Model Hamiltonians and Basic Techniques

Frank Lechermann

I. Institut für Theoretische Physik, Universität Hamburg

Autumn School Hands-on LDA+DMFT

Forschungszentrum Jülich

04.10.2011

Outline

- motivation
- introduction to the single-band Hubbard model
- multi-band Hubbard models
- first approaches: Hartree-Fock and Hubbard I
- slave-boson approach

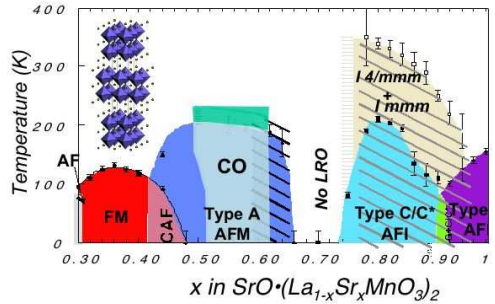
Motivation: Materials

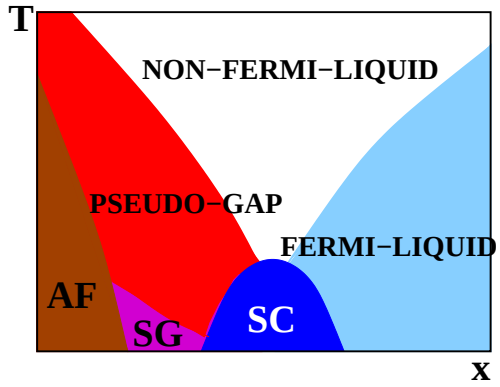
rongly correlated electron systems in alistic condensed matter offer a large ariety of complex phenomena on-Fermi liquid, charge-, spin- and bital order, charge density waves, uperconductivity,...)

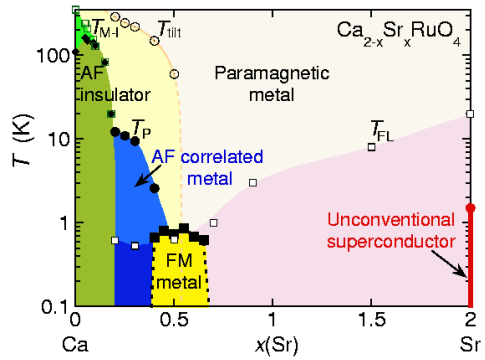
- **manganites**
- **high-T_c superconductors**
- **ruthenates**
- **cobaltates**
- **organic salts**
- **heavy fermions**
- **iron pnictides**

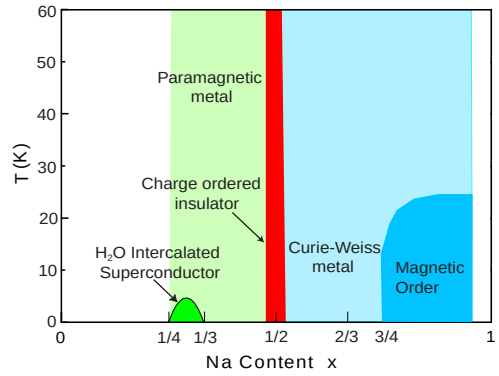
:

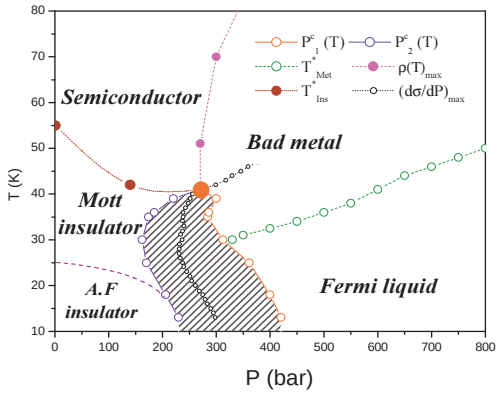
mportant for basic understanding nd future technical applications

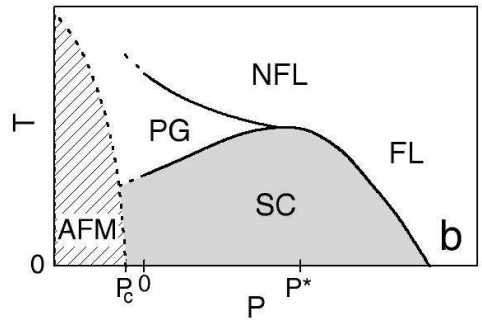












[E. Dagotto, Science 309 (2005)]

Well, lets start from scratch ...

-relativistic Hamiltonian for the Solid State:

$$\mathcal{H} = -\sum_{\alpha}^{N_{\mathrm{K}}} \frac{\hbar^2 \Delta_\alpha}{2M_\alpha} + \frac{1}{2} \sum_{\substack{\alpha\alpha' \\ \alpha\neq\alpha'}} \frac{Z_\alpha Z_{\alpha'} e^2}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|} \qquad (=: \mathcal{T}_{\mathrm{K}} + \mathcal{V}_{\mathrm{KK}} =: \mathcal{H}_{\mathrm{K}})$$

$$-\sum_{\alpha\mu} \frac{Z_\alpha e^2}{|\mathbf{R}_\alpha - \mathbf{r}_\mu|} \qquad (=: \mathcal{V}_{\mathrm{Ke}})$$

$$-\sum_{\mu}^{N_{\mathrm{e}}} \frac{\hbar^2 \Delta_\mu}{2m} + \frac{1}{2} \sum_{\substack{\mu\mu' \\ \mu\neq\mu'}} \frac{e^2}{|\mathbf{r}_\mu - \mathbf{r}_{\mu'}|} \qquad (=: \mathcal{T}_{\mathrm{e}} + \mathcal{V}_{\mathrm{ee}} =: \mathcal{H}_{\mathrm{e}})$$

esides being extremely heavy ($\mathbf{N}_{\mathrm{K}}, \mathbf{N}_{\mathrm{e}} \sim \mathbf{10^{23}}$), intriguing coupling of lattice and electronic degrees of freedom !

Well, lets start from scratch ...

-relativistic Hamiltonian for the Solid State:

$$\mathcal{H} = -\sum_{\alpha}^{N_\mathrm{K}} \frac{\hbar^2 \Delta_\alpha}{2M_\alpha} + \frac{1}{2} \sum_{\substack{\alpha\alpha' \\ \alpha\neq\alpha'}} \frac{Z_\alpha Z_{\alpha'} e^2}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|} \qquad (=: \mathcal{T}_\mathrm{K} + \mathcal{V}_\mathrm{KK} =: \mathcal{H}_\mathrm{K})$$

$$-\sum_{\alpha\mu} \frac{Z_\alpha e^2}{|\mathbf{R}_\alpha - \mathbf{r}_\mu|} \qquad (=: \mathcal{V}_\mathrm{Ke})$$

$$-\sum_{\mu}^{N_\mathrm{e}} \frac{\hbar^2 \Delta_\mu}{2m} + \frac{1}{2} \sum_{\substack{\mu\mu' \\ \mu\neq\mu'}} \frac{e^2}{|\mathbf{r}_\mu - \mathbf{r}_{\mu'}|} \qquad (=: \mathcal{T}_\mathrm{e} + \mathcal{V}_\mathrm{ee} =: \mathcal{H}_\mathrm{e})$$

esides being extremely heavy ($\mathbf{N}_\mathrm{K}, \mathbf{N}_\mathrm{e} \sim \mathbf{10^{23}}$), intriguing coupling of lattice and electronic degrees of freedom !

→ Born-Oppenheimer approximation Decoupling nuclei and electrons

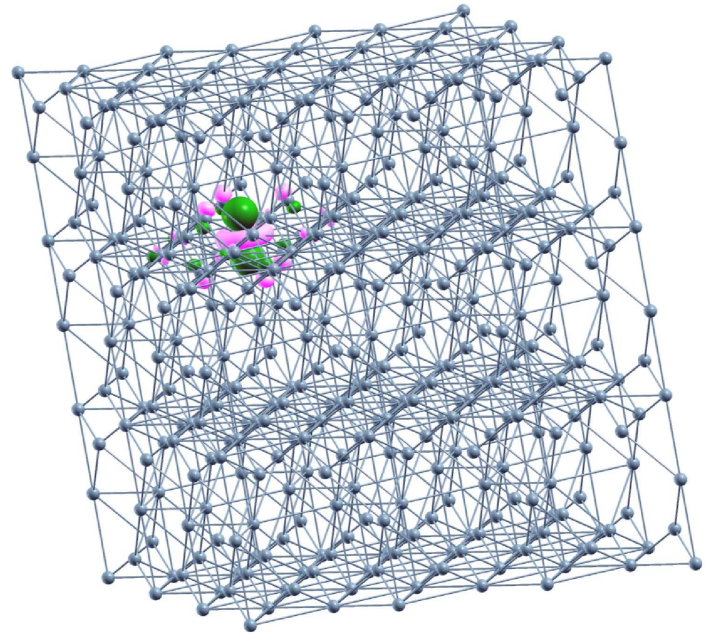
$$H_\mathrm{e} = H_\mathrm{e}(\{\mathbf{R}\}) := \mathcal{H}_\mathrm{e} + \mathcal{V}_\mathrm{Ke}$$

Electrons on the Lattice

tronic Hamiltonian in Second Quantization:

$$H_{\rm e} = -\sum_{\alpha\beta ab\sigma} \mathbf{t}^{\mathbf{L_a L_b}}_{\mathbf{R}_\alpha \mathbf{R}_\beta}\, c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c_{\mathbf{R}_\beta L_b \sigma}$$

$$+\frac{1}{2}\sum_{\substack{\alpha\beta\gamma\delta \\ abcd\sigma\sigma'}} \mathbf{V_{ee}}(\{\mathbf{R},\mathbf{L}\})\, c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c^\dagger_{\mathbf{R}_\beta L_b \sigma'} c_{\mathbf{R}_\delta L_d \sigma'} c_{\mathbf{R}_\gamma L_c \sigma}$$



xed lattice $\mathbf{R}$, orbitals L , spin-projection σ,
ectron creation/annihilation operator $c^{(\dagger)}_{\mathbf{R}L\sigma}$

hopping amplitude $\mathbf{t}^{\mathbf{L_1 L_2}}_{\mathbf{ij}} = \int d\mathbf{r}\, w^*_{iL_1}(\mathbf{r}) \left\{ \frac{\hbar^2 \Delta}{2m} - v(\mathbf{r}) \right\} w_{jL_2}(\mathbf{r})$

