metallic" "insulating"

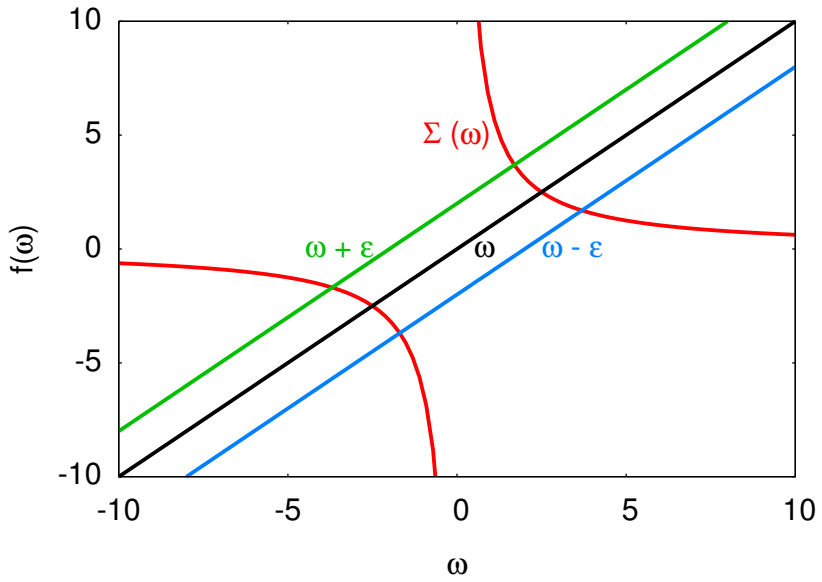
$$I^{\alpha\gamma}_{\boldsymbol{k},\boldsymbol{q}} = \frac{E^\alpha_{\boldsymbol{k}}\ E^\gamma_{\boldsymbol{k}+\boldsymbol{q}}}{(E^+_{\boldsymbol{k}} - E^-_{\boldsymbol{k}})(E^+_{\boldsymbol{k}+\boldsymbol{q}} - E^-_{\boldsymbol{k}+\boldsymbol{q}})} \frac{n(E^\alpha_{\boldsymbol{k}}) - n(E^\gamma_{\boldsymbol{k}+\boldsymbol{q}})}{E^\alpha_{\boldsymbol{k}} - E^\gamma_{\boldsymbol{k}+\boldsymbol{q}}}$$

X_0 term

what about the small t/U limit?

$$\Sigma(i\nu_n) = \mu + \frac{r_U U^2}{4}\frac{1}{i\nu_n}$$

$$G_{\boldsymbol{k}}(i\nu_n) = \frac{1}{i\nu_n - \Sigma(i\nu_n) - \varepsilon_{\boldsymbol{k}}} = \frac{1}{E^+_{\boldsymbol{k}} - E^-_{\boldsymbol{k}}}\left[\frac{E^+_{\boldsymbol{k}}}{i\nu_n - E^+_{\boldsymbol{k}}} - \frac{E^-_{\boldsymbol{k}}}{i\nu_n - E^-_{\boldsymbol{k}}}\right]$$



X_0 term

at the Γ point

$$\chi^0_{zz}(\mathbf{0};0) \sim (g\mu_B)^2 \frac{1}{4}\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}} \frac{r_U\, U^2}{[\varepsilon^2_{\boldsymbol{k}} + r_U\, U^2]^{3/2}} \sim (g\mu_B)^2 \frac{1}{4\sqrt{r_U}\, U}\left[1 - \frac{3}{2}\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}} \frac{\varepsilon^2_{\boldsymbol{k}}}{r_U\, U^2} + \dots\right]$$

at the M point

$$\chi_0(\boldsymbol{q}_C;0) \sim (g\mu_B)^2 \frac{1}{4\sqrt{r_U}U}\left[1 - \frac{1}{2}\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}} \frac{\varepsilon^2_{\boldsymbol{k}}}{r_U U^2}\right]$$

in general

$$\chi_0(\boldsymbol{q};0) \sim (g\mu_B)^2 \frac{1}{4\sqrt{r_U}U}\left[1 - \frac{1}{2}\frac{J_{\mathbf{0}}}{\sqrt{r_U}U} - \frac{1}{4}\frac{J_{\boldsymbol{q}}}{\sqrt{r_U}U}\right]$$

$$J_{\boldsymbol{q}} = 2J[\cos q_x + \cos q_y], \quad J \propto t^2/U$$

local term and vertex

(replace susceptibility tensors with physical susceptibilities)

local magnetic susceptibility

result after Matsubara sums

$$\chi_{zz}(\boldsymbol{q};0) = (g\mu_B)^2 \, \frac{1}{4k_BT} \, \frac{e^{\beta U/2}}{1+e^{\beta U/2}}$$