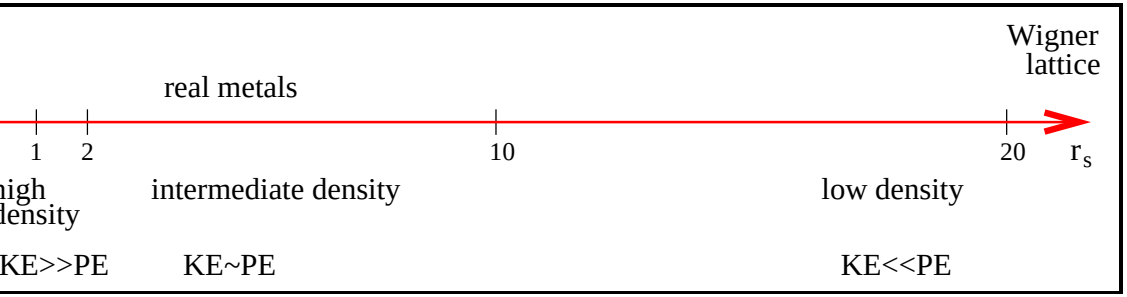
Coulomb interaction $\mathbf{V_{ee}}(\{\mathbf{R},\mathbf{L}\}) = e^2 \int d\mathbf{r} d\mathbf{r}'\, \frac{w^*_{iL_1\sigma}(\mathbf{r})\, w^*_{jL_2\sigma'}(\mathbf{r}')\, w_{kL_3\sigma'}(\mathbf{r}')\, w_{lL_4\sigma}(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}$

$_{\mathbf{R}L}(\mathbf{r}) := w_L(\mathbf{r}-\mathbf{R})$: **Wannier function**

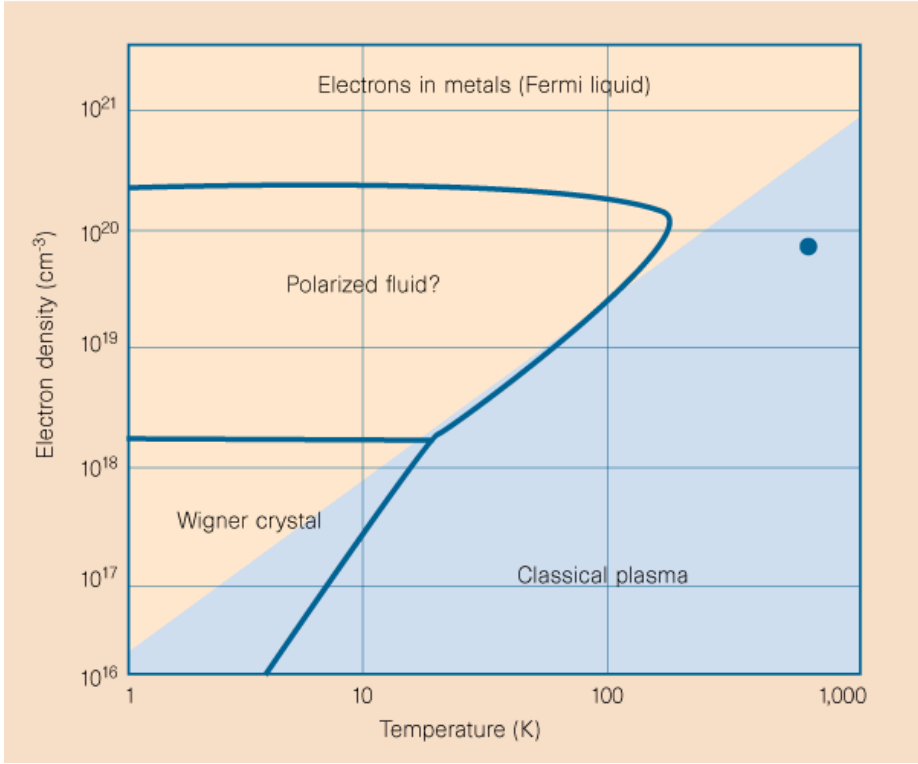
(→ presentation by J. Kunes)

The Big Problem

ow do we go from the manageable homogeneous electron gas ...



om [R.D. Mattuck: A Guide to Feynman Diagrams, McGraw-Hill (1976)]



to the notoriously complex inhomogeneous, realistic electron gas:

- density functional theory (LDA, GGA, . . .) *(→ presentation by P. Blöchl)*
- quantum chemistry (CI, CC, MP, . . .)

⋮

The Lesson

Because of the complexity of the interacting problem in condensed matter (i.e. exponential grow of the Hilbert space in a complicated potential landscape), simplified model Hamiltonians are needed to get access to the essential physics !

Introduction to the single-band Hubbard model

Theory Reminder: Green's Functions

ensity Functional Theory (LDA, GGA, SIC, OEP, . . .) : (ground-state) electronic charge density $n(\mathbf{r})$

uantum Chemistry (CI, CC, MP, . . .) : many-particle wave function $|\Psi\rangle$ *(landlord view)*

Theory Reminder: Green's Functions

ensity Functional Theory (LDA, GGA, SIC, OEP, . . .)	:	(ground-state) electronic charge density $n(\mathbf{r})$
uantum Chemistry (CI, CC, MP, . . .)	:	many-particle wave function $\vert\Psi\rangle$ *(landlord view)*
Solid-State Many-Body Formalism	:	**Green's functions (propagators)**

ne-particle Green's function: **"collecting events in the life of an electron"***(tenant view)*

$$G(\mathbf{k},t) = -i\,\langle\Psi_0|\mathcal{T}\,c_{\mathbf{k}}(t)c^{\dagger}_{\mathbf{k}}(0)|\Psi_0\rangle \quad \overset{t\gtrless 0}{\Rightarrow} \quad \text{free electrons with dispersion } \varepsilon_{\mathbf{k}} \quad \begin{cases} G_0(\mathbf{k},t) = -i\,\Theta_{\varepsilon_{\mathbf{k}}-\varepsilon_{\mathrm{F}}}\,\Theta_t\,e^{-i\varepsilon_{\mathbf{k}}t} \\ \mathbf{G_0}(\mathbf{k},\omega) = \frac{1}{\omega-\varepsilon_{\mathbf{k}}+\mathbf{i}\delta} \end{cases}$$

Theory Reminder: Green's Functions

ensity Functional Theory (LDA, GGA, SIC, OEP, . . .)	:	(ground-state) electronic charge density $n(\mathbf{r})$
uantum Chemistry (CI, CC, MP, . . .)	:	many-particle wave function $\|\Psi\rangle$ *(landlord view)*
Solid-State Many-Body Formalism	:	**Green's functions (propagators)**

ne-particle Green's function: **"collecting events in the life of an electron"***(tenant view)*

$$G(\mathbf{k},t) = -i\,\langle\Psi_0|\mathcal{T}\,c_{\mathbf{k}}(t)c^{\dagger}_{\mathbf{k}}(0)|\Psi_0\rangle \quad \overset{\substack{t\gtrless 0\\ \Rightarrow\\ \text{free electrons}\\ \text{with dispersion } \varepsilon_{\mathbf{k}}}}{} \quad \begin{cases} G_0(\mathbf{k},t) = -i\,\Theta_{\varepsilon_{\mathbf{k}}-\varepsilon_{\mathrm{F}}}\,\Theta_t\,e^{-i\varepsilon_{\mathbf{k}}t} \\ \mathbf{G_0(k,\omega) = \frac{1}{\omega-\varepsilon_{\mathbf{k}}+i\delta}} \end{cases}$$

$$\begin{aligned} \mathbf{G}(\mathbf{k},\omega) &= G_0 + G_0\Sigma G = G_0 + G_0\Sigma G_0 + G_0\Sigma G_0\Sigma G_0 + \cdots = G_0(1 + G_0\Sigma + G_0^2\Sigma^2 + \cdots) \\ &= G_0\frac{1}{1-G_0\Sigma} = \frac{1}{G_0^{-1}-\Sigma} = \frac{\mathbf{1}}{\omega - \varepsilon_{\mathbf{k}} - \mathbf{\Sigma}(\mathbf{k},\omega)} \quad , \qquad \mathbf{\Sigma}(\mathbf{k},\omega) \text{ : self-energy} \end{aligned}$$

Theory Reminder: Green's Functions

ensity Functional Theory (LDA, GGA, SIC, OEP, . . .)	:	(ground-state) electronic charge density $n(\mathbf{r})$
uantum Chemistry (CI, CC, MP, . . .)	:	many-particle wave function $\vert\Psi\rangle$ *(landlord view)*
Solid-State Many-Body Formalism	:	**Green's functions (propagators)**

ne-particle Green's function: **"collecting events in the life of an electron"** *(tenant view)*

$$G(\mathbf{k},t) = -i\,\langle\Psi_0|\mathcal{T}\,c_{\mathbf{k}}(t)c^{\dagger}_{\mathbf{k}}(0)|\Psi_0\rangle \quad \overset{\substack{t\gtrless 0\\ \Rightarrow\\ \text{free electrons}\\ \text{with dispersion } \varepsilon_{\mathbf{k}}}}{} \quad \begin{cases} G_0(\mathbf{k},t) = -i\,\Theta_{\varepsilon_{\mathbf{k}}-\varepsilon_{\mathrm{F}}}\,\Theta_t\,e^{-i\varepsilon_{\mathbf{k}}t} \\ \mathbf{G_0}(\mathbf{k},\omega) = \frac{1}{\omega-\varepsilon_{\mathbf{k}}+\mathbf{i}\delta} \end{cases}$$

$$\begin{aligned} \mathbf{G}(\mathbf{k},\omega) &= G_0 + G_0\Sigma G = G_0 + G_0\Sigma G_0 + G_0\Sigma G_0\Sigma G_0 + \cdots = G_0(1 + G_0\Sigma + G_0^2\Sigma^2 + \cdots) \\ &= G_0\frac{1}{1-G_0\Sigma} = \frac{1}{G_0^{-1}-\Sigma} = \frac{\mathbf{1}}{\omega - \varepsilon_{\mathbf{k}} - \mathbf{\Sigma}(\mathbf{k},\omega)} \quad , \qquad \mathbf{\Sigma}(\mathbf{k},\omega) \text{ : self-energy} \end{aligned}$$

pectral function: **"reading out the energy dependence"**

$$A(\mathbf{k},\omega) = \begin{cases} A^{+}(\mathbf{k},\omega) = \sum_m |\langle\Psi_m^{(N_\mathrm{e}+1)}|c^{\dagger}_{\mathbf{k}}|\Psi_0\rangle|^2\,\delta(\omega-\omega_{m0}) & \text{for } \omega \geq 0 \\ A^{-}(\mathbf{k},\omega) = \sum_m |\langle\Psi_m^{(N_\mathrm{e}-1)}|c_{\mathbf{k}}|\Psi_0\rangle|^2\,\delta(\omega-\omega_{0m}) & \text{for } \omega < 0 \end{cases}$$

k-summed version: $\rho(\omega) = \sum_{\mathbf{k}} A(\mathbf{k},\omega)$

Chopping off hoppings and interactions

rt from full electronic Hamiltonian on the lattice:

$$H_{\rm e} = -\sum_{\alpha\beta ab\sigma} t^{L_a L_b}_{\mathbf{R}_\alpha \mathbf{R}_\beta}\, c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c_{\mathbf{R}_\beta L_b \sigma} + \frac{1}{2} \sum_{\substack{\alpha\beta\gamma\delta \\ abcd\sigma\sigma'}} V_{ee}(\{\mathbf{R}, L\})\, c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c^\dagger_{\mathbf{R}_\beta L_b \sigma'} c_{\mathbf{R}_\delta L_d \sigma'} c_{\mathbf{R}_\gamma L_c \sigma}$$

$\rightarrow$ **1. Approximation:** only single orbital with nearest-neighbor (NN) hopping

$$H'_{\rm e} = -\sum_{\langle\alpha\beta\rangle\sigma} t_{\mathbf{R}_\alpha \mathbf{R}_\beta}\, c^\dagger_{\mathbf{R}_\alpha \sigma} c_{\mathbf{R}_\beta \sigma} + \frac{1}{2} \sum_{\substack{\alpha\beta\gamma\delta \\ \sigma\sigma'}} V_{ee}(\{\mathbf{R}\})\, c^\dagger_{\mathbf{R}_\alpha \sigma} c^\dagger_{\mathbf{R}_\beta \sigma'} c_{\mathbf{R}_\delta \sigma'} c_{\mathbf{R}_\gamma \sigma}$$

$\rightarrow$ **2. Approximation:** keep only local Coulomb interaction $V_{ee}(\mathbf{R}_\alpha, \mathbf{R}_\alpha, \mathbf{R}_\alpha, \mathbf{R}_\alpha)$

$$H''_{\rm e} = -\sum_{\langle\alpha\beta\rangle\sigma} t_{\mathbf{R}_\alpha \mathbf{R}_\beta}\, c^\dagger_{\mathbf{R}_\alpha \sigma} c_{\mathbf{R}_\beta \sigma} + \frac{1}{2} \sum_{\alpha\sigma\sigma'} V_{ee}(\mathbf{R}_\alpha, \mathbf{R}_\alpha, \mathbf{R}_\alpha, \mathbf{R}_\alpha)\, c^\dagger_{\mathbf{R}_\alpha \sigma} c^\dagger_{\mathbf{R}_\alpha \sigma'} c_{\mathbf{R}_\alpha \sigma'} c_{\mathbf{R}_\alpha \sigma}$$

Chopping off hoppings and interactions

rt from full electronic Hamiltonian on the lattice:

$$H_{\rm e} = -\sum_{\alpha\beta ab\sigma} t^{L_a L_b}_{\mathbf{R}_\alpha \mathbf{R}_\beta}\, c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c_{\mathbf{R}_\beta L_b \sigma} + \frac{1}{2} \sum_{\substack{\alpha\beta\gamma\delta \\ abcd\sigma\sigma'}} V_{ee}(\{\mathbf{R}, L\})\, c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c^\dagger_{\mathbf{R}_\beta L_b \sigma'} c_{\mathbf{R}_\delta L_d \sigma'} c_{\mathbf{R}_\gamma L_c \sigma}$$

$\rightarrow$ **1. Approximation:** only single orbital with nearest-neighbor (NN) hopping

$$H'_{\rm e} = -\sum_{\langle\alpha\beta\rangle\sigma} t_{\mathbf{R}_\alpha \mathbf{R}_\beta}\, c^\dagger_{\mathbf{R}_\alpha \sigma} c_{\mathbf{R}_\beta \sigma} + \frac{1}{2} \sum_{\substack{\alpha\beta\gamma\delta \\ \sigma\sigma'}} V_{ee}(\{\mathbf{R}\})\, c^\dagger_{\mathbf{R}_\alpha \sigma} c^\dagger_{\mathbf{R}_\beta \sigma'} c_{\mathbf{R}_\delta \sigma'} c_{\mathbf{R}_\gamma \sigma}$$

$\rightarrow$ **2. Approximation:** keep only local Coulomb interaction $V_{ee}(\mathbf{R}_\alpha, \mathbf{R}_\alpha, \mathbf{R}_\alpha, \mathbf{R}_\alpha)$

$$H''_{\rm e} = -\sum_{\langle\alpha\beta\rangle\sigma} t_{\mathbf{R}_\alpha \mathbf{R}_\beta}\, c^\dagger_{\mathbf{R}_\alpha \sigma} c_{\mathbf{R}_\beta \sigma} + \frac{1}{2} \sum_{\alpha\sigma\sigma'} V_{ee}(\mathbf{R}_\alpha, \mathbf{R}_\alpha, \mathbf{R}_\alpha, \mathbf{R}_\alpha)\, c^\dagger_{\mathbf{R}_\alpha \sigma} c^\dagger_{\mathbf{R}_\alpha \sigma'} c_{\mathbf{R}_\alpha \sigma'} c_{\mathbf{R}_\alpha \sigma}$$

mplify notation: $\mathbf{R}_\alpha, \mathbf{R}_\beta \rightarrow i, j \quad , \quad t_{ij} =: t \quad , \quad V_{ee}(i,i,i,i) =: U \quad , \quad n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$

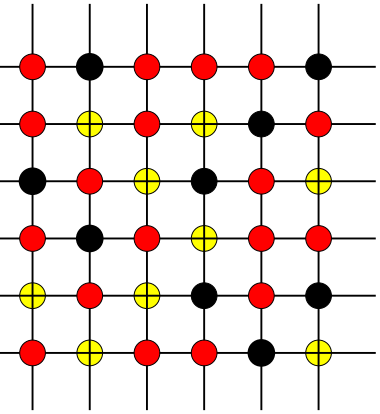
$\Rightarrow$ Hubbard model: $$H_{\rm hub} = -\mathbf{t} \sum_{\langle ij\rangle\sigma} c^\dagger_{i\sigma} c_{j\sigma} + \mathbf{U} \sum_i n_{i\uparrow} n_{i\downarrow}$$

[J. Hubbard, Proc. Royal Soc. London A 276, 238 (1963)]

Itinerancy versus Localization

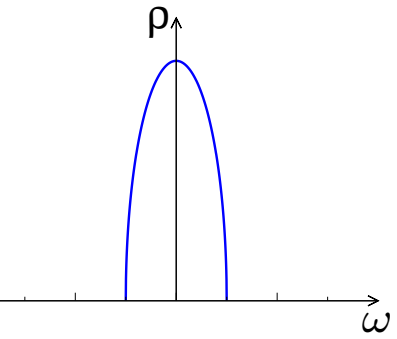
Hubbard model: $H_{\rm hub} = -\mathbf{t} \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + \mathbf{U} \sum_i n_{i\uparrow} n_{i\downarrow}$, for filling $n = 1$ (half filling)

oninteracting limit $(U = 0)$



occupation
- empty
- single
- double

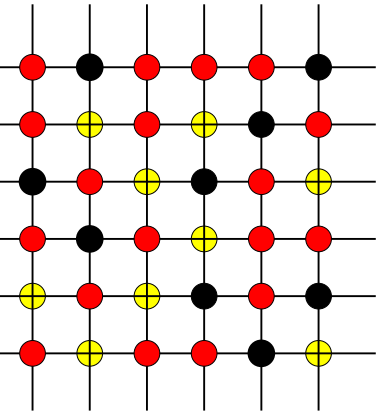
- $H_{\rm hub} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$
- ideal metal, Fermi gas



Itinerancy versus Localization

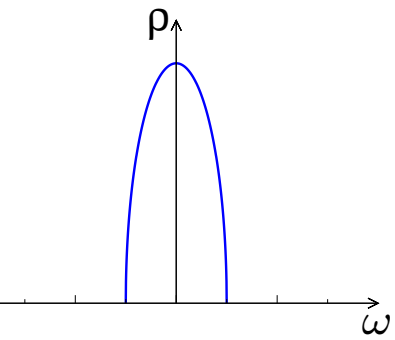
Hubbard model: $H_{\rm hub} = -\mathbf{t} \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + \mathbf{U} \sum_i n_{i\uparrow} n_{i\downarrow}$, for filling $n = 1$ (half filling)

noninteracting limit $(U = 0)$

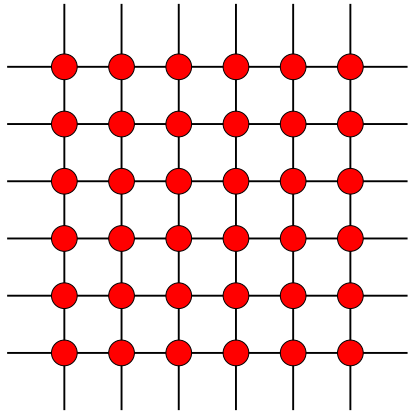


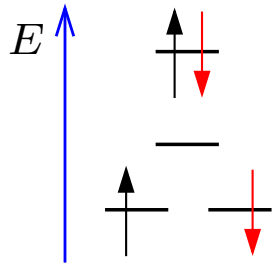
occupation
- empty
- single
- double

- $H_{\rm hub} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$
- ideal metal, Fermi gas



atomic limit $(t = 0)$



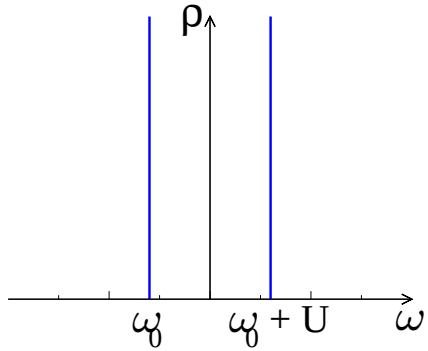


$|\psi_d\rangle$, $2\varepsilon_0 + U$

$|\psi_e\rangle$, 0

$|\psi_\sigma\rangle$, ε_0

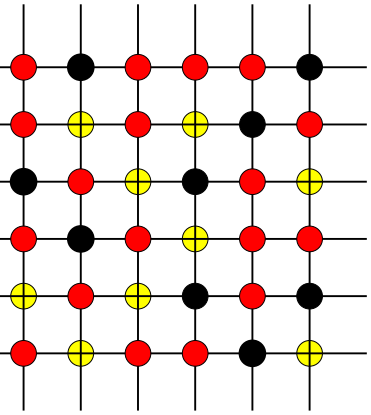
- disconnected sites
- only single-occupied sites populated in ground state



Itinerancy versus Localization

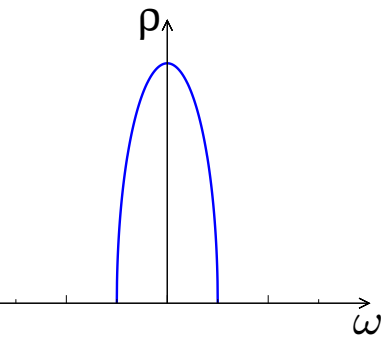
Hubbard model: $H_{\rm hub} = -\mathbf{t} \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + \mathbf{U} \sum_i n_{i\uparrow} n_{i\downarrow}$, for filling $n = 1$ (half filling)