Curie-like temperature behavior

infinite U limit: emergence of spin

X_0 term & the local vertex Γ

use atomic susceptibility as local susceptibility to determine the vertex via the local Bethe-Salpeter equation

$$\Gamma \sim \left[\frac{1}{\chi^0_{zz}(0)} - \frac{1}{\chi_{zz}(0)}\right] \sim \frac{1}{(g\mu_B)^2}\left[4\sqrt{r_U}U\left(1+\frac{1}{2}\frac{J_{\mathbf{0}}}{\sqrt{r_U}U}\right) - 4k_BT\right]$$

the expected Curie-Weiss behavior

$$\chi_{zz}(\boldsymbol{q};0) = \frac{1}{[\chi^0_{zz}(\boldsymbol{q};0)]^{-1} - \Gamma} \sim (g\mu_B)^2 \frac{1}{4}\frac{1}{k_BT + J_{\boldsymbol{q}}/4} = \frac{(g\mu_B)^2}{k_B}\frac{1}{4}\frac{1}{T - T_{\boldsymbol{q}}}$$

what happens if we neglect the vertex?

example: **atomic limit**

finite temperature Green function

$$G_\sigma(\tau) = -\frac{1}{2}\frac{1}{1+e^{\beta U/2}}\left[e^{\tau U/2} + e^{(\beta-\tau)U/2}\right]$$

$$G_\sigma(i\nu_n) = \frac{1}{2}\left[\frac{1}{i\nu_n + U/2} + \frac{1}{i\nu_n - U/2}\right]$$

X_0 term

atomic limit

$$\chi^0_{zz}(0) = \frac{1}{4}(g\mu_B)^2 \sum_\sigma \frac{1}{\beta^2} \sum_n \chi^{\sigma\sigma}_{n,n}(0) = \frac{1}{4}(g\mu_B)^2 \frac{\beta e^{\beta U/2}}{1+e^{\beta U/2}} \left[\frac{1}{1+e^{\beta U/2}} + \frac{1}{U\beta} \left(\frac{1-e^{-\beta U}}{1+e^{-\beta U/2}} \right) \right]$$

large U: weakly temperature dependent

$$\chi^0_{zz}(0) \sim (g\mu_B)^2/4U$$

Curie behavior? Local moments?

local magnetic susceptibility

result after Matsubara sums

$$\chi_{zz}(\boldsymbol{q};0) = (g\mu_B)^2 \frac{1}{4k_BT} \frac{e^{\beta U/2}}{1+e^{\beta U/2}}$$

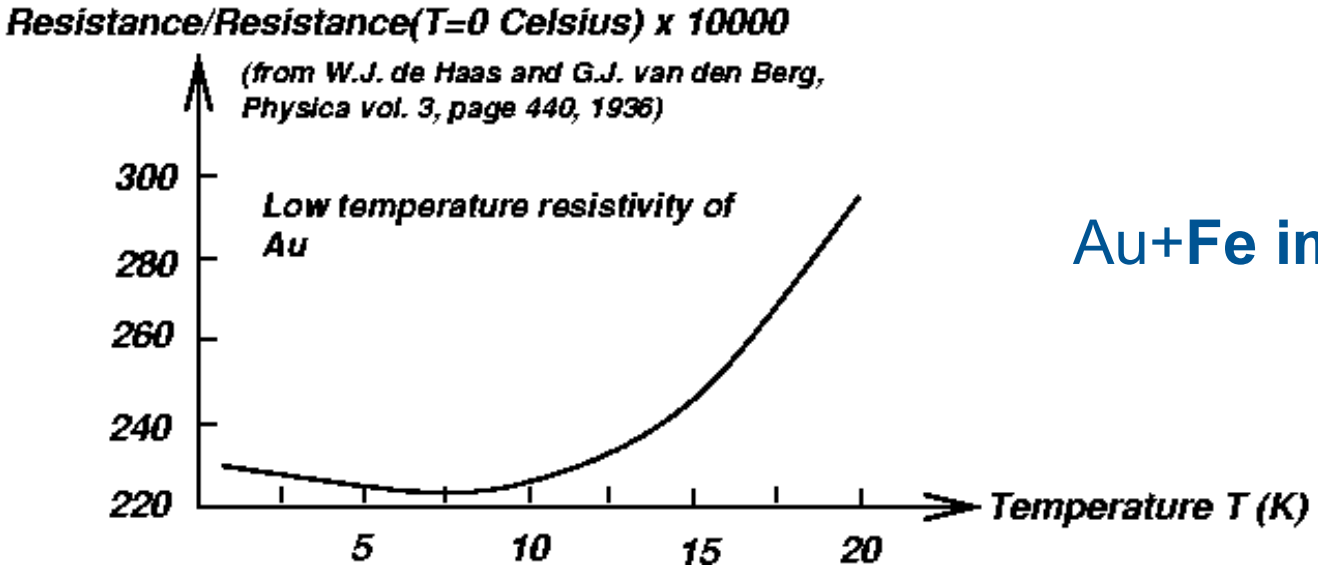
Curie-like temperature behavior

infinite U limit: **emergence** of spin

the Kondo effect

the Kondo effect

diluted magnetic alloys: metal+**magnetic** impurities



Au+**Fe impurities**

minimum in resistivity

high-temperature: impurity local moments, Curie susceptibility

low temperature: effective magnetic moment disappears
(Fermi-liquid susceptibility)

characteristic temperature: Kondo temperature T_K

Anderson model

metal impurity

$$H_{\mathrm{A}} = \sum_{\sigma}\sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_{\sigma} \varepsilon_f n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow}$$

$$+ \sum_{\sigma}\sum_{\boldsymbol{k}} \left[V_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{f\sigma} + h.c. \right]$$

hybridization

Kondo regime: $n_f \sim 1$

canonical transformation (Schrieffer-Wolff) to Kondo model

$$H_{\mathrm{K}} = \sum_{\sigma}\sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \Gamma \boldsymbol{S}_f \cdot \boldsymbol{s}_c(\boldsymbol{0}) = H_0 + H_{\Gamma}$$

$$\Gamma \sim -2|V_{k_F}|^2 \left[\frac{1}{\varepsilon_f} - \frac{1}{\varepsilon_f + U} \right] > 0$$

antiferromagnetic coupling

Schrieffer-Wolff transformation

Through the Schrieffer-Wolff canonical transformation [28] one can map the Anderson model onto the Kondo model, in which only the effective spin of the impurity enters

$$H_{\mathrm{K}} = H_0' + \Gamma \boldsymbol{S}_f \cdot \boldsymbol{s}_c(\mathbf{0}) = H_0' + H_\Gamma, \tag{30}$$

where

$$\Gamma \sim -2|V_{k_F}|^2 \left[\frac{1}{\varepsilon_f} - \frac{1}{\varepsilon_f + U}\right] > 0$$

is the antiferromagnetic coupling arising from the hybridization, $\boldsymbol{S}_f$ the spin of the impurity ($S_f = 1/2$), and $\boldsymbol{s}_c(\mathbf{0})$ is the spin-density of the conduction band at the impurity site. For convenience we set the Fermi energy to zero; k_F is a $\boldsymbol{k}$ vector at the Fermi level. The Schrieffer-Wolff canonical transformation works as follows. We introduce the operator S that transforms the Hamiltonian H into H_S

$$H_S = e^S H e^{-S}.$$

Schrieffer-Wolff transformation

$$[S, H_0] = -H_1. \tag{31}$$

From Eq. (31) one finds that the operator S is given by

$$S = \sum_{\boldsymbol{k}\sigma} \left[\frac{1 - n_{f-\sigma}}{\varepsilon_{\boldsymbol{k}} - \varepsilon_f} + \frac{n_{f-\sigma}}{\varepsilon_{\boldsymbol{k}} - \varepsilon_f - U} \right] V_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{f\sigma} - \text{h.c.}.$$