oninteracting limit $(U = 0)$

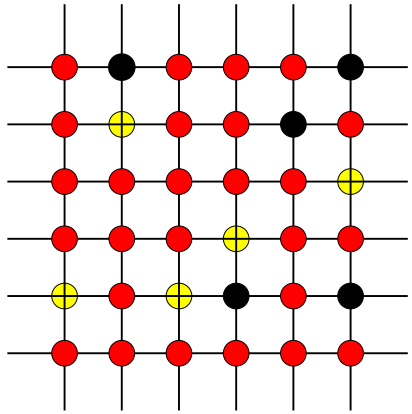


$H_{\rm hub} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$

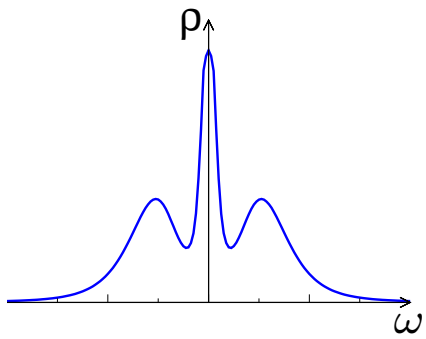
ideal metal, Fermi gas



intermediate $(U \sim t)$

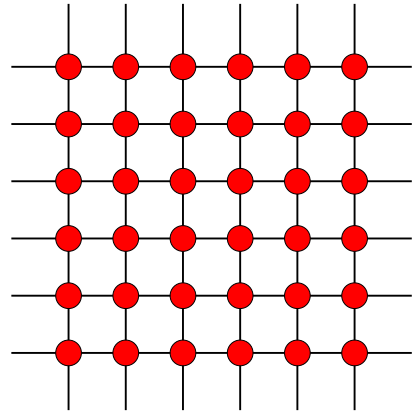


– correlated metal
– dominant population of single-occupied sites

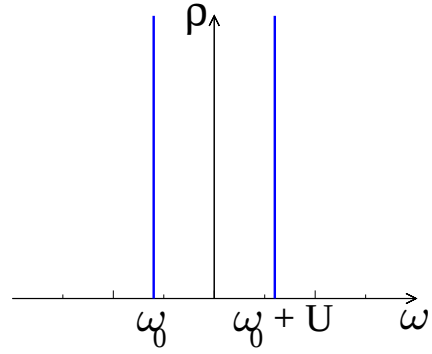


"Three-Peak Structure"

atomic limit $(t = 0)$



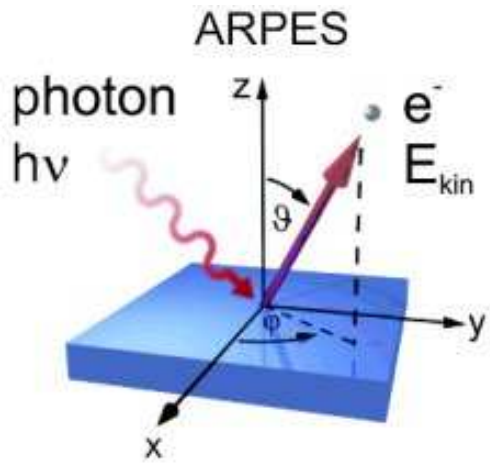
– disconnected sites
– only single-occupied sites populated in ground state

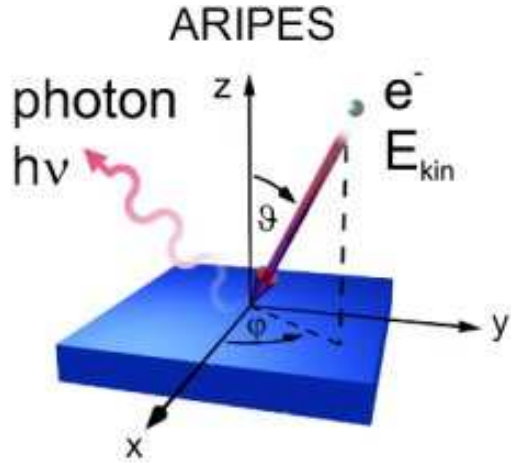


Spectral Function $A(\mathbf{k}, \omega)$

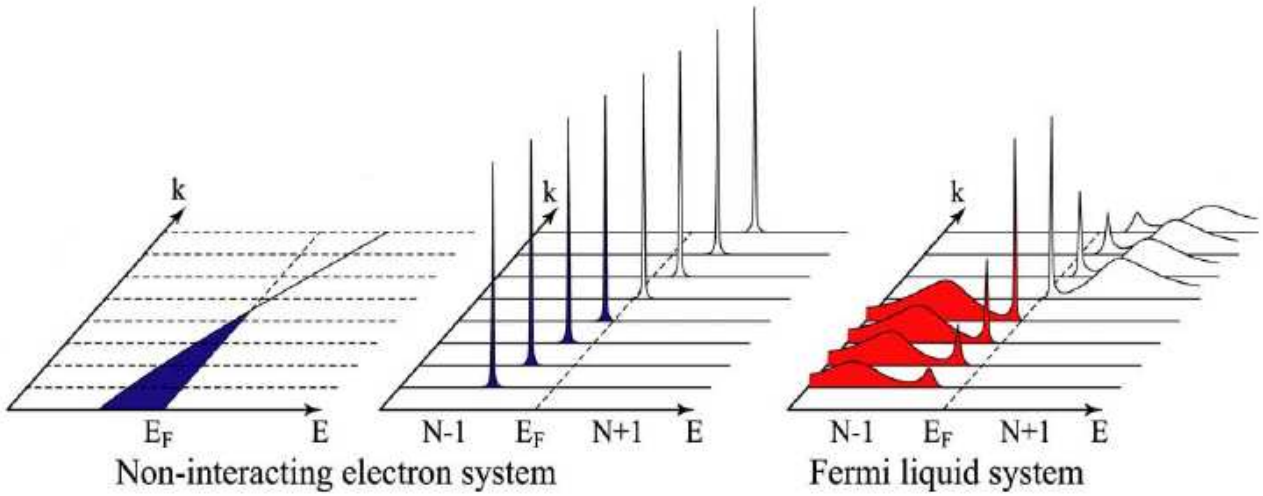
he spectral function $A(\mathbf{k}, \omega)$ is of cen-
al interest and can be interpreted
s the many-particle generalization of
e band-structure and density-of-states
oncept for a solid. Measured by:

ngle-resolved (inverse) photoemission.





$A(\mathbf{k}, \omega)$ with and without interactions:



Correlated condensed matter

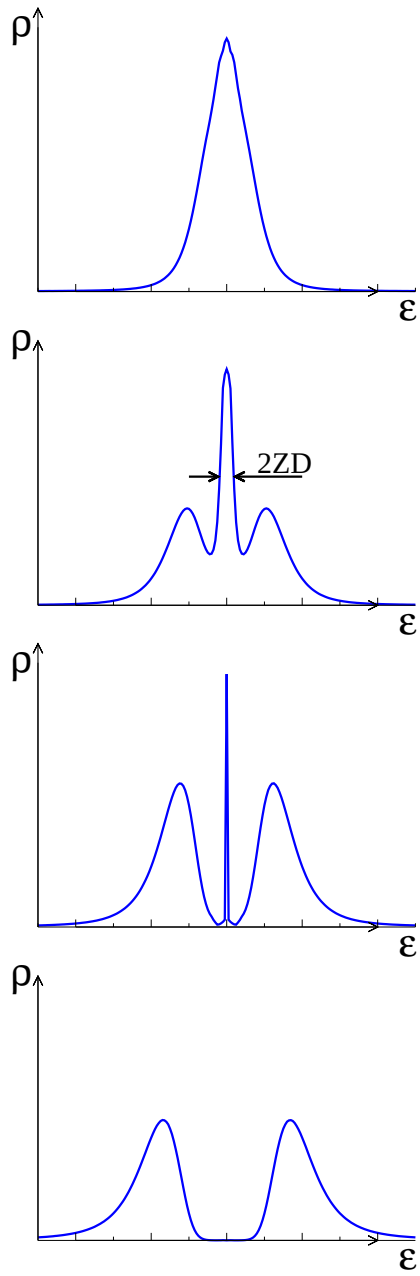
- $\mathbf{k}$ is not always a good quantum number
- finite lifetime of states away from Fermi level
- band-narrowing close to Fermi level
- filling of states affects the **whole** spectrum

Main Excitations

n strongly correlated solids there are in principle
wo dominant types of excitations:

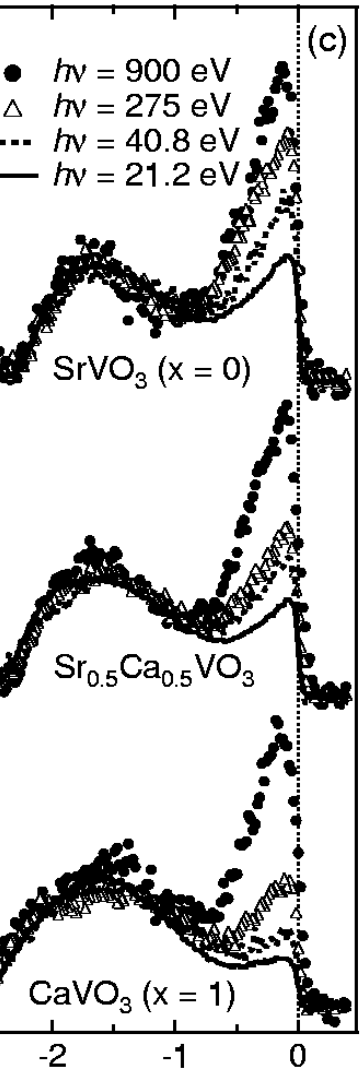
- **low-energy (coherent) quasiparticles with well-defined wave vector**
  - energy shift from the noninteracting eigenvalue
  - exist on a long but still finite timescale
  - band narrowing by $ZD \sim \varepsilon_F^\star$
  - will be destroyed at high temperature
- **high-energy (incoherent) atomic-like excitations**
  - form Hubbard bands around atomic levels
  - exist on a short time scale
  - lower and upper Hubbard band are separated by U
  - Mott insulating state for small t/U

$\Rightarrow$ **Theory has to describe the interplay of different energy scales !**



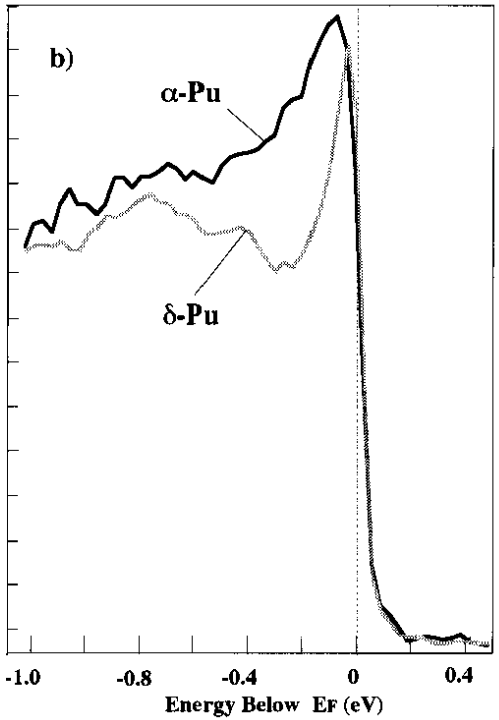
Experimental Evidence

$Sr/CaVO_3$

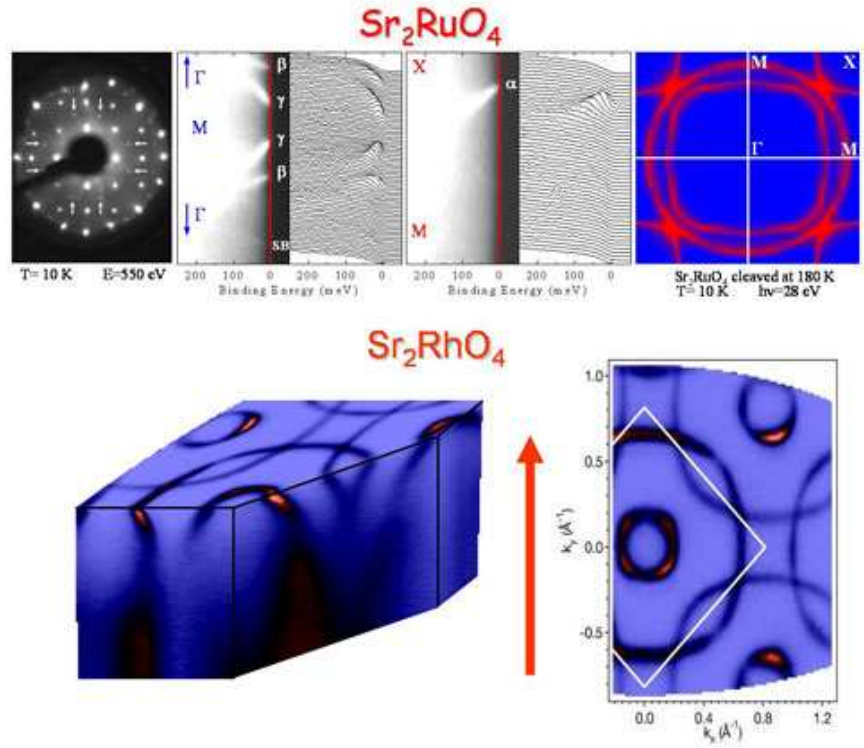


ekiyama et al. PRL 93 (2004)]