The transformed Hamiltonian is complicated, as can be seen from explicitly writing the series for a transformation satisfying Eq. (31)

$$H_S = H_0 + \frac{1}{2}[S, H_1] + \frac{1}{3}\Big[S, [S, H_1]\Big] + \ldots.$$

In the limit in which the hybridization strength Γ is small this series can, however, be truncated at second order. The resulting Hamiltonian has the form $H_S = H_0 + H_2$, with $H_2 = H_\Gamma + H_{\text{dir}} + \Delta H_0 + H_{\text{ch}}$. The first term is the exchange interaction

$$H_\Gamma = \frac{1}{4} \sum_{\boldsymbol{k}\boldsymbol{k}'} \Gamma_{\boldsymbol{k}\boldsymbol{k}'} \left[\sum_{\sigma_1\sigma_2} c^\dagger_{\boldsymbol{k}'\sigma_1} \langle \sigma_1 | \hat{\sigma} | \sigma_2 \rangle c_{\boldsymbol{k}\sigma_2} \cdot \sum_{\sigma_3\sigma_4} c^\dagger_{f\sigma_3} \langle \sigma_3 | \hat{\sigma} | \sigma_4 \rangle c_{f\sigma_4} \right]$$

where

$$\Gamma_{\boldsymbol{k}\boldsymbol{k}'} = V^*_{\boldsymbol{k}} V_{\boldsymbol{k}'} \left[\frac{1}{\varepsilon_{\boldsymbol{k}} - \varepsilon_f} + \frac{1}{\varepsilon_{\boldsymbol{k}'} - \varepsilon_f} + \frac{1}{U + \varepsilon_f - \varepsilon_{\boldsymbol{k}}} + \frac{1}{U + \varepsilon_f - \varepsilon_{\boldsymbol{k}'}} \right].$$

susceptibility

high-temperature impurity susceptibility

$$\chi^f_{zz}(T) \sim \frac{(g\mu_B)^2 S_f(S_f+1)}{3k_BT}\left\{1 - \frac{1}{\ln\left(T/T_{\rm K}\right)}\right\}$$

Kondo temperature

$$k_B T_{\rm K} \sim D e^{-2/\rho(\varepsilon_F)\Gamma}$$

low-temperature impurity susceptibility

$$\chi^f_{zz}(T) \sim \frac{C_{1/2}}{\mathcal{W}T_{\rm K}}\left\{1 - \alpha T^2 + \dots\right\}$$

Fermi liquid!