α- and δ-Pu



[Arko et al. PRB bf 62 (2000)]



[Shen group, Standford]

Some properties of the Hubbard model

- parameters: t, U (filling n, lattice type)
- spin-rotational invariant
- analytically exact solvable in one dimension and numerically exact in infinite dimensions
- $U = 0$: Fermi gas, t=0: atomic limit
- limit $U/t \gg 1$: perturbation approach in t/U
  - half filling: Hubbard model $\rightarrow$ antiferromagnetic quantum Heisenberg model

$$H_{\mathrm{heis}} = \frac{2t^2}{U} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S_j}$$

  - doped case: Hubbard model $\rightarrow$ t-J model

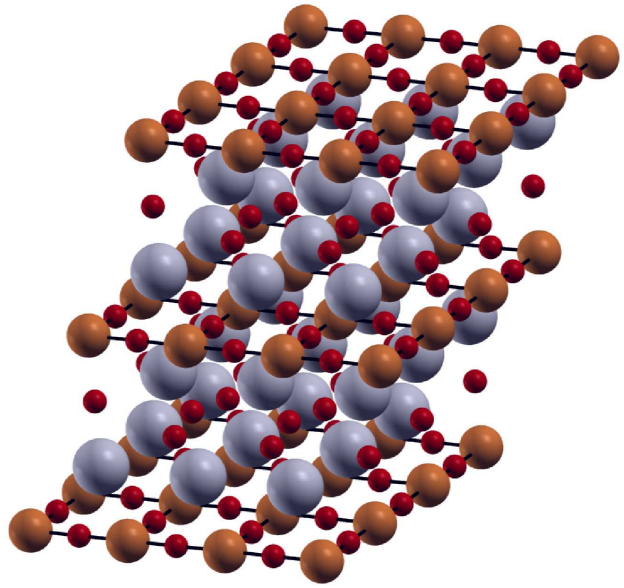
$$H_{\mathrm{tj}} = P \left[-t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} - \frac{t^2}{U} \sum_{\langle ijk \rangle} \left(c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} - c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} \right) \left(c_{j\downarrow} c_{k\uparrow} - c_{j\uparrow} c_{k\downarrow} \right) \right] P$$

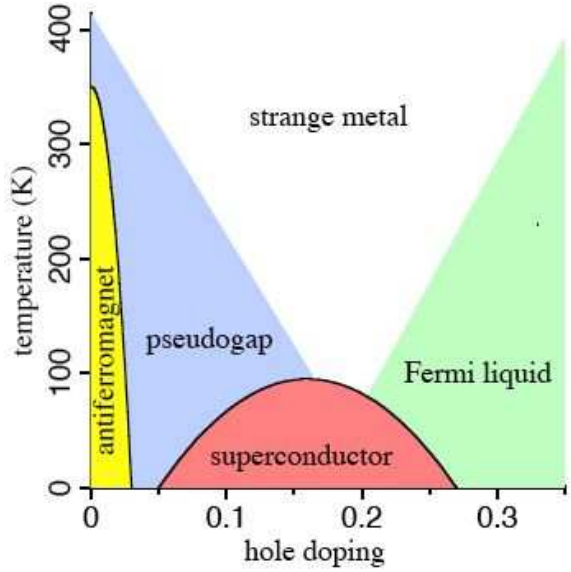
- Mott transition at half filling for larger U/t : complete breakdown of Bloch picture !

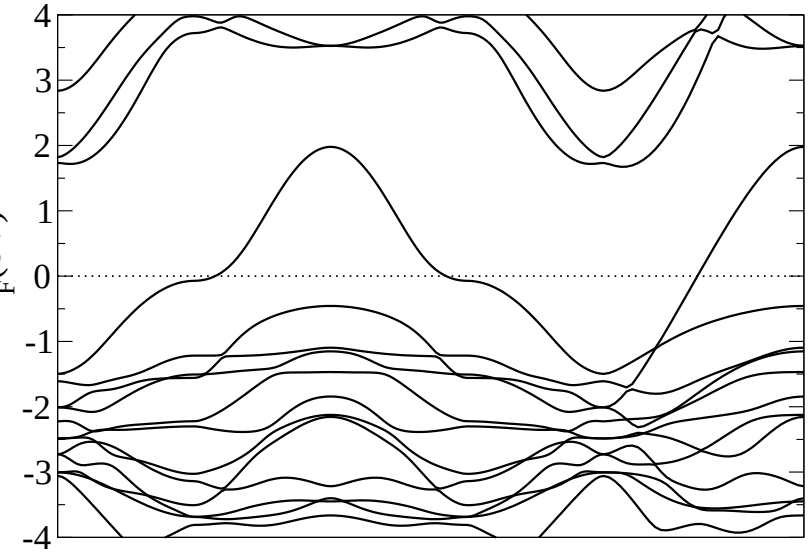
ometimes single-band may indeed be ok ...

High-Temperature

Cuprate Superconductors:



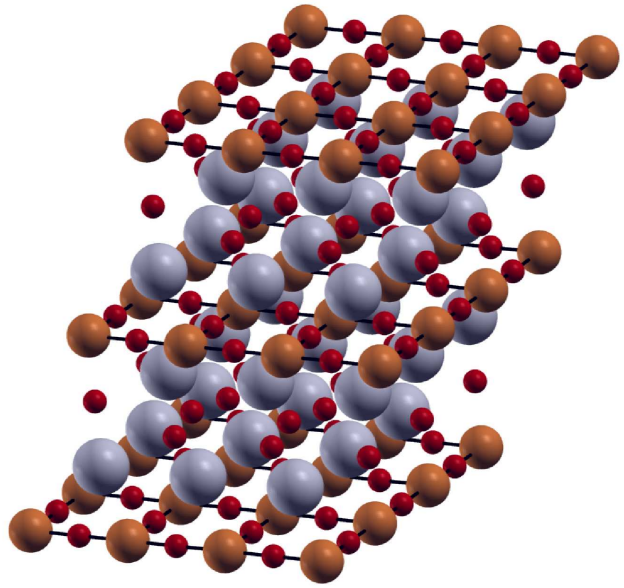


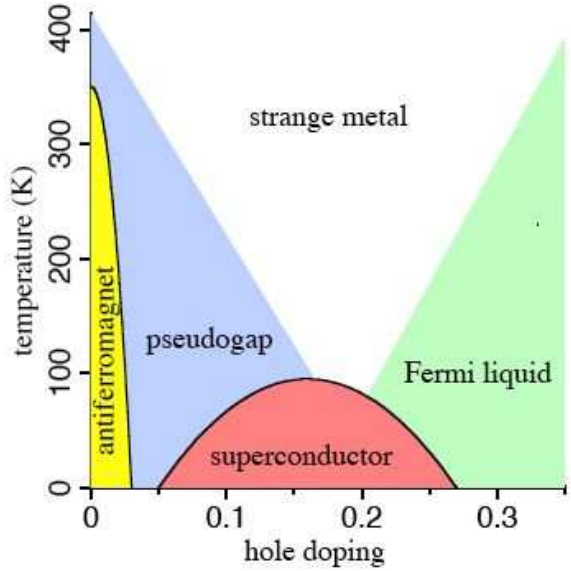


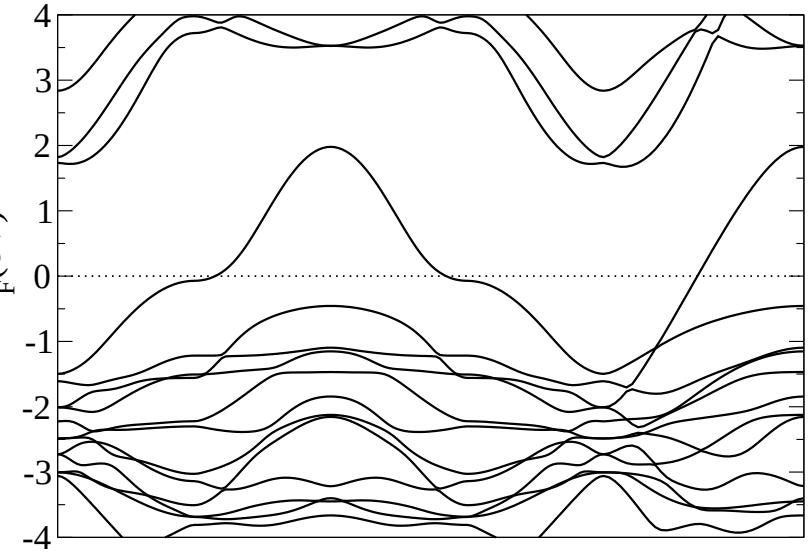
ometimes single-band may indeed be ok ...

High-Temperature

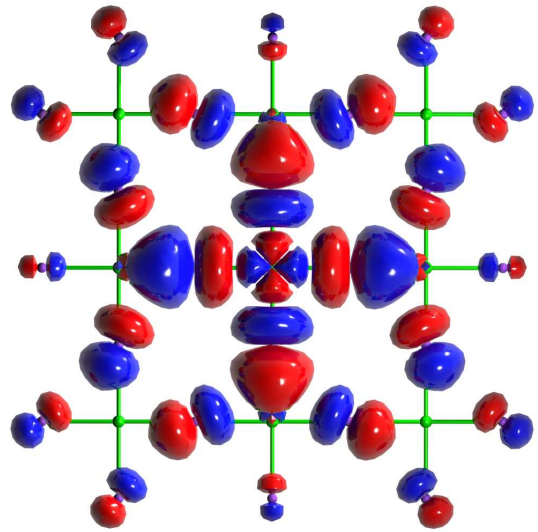
Cuprate Superconductors:







$\Rightarrow$



However ...

Wannier function for the band at the Fermi level with strong Cu$(3d_{x^2-y^2})$ character

[O. K. Andersen et al.]