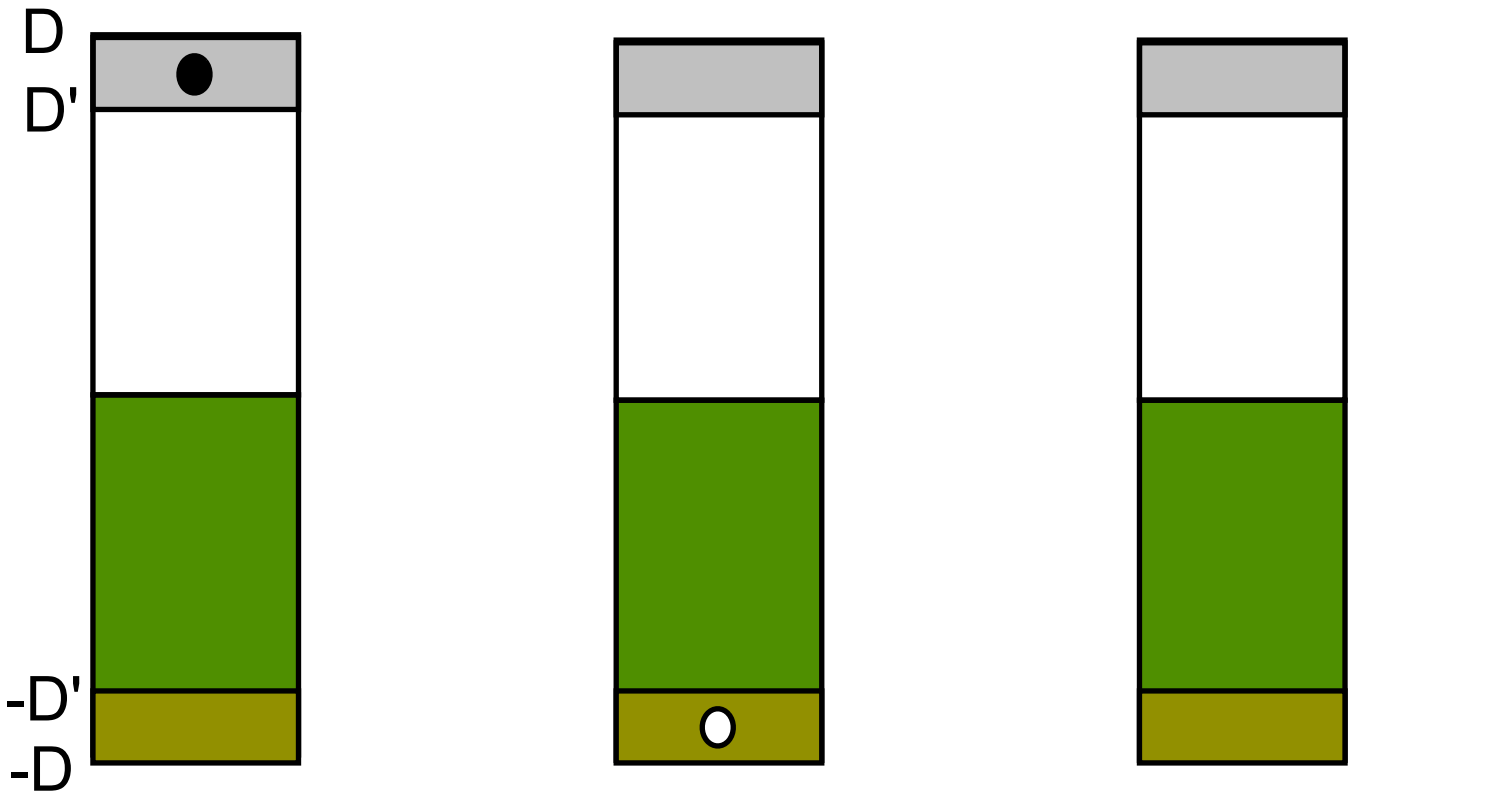
$$\mu^2_{\rm eff}(T) \equiv 3k_BT\chi^f_{zz}(T) \propto \langle S^f_z S^f_z\rangle + \langle S^f_z s^c_z\rangle$$

magnetic moment screened, S=0

poor's man scaling

eliminate high-energy states, i.e., the states with

- at least one electron in high-energy region
- at least one hole in high-energy region



- one electron
- one hole
- low-energy state

downfolding

electron case: projectors

$$P_H \sim \sum_{\sigma} \sum_{\boldsymbol{q}} c^{\dagger}_{\boldsymbol{q}\sigma} |FS\rangle\langle FS| c_{\boldsymbol{q}\sigma}$$

high-energy sector

$$P_L \sim \sum_{\sigma} \sum_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} |FS\rangle\langle FS| c_{\boldsymbol{k}\sigma}$$

low-energy sector

effect of downfolding high sector at second order

$$\delta H_L^{(2)} \sim P_L H_\Gamma P_H (\omega - P_H H_0 P_H)^{-1} P_H H_\Gamma P_L$$

electron contribution

$$\begin{aligned} \delta H_L^{(2)} &= -\frac{1}{2}\Gamma^2 \sum_{\boldsymbol{q}} \frac{1}{\omega - \varepsilon_{\boldsymbol{q}}} \boldsymbol{S}_f \cdot \boldsymbol{s}_c(\boldsymbol{0}) + \ldots \\ &\sim \frac{1}{4}\rho(\varepsilon_F)\Gamma^2 \frac{\delta D}{D} \boldsymbol{S}_f \cdot \boldsymbol{s}_c(\boldsymbol{0}) + \ldots \end{aligned}$$

scaling equations

thus the Kondo Hamiltonian is modified as follows

$$\begin{aligned} \Gamma &\rightarrow \Gamma' = \Gamma + \delta\Gamma, \\ \frac{\delta\Gamma}{\delta \ln D} &= \frac{1}{2}\rho(\varepsilon_F)\Gamma^2 \end{aligned}$$

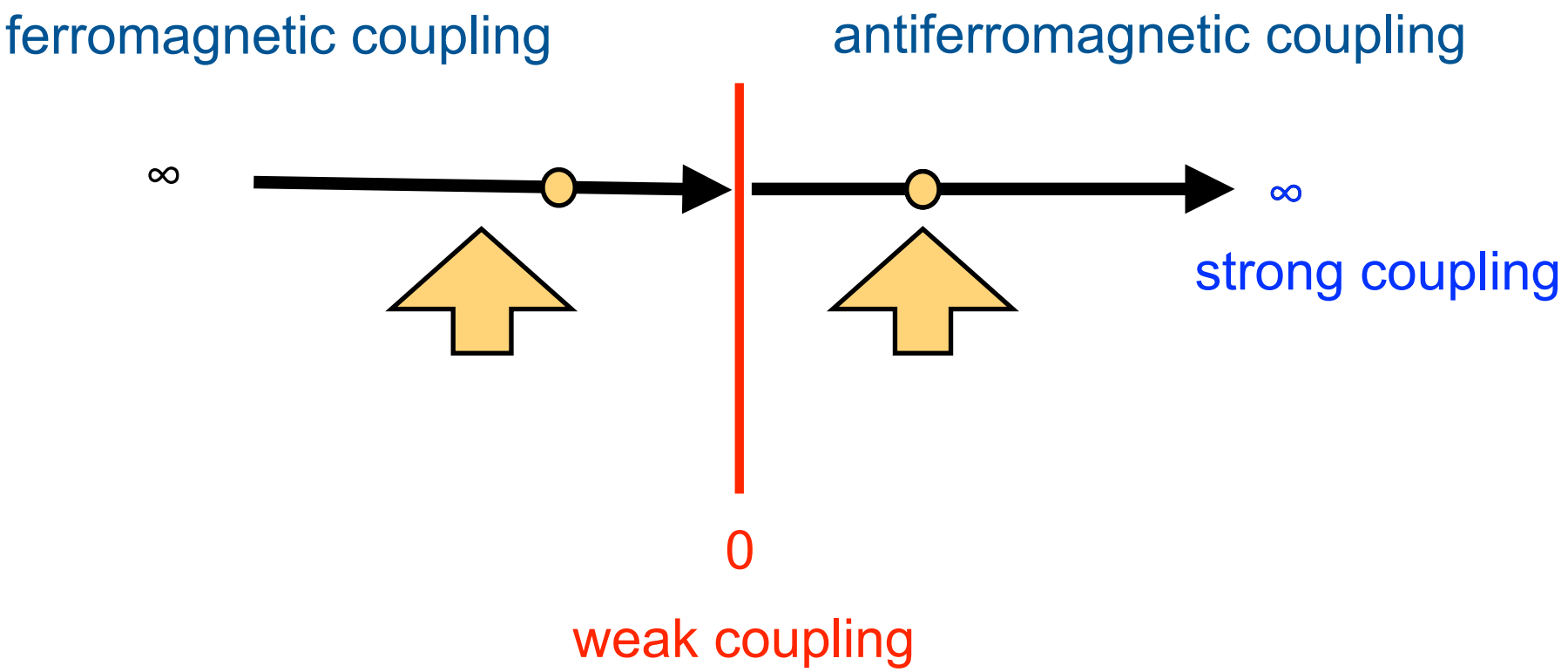
scaling equations

$$\Gamma' = \frac{\Gamma}{1 + \frac{1}{2}\rho(\varepsilon_F)\Gamma \ln \frac{D'}{D}}.$$

scaling equations

$$\Gamma \rightarrow \Gamma' = \Gamma + \delta\Gamma,$$

$$\frac{\delta\Gamma}{\delta \ln D} = \frac{1}{2}\rho(\varepsilon_F)\Gamma^2$$



strong coupling case

one electron screens local moment

spin zero system!