Multi-orbital Hubbard models

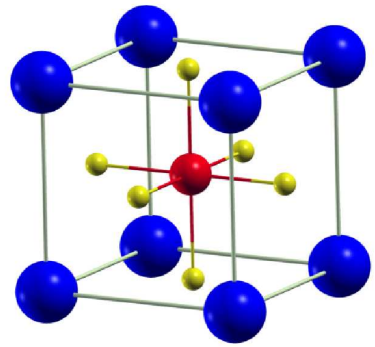
Atoms on the Lattice: Crystal Field

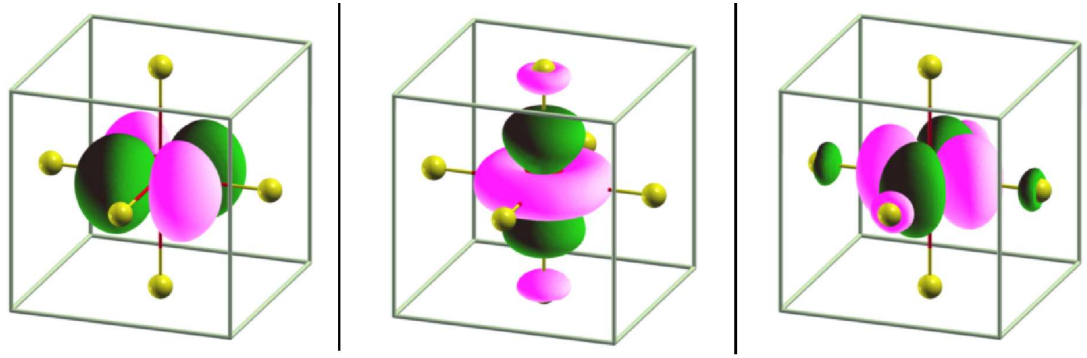
ingle-Band modeling often insufficient, since usually several bands live at low energy ...

. how can one decide which bands/orbitals to consider ?

example:

atom with correlated $3d$ shell in cubic structure

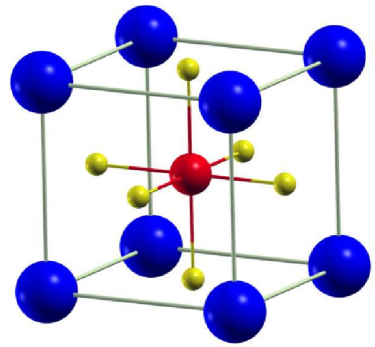




Atoms on the Lattice: Crystal Field

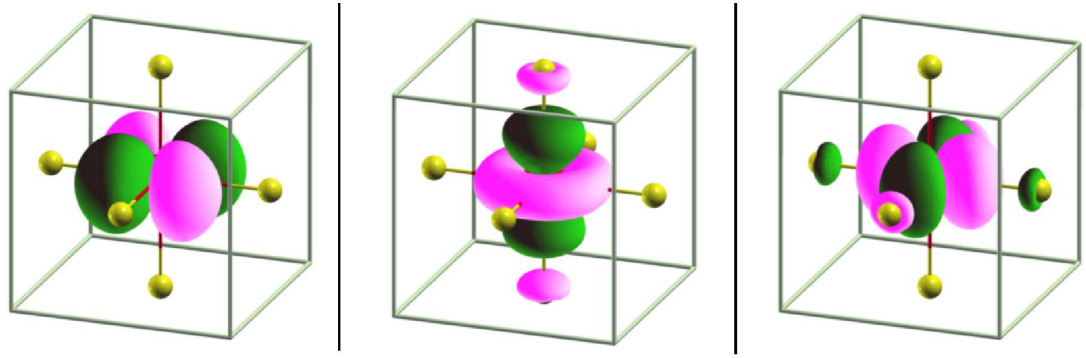
ingle-Band modeling often insufficient, since usually several bands live at low energy ...

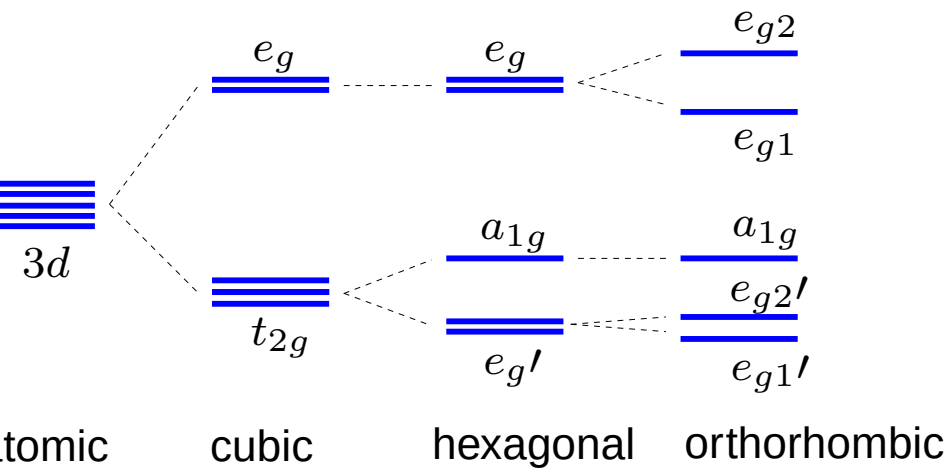
. how can one decide which bands/orbitals to consider ?



example:

atom with correlated $3d$ shell in cubic structure





atomare Zustände spalten anhand der Punktgruppe des Kristalls energetisch auf, dadurch reduzieren sich viele realistische Probleme auf einen orbitalen Unterraum

(e_g,t_{2g}) generalized Hubbard Hamiltonian

rt again from full electronic Hamiltonian on the lattice:

$$H_{\rm e} = -\sum_{\alpha\beta ab\sigma} t^{L_a L_b}_{\mathbf{R}_\alpha \mathbf{R}_\beta}\, c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c_{\mathbf{R}_\beta L_b \sigma} + \frac{1}{2} \sum_{\substack{\alpha\beta\gamma\delta \\ abcd\sigma\sigma'}} V_{ee}(\{\mathbf{R}, L\})\, c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c^\dagger_{\mathbf{R}_\beta L_b \sigma'} c_{\mathbf{R}_\delta L_d \sigma'} c_{\mathbf{R}_\gamma L_c \sigma}$$

$\rightarrow$ **Approximation:** keep two/three orbitals with local rotationally invariant Coulomb interactions

otation: $\mathbf{R}_\alpha, \mathbf{R}_\beta \rightarrow i, j \quad , \quad a, b \rightarrow m, m' \quad , \quad n_{im\sigma} = c^\dagger_{im\sigma} c_{im\sigma}$

$$H_{\rm cub} = \sum_{ijmm'\sigma} t^{mm'}_{ij}\, c^\dagger_{im\sigma} c_{jm'\sigma} + U \sum_{im} n_{im\uparrow} n_{im\downarrow} + \frac{1}{2} \sum_{i, m\neq m', \sigma} \left[U'\, n_{im\sigma} n_{im'\bar{\sigma}} + U''\, n_{im\sigma} n_{im'\sigma} \right]$$
$$+ \frac{1}{2} \sum_{m\neq m', \sigma} \left[J\, c^\dagger_{im\sigma} c^\dagger_{im'\bar{\sigma}} c_{im\bar{\sigma}} c_{im'\sigma} + J_{\rm C}\, c^\dagger_{im\sigma} c^\dagger_{im\bar{\sigma}} c_{im'\bar{\sigma}} c_{im'\sigma} \right]$$

(e_g,t_{2g}) generalized Hubbard Hamiltonian

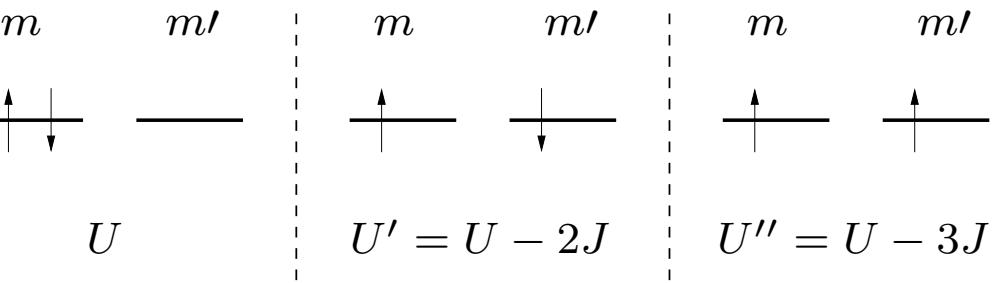
rt again from full electronic Hamiltonian on the lattice:

$$H_{\rm e} = -\sum_{\alpha\beta ab\sigma} t^{L_a L_b}_{\mathbf{R}_\alpha \mathbf{R}_\beta}\, c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c_{\mathbf{R}_\beta L_b \sigma} + \frac{1}{2} \sum_{\substack{\alpha\beta\gamma\delta \\ abcd\sigma\sigma'}} V_{ee}(\{\mathbf{R}, L\})\, c^\dagger_{\mathbf{R}_\alpha L_a \sigma} c^\dagger_{\mathbf{R}_\beta L_b \sigma'} c_{\mathbf{R}_\delta L_d \sigma'} c_{\mathbf{R}_\gamma L_c \sigma}$$

$\rightarrow$ **Approximation:** keep two/three orbitals with local rotationally invariant Coulomb interactions

otation: $\mathbf{R}_\alpha, \mathbf{R}_\beta \rightarrow i, j \quad , \quad a, b \rightarrow m, m' \quad , \quad n_{im\sigma} = c^\dagger_{im\sigma} c_{im\sigma}$

$$H_{\rm cub} = \sum_{ijmm'\sigma} t^{mm'}_{ij}\, c^\dagger_{im\sigma} c_{jm'\sigma} + U \sum_{im} n_{im\uparrow} n_{im\downarrow} + \frac{1}{2} \sum_{i, m\neq m', \sigma} \left[U'\, n_{im\sigma} n_{im'\bar\sigma} + U''\, n_{im\sigma} n_{im'\sigma} \right]$$
$$+ \frac{1}{2} \sum_{m\neq m', \sigma} \left[J\, c^\dagger_{im\sigma} c^\dagger_{im'\bar\sigma} c_{im\bar\sigma} c_{im'\sigma} + J_{\rm C}\, c^\dagger_{im\sigma} c^\dagger_{im\bar\sigma} c_{im'\bar\sigma} c_{im'\sigma} \right]$$



establishing Hund's rule

full-shell Hubbard Hamiltonian

$$H_{\rm d} = \sum_{ijmm'\sigma} t_{ij}^{mm'} c_{im\sigma}^{\dagger} c_{jm'\sigma} + \frac{1}{2} \sum_{i,mm'm''m''',\sigma\sigma'} U_{mm'm''m'''} c_{im\sigma}^{\dagger} c_{im'\sigma'}^{\dagger} c_{im'''\sigma'} c_{im''\sigma}$$

$U_{mm'm''m'''}$ via Slater integrals F_k: $U_{mm'm''m'''} = \langle mm'|V_{ee}^{\rm loc}|m''m'''\rangle = \sum_{k=0} a_k(m,m',m'',m''')\, F_k$