starting point for perturbation theory

nearby electrons polarize moment via virtual excitations

effective repulsive on-site Coulomb interaction

Nozières Fermi liquid

weak coupling case

asymptotic freedom

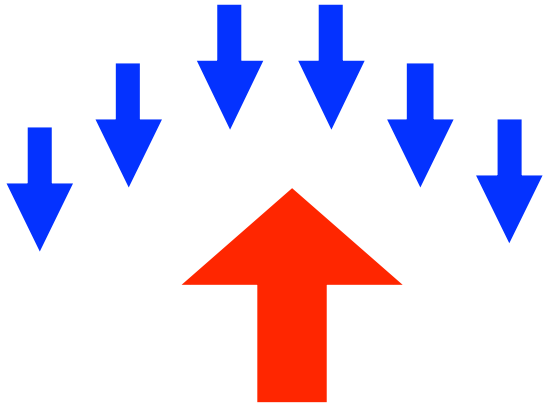
non-interacting local moment

Curie susceptibility

magnetic interaction as perturbation

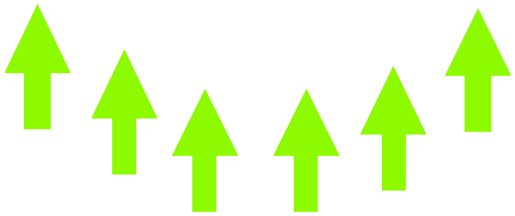
scaling: two-channel case

conduction band A



kinetic exchange: AFM

conduction band B



Coulomb exchange: FM

situation realized in some Ce and Yb alloys

Kondo or Curie?

scaling: two-channel case

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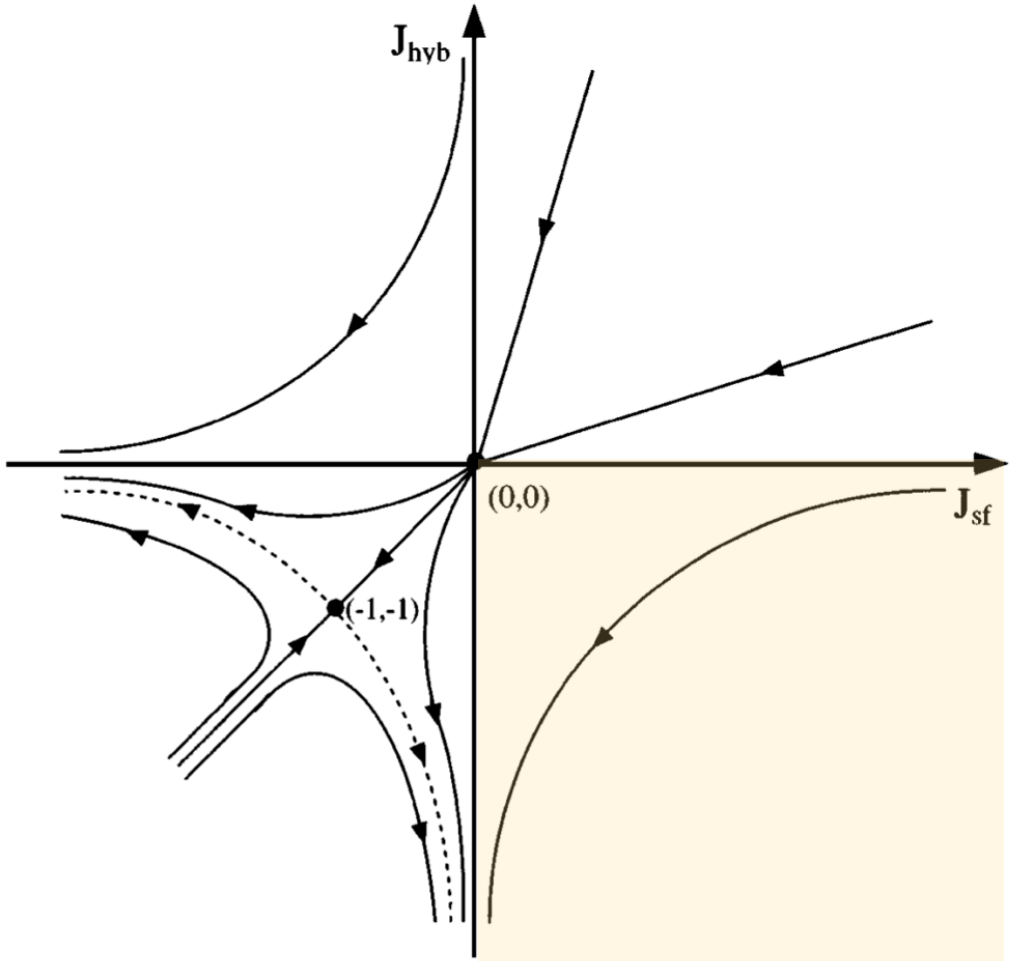
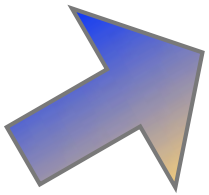
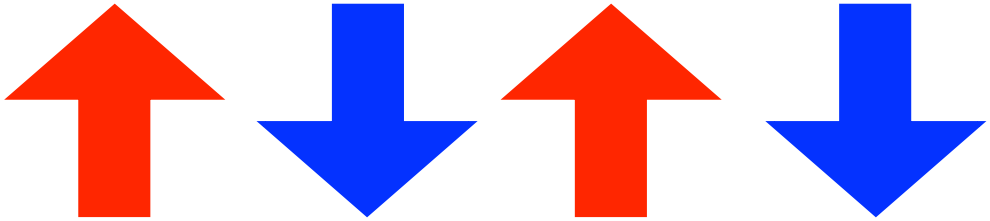
Hybridization versus Local Exchange Interaction in the Kondo Problem: A Two-Band Model

Eva Pavarini and Lucio Claudio Andreani

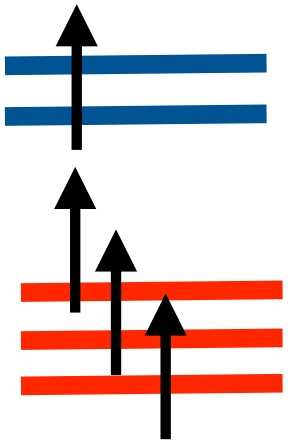


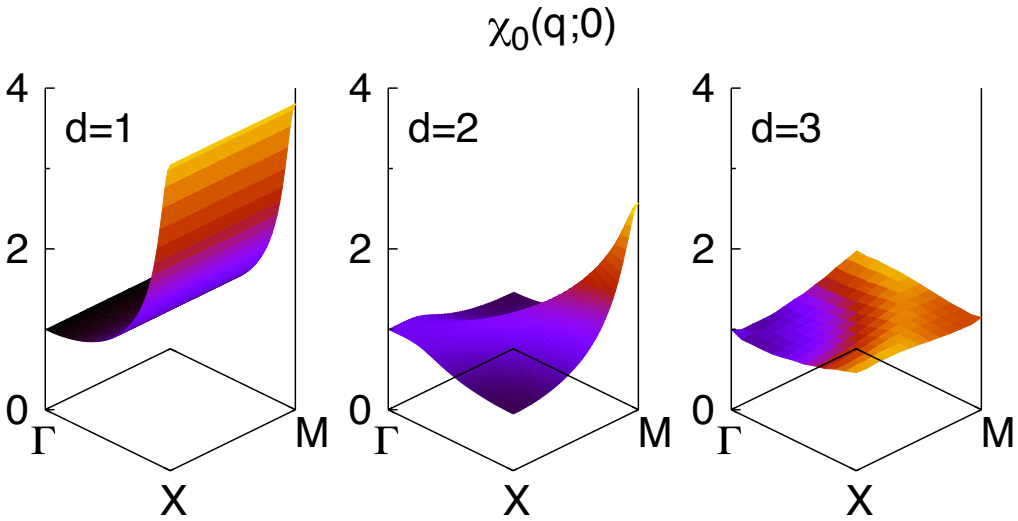
conclusion





- emergence of spin
- emergence of long-range order





- local moment regime
  Curie and Curie-Weiss susceptibility
  Heisenberg model
- itinerant regime
  Pauli susceptibility
  Stoner instabilities

in strongly correlated system both local and delocalized features present

conclusion

lattice model

$$H = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U$$

large U limit, n=1

$$H = \frac{1}{2} \Gamma \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

quantum impurity model

$$H_{\mathrm{A}} = \sum_\sigma \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_\sigma \varepsilon_f n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow}$$

$$+ \sum_\sigma \sum_{\boldsymbol{k}} \left[V_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{f\sigma} + h.c. \right]$$

large U limit, n=1

$$H = \Gamma \, \mathbf{S}_f \cdot \mathbf{s}_c(\mathbf{0})$$

self-consistency loop

thank you!