→ **spherical approximation to the local Coulomb interaction**

Depending on angular-momentum quantum number l:

$$l = 1 \quad : \quad U = F_0 \ , \ J = \frac{1}{5} F_2 \quad ,$$

$$l = 2 \quad : \quad U = F_0 \ , \ J = \frac{1}{14}(F_2 + F_4) \ , \ F_4 = 0.625 F_2$$

$$l = 3 \quad : \quad U = F_0 \ , \ J = \frac{1}{6435}(286 F_2 + 195 F_4 + 250 F_6) \ , \ F_4 = 0.668 F_2 \ , \ F_6 = 0.494 F_2$$

full-shell Hubbard Hamiltonian

$$H_{\rm d} = \sum_{ijmm'\sigma} t_{ij}^{mm'} c_{im\sigma}^\dagger c_{jm'\sigma} + \frac{1}{2} \sum_{i,mm'm''m''',\sigma\sigma'} U_{mm'm''m'''} c_{im\sigma}^\dagger c_{im'\sigma'}^\dagger c_{im'''\sigma'} c_{im''\sigma}$$

$U_{mm'm''m'''}$ via Slater integrals F_k: $U_{mm'm''m'''} = \langle mm'|V_{ee}^{\rm loc}|m''m'''\rangle = \sum_{k=0} a_k(m,m',m'',m''')\, F_k$

→ **spherical approximation to the local Coulomb interaction**

Depending on angular-momentum quantum number l:

$$l=1 \quad : \quad U = F_0 \ , \ J = \frac{1}{5} F_2 \quad ,$$

$$l=2 \quad : \quad U = F_0 \ , \ J = \frac{1}{14}(F_2 + F_4) \ , \ F_4 = 0.625 F_2$$

$$l=3 \quad : \quad U = F_0 \ , \ J = \frac{1}{6435}(286F_2 + 195F_4 + 250F_6) \ , \ F_4 = 0.668F_2 \ , \ F_6 = 0.494F_2$$

Advances for realistic models, especially in the LDA+DMFT context:

- computing $U_{mm'm''m'''}(\omega)$ from first principles *(→ presentation by F. Aryasetiawan)*
- many-body technique to handle $U = U(\omega)$ *(→ presentation by P. Werner)*

Basic techniques
1. Hartree Fock

Mean-Field Approach

Hubbard model: $H_{\rm hub} = -\mathbf{t} \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + \mathbf{U} \sum_i n_{i\uparrow} n_{i\downarrow}$

ewrite particle-number operator: $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma} = \underbrace{\langle n_{i\sigma} \rangle}_{\text{expectation value}} + \underbrace{\delta n_{i\sigma}}_{\text{fluctuations}}$ **(decoupling ansatz)**

nteraction kernel: $n_{i\uparrow} n_{i\downarrow} = \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + \langle n_{i\downarrow} \rangle \delta n_{i\uparrow} + \langle n_{i\uparrow} \rangle \delta n_{i\downarrow} + \delta n_{i\uparrow} \delta n_{i\downarrow} =: A(n_{i\uparrow} n_{i\downarrow}) + \delta n_{i\uparrow} \delta n_{i\downarrow}$

approximation: neglecting $\delta n_{i\uparrow} \delta n_{i\downarrow}$

$$\Rightarrow \quad U \sum_i n_{i\uparrow} n_{i\downarrow} \approx U \sum_i A(n_{i\uparrow} n_{i\downarrow}) = U \sum_i \left(n_{i\uparrow} \langle n_{i\downarrow} \rangle + n_{i\downarrow} \langle n_{i\uparrow} \rangle - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \right)$$

→ **essence of mean-field theory on the atomistic level:** **neglect of the correlations of fluctuations !**

Mean-Field Approach

Hubbard model: $H_{\rm hub} = -\mathbf{t} \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + \mathbf{U} \sum_i n_{i\uparrow} n_{i\downarrow}$

ewrite particle-number operator: $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma} = \underbrace{\langle n_{i\sigma} \rangle}_{\text{expectation value}} + \underbrace{\delta n_{i\sigma}}_{\text{fluctuations}}$ **(decoupling ansatz)**

nteraction kernel: $n_{i\uparrow} n_{i\downarrow} = \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + \langle n_{i\downarrow} \rangle \delta n_{i\uparrow} + \langle n_{i\uparrow} \rangle \delta n_{i\downarrow} + \delta n_{i\uparrow} \delta n_{i\downarrow} =: A(n_{i\uparrow} n_{i\downarrow}) + \delta n_{i\uparrow} \delta n_{i\downarrow}$

approximation: neglecting $\delta n_{i\uparrow} \delta n_{i\downarrow}$

$$\Rightarrow \quad U \sum_i n_{i\uparrow} n_{i\downarrow} \approx U \sum_i A(n_{i\uparrow} n_{i\downarrow}) = U \sum_i \left(n_{i\uparrow} \langle n_{i\downarrow} \rangle + n_{i\downarrow} \langle n_{i\uparrow} \rangle - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \right)$$

→ **essence of mean-field theory on the atomistic level:** **neglect of the correlations of fluctuations !**

problem: decoupling of operators not unique in any case here rotational invariance is lost !

$$c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} = - c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{i\uparrow} c_{i\downarrow} \quad \overset{\text{Wick}}{\rightarrow} \quad - \langle c^\dagger_{i\uparrow} c_{i\downarrow} \rangle c^\dagger_{i\downarrow} c_{i\uparrow} - \langle c^\dagger_{i\downarrow} c_{i\uparrow} \rangle c^\dagger_{i\uparrow} c_{i\downarrow} + \langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle c^\dagger_{i\downarrow} c_{i\downarrow} + \langle c^\dagger_{i\downarrow} c_{i\downarrow} \rangle c^\dagger_{i\uparrow} c_{i\uparrow}$$
$$+ \langle c^\dagger_{i\uparrow} c_{i\downarrow} \rangle \langle c^\dagger_{i\downarrow} c_{i\uparrow} \rangle - \langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle \langle c^\dagger_{i\downarrow} c_{i\downarrow} \rangle$$

Hartree-Fock representation

he local decoupling of the interaction kernel in

$$n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma} \qquad \wedge \qquad S^+_i = c^\dagger_{i\downarrow} c_{i\uparrow} \;\;,\;\; S^-_i = c^\dagger_{i\downarrow} c_{i\uparrow}$$

ads to Hartree-Fock (HF) theory of the mean-field approach to the Hubbard model:

$$H^{\rm HF}_{\rm hub} = -t \sum_{\langle ij\rangle\sigma} c^\dagger_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_i \left\{ n_i \langle n_i\rangle - 4 \mathbf{S}_i \langle \mathbf{S}_i\rangle - \frac{1}{2}\langle n_i\rangle^2 - 2\langle \mathbf{S}_i\rangle^2 \right\} \qquad n_i = \textstyle\sum_\sigma n_{i\sigma}$$

$$\Rightarrow \quad \text{modified dispersion} \quad \varepsilon^{\rm HF}_{\mathbf{k}\sigma} := \frac{\partial E^{\rm HF}_{\rm hub}}{\partial \langle n_{\mathbf{k}\sigma}\rangle} = \frac{\partial \langle H^{\rm HF}_{\rm hub}\rangle}{\partial \langle n_{\mathbf{k}\sigma}\rangle} = \begin{cases} \varepsilon_{\mathbf{k}} + U\left(\frac{n}{2} - m\right) & \text{for } \sigma = \uparrow \\ \varepsilon_{\mathbf{k}} + U\left(\frac{n}{2} + m\right) & \text{for } \sigma = \downarrow \end{cases}$$

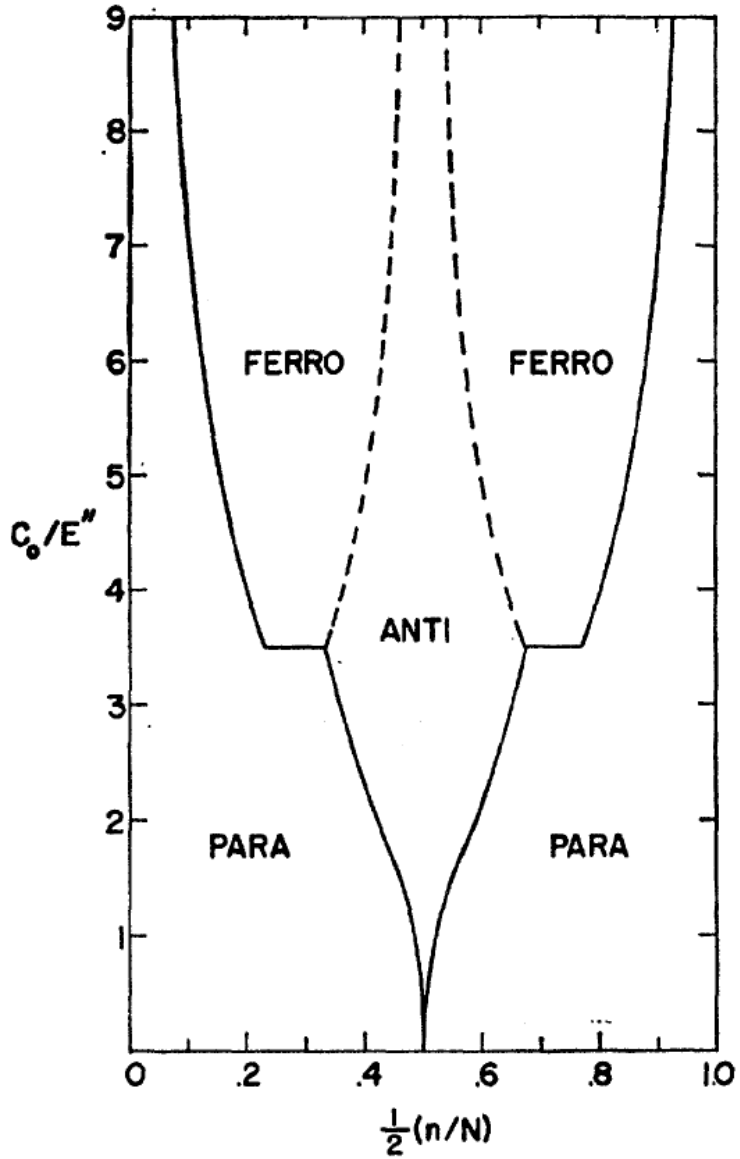
$$\left(\text{using } \sum_i n_{i\sigma} = \sum_{\mathbf{k}} n_{\mathbf{k}\sigma} \quad , \quad m = \frac{1}{2}(\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle) \right)$$

- simple approximation, numerically very efficient
- in principle no correlations in HF, ill-defined for metallic systems
- can be useful for long-range ordered Mott insulators ($\rightarrow$ LDA+U !)
- other decoupling schemes possible (e.g., to describe superconductivity)

HF phase diagram for the Hubbard model

ngle-band Hubbard model on the 3D simple cubic lattice without non-collinear phases

R. Penn, Phys. Rev. 142, 350 (1966)]



Basic techniques
2. Hubbard I

Employing the Green's function

one-particle Green's function: $G_\sigma(\mathbf{k},t) = -i\,\langle\Psi_0|\mathcal{T}\,c_{\mathbf{k}\sigma}(t)c^\dagger_{\mathbf{k}\sigma}(0)|\Psi_0\rangle$

ehmann representation:

$$_\sigma(\mathbf{k},\omega) = \sum_m \frac{|\langle\Psi_m^{(N_\mathrm{e}+1)}|c^\dagger_{\mathbf{k}\sigma}|\Psi_0\rangle|^2}{\omega+\mu-\omega_{m0}+i\eta} + \sum_m \frac{|\langle\Psi_m^{(N_\mathrm{e}-1)}|c_{\mathbf{k}\sigma}|\Psi_0\rangle|^2}{\omega+\mu-\omega_{0m}-i\eta} \;\to\; \int_{-\infty}^{\infty} \frac{d\omega'\,A_\sigma(\mathbf{k},\omega)}{\omega+\mu-\omega'+\mathrm{sgn}(\omega')i0^+}$$

xample: Fermi-gas limit $A_\sigma(\mathbf{k},\omega) = \delta(\omega-\varepsilon_\mathbf{k})$

$$\Rightarrow \quad G^{\mathrm{FG}}_\sigma(\mathbf{k},\omega) = \int_{-\infty}^{\infty} d\omega' \,\frac{\delta(\omega'-\varepsilon_\mathbf{k})}{\omega+\mu-\omega'+\mathrm{sgn}(\omega')i0^+} = \frac{1}{\omega+\mu-\varepsilon_\mathbf{k}+i\eta_\mathbf{k}}$$

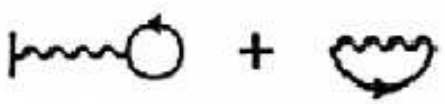
general

$$G_\sigma(\mathbf{k},\omega) = \frac{1}{\omega+\mu-\varepsilon_\mathbf{k}-\Sigma_\sigma(\mathbf{k},\omega)}$$

elf-energy $\Sigma_\sigma(\mathbf{k},\omega)$ carries all many-body effects !

xample: Hartree-Fock approximation (first order diagrammatic expansion)

$$\Sigma^{\mathrm{HF}} = \Sigma(\mathbf{k}) = \Sigma^{\mathrm{Hartree}} + \Sigma^{\mathrm{Fock}} =$$

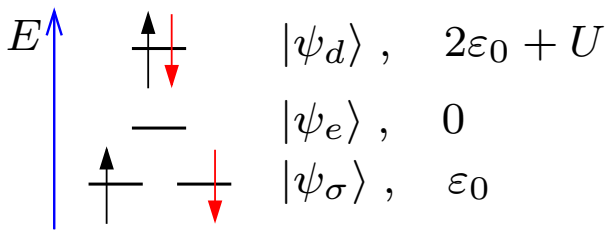


Computing the atomic self-energy

oncentrate on the local Green's function: $G_{i\sigma}(\omega) = \sum_{\mathbf{k}} G_\sigma(\mathbf{k},\omega)$

half filling the local spectral function $\rho(\omega)$ in the atomic limit is given by

$$\rho_\sigma(\omega) = \begin{cases} \sum_i \langle n_{i\bar\sigma}\rangle |\langle\psi_d|c^\dagger_{i\sigma}|\psi_{\bar\sigma}\rangle|^2\,\delta(\omega-\omega_{d\bar\sigma}) = \sum_i \langle n_{i\bar\sigma}\rangle\,\delta(\omega-(\varepsilon_0+U)) \\ \sum_i \langle n_{i\sigma}\rangle |\langle\psi_e|c_{i\sigma}|\psi_\sigma\rangle|^2\,\delta(\omega-\omega_{e\sigma}) = \sum_i \langle n_{i\sigma}\rangle\,\delta(\omega-\varepsilon_0) \end{cases}$$



$$\Rightarrow \quad G_{i\sigma}(\omega) = \int_{-\infty}^{0} d\omega' \frac{(1-\langle n_{i\bar\sigma}\rangle)\,\delta(\omega'-\varepsilon_0)}{\omega+\mu-\omega'-i0^+} + \int_0^\infty d\omega' \frac{\langle n_{i\bar\sigma}\rangle\,\delta(\omega'-(\varepsilon_0+U))}{\omega+\mu-\omega'+i0^+}$$

$$= \frac{1-\langle n_{i\bar\sigma}\rangle}{\omega+\mu-\varepsilon_0-i0^+} + \frac{\langle n_{i\bar\sigma}\rangle}{\omega+\mu-\varepsilon_0-U+i0^+}$$

now adapt to $G_{i\sigma}(\omega) = \dfrac{1}{\omega+\mu-\Sigma^{\rm atom}_{i\sigma}(\omega)}$

$$\Sigma^{\rm atom}_{i\sigma}(\omega) = U n_{i\bar\sigma} + U^2 \frac{n_{i\bar\sigma}(1-n_{i\bar\sigma})}{\omega+\mu-U(1-n_{i\bar\sigma})}$$

atomic-limit self-energy of the half-filled Hubbard model

Hubbard-I approximation

se structure of atomic self-energy for the crystal Green's function:

$$G_\sigma^{\mathrm{HI}}(\mathbf{k},\omega) = \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma_{i\sigma}^{\mathrm{atom}}(\omega)}$$

oots of the denominator (poles) yield the excitations of the system:

$$\varepsilon_{\mathbf{k}\sigma}^{\mathrm{HI}} = \frac{1}{2}\left\{\varepsilon_{\mathbf{k}} + U \vee \pm\sqrt{(\varepsilon_{\mathbf{k}} + U)^2 + 4U\langle n_{i\bar{\sigma}}\rangle}\right\}$$

- simple approximation, numerically very efficient
- atomic reference point, does not reduce to Hartree-Fock
- appropriate for paramagnetic Mott insulators
- dispersing Hubbard bands, but no quasiparticle peak
- violates particle-hole symmetry

Basic techniques
3. Slave Bosons

Introducing additional degrees of freedom

half-filled single-band Hubbard model in the $U \to \infty$ limit: $H = -t \sum_{\langle ij \rangle \sigma} P\, c^\dagger_{i\sigma} c_{j\sigma}\, P$

oubly occupied sites are forbidden: $\sum_\sigma n_{i\sigma} < 2$ **not easy to handle !**

new auxiliary quantum degrees of freedom $\phi_i^{(\dagger)}$ $\quad c^\dagger_{i\sigma} = f^\dagger_{i\sigma}\phi_i \quad \wedge \quad c_{i\sigma} = f_{i\sigma}\phi^\dagger_i$

decomposition of original electron operator into fermionic f part and bosonic ϕ part

$$\begin{aligned} \phi_i^\dagger|\mathrm{vac}\rangle &= |0_i\rangle \\ f^\dagger_{i\sigma}|\mathrm{vac}\rangle &= |\sigma_i\rangle \end{aligned}$$

$$\begin{aligned} |0_i\rangle &: \quad n_b = 1 \quad \wedge \quad n_{f\sigma} = 0 \\ |\uparrow_i\rangle &: \quad n_b = 0 \quad \wedge \quad n_{f\uparrow} = 1 \\ |\downarrow_i\rangle &: \quad n_b = 0 \quad \wedge \quad n_{f\downarrow} = 1 \end{aligned}$$

ecessary constraint for $U \to \infty$: $\sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} + \phi^\dagger_i \phi_i = 1 =: \mathcal{Q}$

Hamiltonian problem may then be expressed as $H = -t \sum_{\langle ij \rangle \sigma} \phi_i \phi^\dagger_j f^\dagger_{i\sigma} f_{j\sigma}$

lave boson $\phi_i^{(\dagger)}$ takes care of high-energy excitations, while $f_{i\sigma}^{(\dagger)}$ carries the sole quasiparticle part at low energy

Slave-Boson Mean-Field Approximation

$$U \to \infty : \qquad H_{\rm hub} = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad \to \quad H^{\rm SB}_{\rm hub} = -t \sum_{\langle ij \rangle \sigma} \phi_i \phi^\dagger_j f^\dagger_{i\sigma} f_{j\sigma}$$

Mean-field approach: condensing the slave bosons (saddle-point approximation)

$$r := \langle \phi_i \rangle \quad , \qquad \sum_\sigma \langle n_{f\sigma} \rangle + |r|^2 = 1 \quad , \qquad H_{\rm eff} = -|r|^2 \, t \sum_{\langle ij \rangle \sigma} f^\dagger_{i\sigma} f_{j\sigma}$$

Brinkman-Rice effect: $|r|^2 = 1 - \langle n_f \rangle := \delta \quad \Rightarrow \quad t_{\rm eff} = \delta t$ (strong bandwidth reduction at doping δ)

Interacting ground state may be found my minimizing the grand potential with constraint:

$$\Omega = \langle H_{\rm eff} \rangle + \lambda \left(\sum_\sigma \langle n_{f\sigma} \rangle + |r|^2 - 1 \right) - \mu \sum_\sigma \langle n_{f\sigma} \rangle$$

Generalization to finite-U and multi-orbital Hubbard problems possible !

$$\to \quad \underline{H}_{\rm hub} = -t \sum_{\langle ij \rangle \sigma} r_i r^*_j f^\dagger_{i\sigma} f_{j\sigma} + U \sum_i \phi^\dagger_{\uparrow\downarrow i} \, \phi_{\uparrow\downarrow i}$$

Green's Function and Self-Energy

quasiparticle dispersion: $\varepsilon_{\mathbf{k}\sigma}^{\mathrm{SBMF}} := \dfrac{\partial E^{\mathrm{SBMF}}}{\partial \langle n_{\mathbf{k}\sigma}^{f} \rangle} = |r|^2 \varepsilon_{\mathbf{k}\sigma} + \lambda$

- **Green's function of non-interacting quasiparticles:**

$$G_f(\mathbf{k},\omega) = \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}\sigma}^{\mathrm{SBMF}}} = \frac{1}{\omega + \mu - |r|^2 \varepsilon_{\mathbf{k}} - \lambda}$$

Full electronic Green's function and local self-energy:

$$\begin{aligned} G^{\mathrm{SBMF}}(\mathbf{k},\omega) &= |r|^2 G_f(\mathbf{k},\omega) = \frac{|r|^2}{\omega + \mu - |r|^2 \varepsilon_{\mathbf{k}} - \lambda} =: \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma^{\mathrm{SBMF}}(\omega)} \\ \Sigma^{\mathrm{SBMF}}(\omega) &= \omega \left(1 - \frac{1}{|r|^2}\right) + \mu - \frac{\mu - \lambda}{|r|^2} \end{aligned}$$

- still simple approximation, numerically very efficient
- good description of renormalized quasiparticles at low energy
- Hubbard excitations only via static multiplets $\rightarrow$ no complete spectral function !

Conclusions

- Models
  - are needed to investigate complex physics beyond effective single-particle problems
  - are still very difficult to solve, most often only in approximations manageable
  - Hubbard-like models are at the heart of describing the competition between localization and itinerancy
- Techniques
  - static mean-field approaches are simple, but most often a good starting point
  - central goal: modeling self-energy $\Sigma(\mathbf{k}, \omega)$ as good as possible
  - many approaches concentrate on certain limits/energy-ranges
  - one needs to describe strong/weak interacting limit as well as all relevant energy scales
  - Hartree-Fock and Hubbard-I are ok for the start, but one has to understand their limits
  - Slave-Boson Mean-Field ok when explicit quantum-fluctuactions are negligible and dynamic Hubbard bands are irrelevant