

# *The Hubbard Model for Dummies*

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- Some math
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  - $U = 0$
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- Extensions of the Hubbard model

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13.6.07

# The Hubbard Model: Introduction

- J. Hubbard, Proc. Roy. Soc. London, A266, 238 (1963).
- Simplest model of interacting particles in a lattice: extension of the „tight-binding“ model to include short-range el-el interactions.
- „One-band“ Hubbard Hamiltonian (one orbital per site):

$$H = -t \sum_{\langle ij \rangle \sigma} c_{j\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

hopping term      interaction term

„ $\langle ij \rangle$ “ implies adjacent sites

- „Half-filling“: on average one electron per site.
- Electrons may hop from site to site, but for large  $U/t$ , we get a „Mott insulator“.
- Note: One of the first correlated electron calculations: Heitler+London treatment of  $H_2$ -molecule (1927).

# Second Quantization

- **Boson** annihilation and creation operators for the harmonic oscillator:

$$a = \sqrt{\frac{m\omega}{2\hbar}}x + i\sqrt{\frac{1}{2m\omega\hbar}}p$$
$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - i\sqrt{\frac{1}{2m\omega\hbar}}p$$

- From  $[x, p] = i\hbar$ , we verify that  $[a, a^\dagger] = 1$  and that the oscillator Hamiltonian is:

$$H_{osc} = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}x^2$$
$$= \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) = \hbar\omega\left(n + \frac{1}{2}\right)$$

n=a<sup>†</sup>a = „number operator“.

- From the ground state  $|0\rangle$ , we build up the excited states:

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \quad H_{osc}|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle$$

- Electron states for the (N=8) Hubbard model in terms of ***fermionic*** operators:

$$c_{1\uparrow}^\dagger |0\rangle = |\uparrow, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot\rangle$$

$$c_{5\downarrow}^\dagger |0\rangle = |\cdot, \cdot, \cdot, \cdot, \downarrow, \cdot, \cdot, \cdot\rangle \quad c_{1\uparrow}^\dagger c_{1\uparrow} |\uparrow, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot\rangle \equiv n_{1\uparrow} |\uparrow, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot\rangle = 1 |\uparrow, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot\rangle$$

$$c_{5\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle = |\uparrow, \cdot, \cdot, \cdot, \downarrow, \cdot, \cdot, \cdot\rangle \quad c_{5\downarrow}^\dagger c_{5\downarrow} |\uparrow, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot\rangle \equiv n_{5\downarrow} |\uparrow, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot\rangle = 0 |\uparrow, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot\rangle$$

$$c_{4\uparrow}^\dagger c_{4\downarrow}^\dagger |0\rangle = |\cdot, \cdot, \cdot, \uparrow \downarrow, \cdot, \cdot, \cdot, \cdot\rangle$$

$$c_{1\uparrow} |0\rangle = 0$$

$$c_{1\uparrow}^\dagger c_{1\uparrow} |0\rangle = 0$$

$$\{c_{i\sigma}, c_{j\sigma'}\} \equiv c_{i\sigma} c_{j\sigma'} + c_{j\sigma'} c_{i\sigma} = 0$$

$$\{c_{i\sigma}^\dagger, c_{j\sigma'}^\dagger\} = 0 \quad \{ \} = \text{„anticommutator“}$$

$$\{c_{i\sigma}, c_{j\sigma'}^\dagger\} = \delta_{ij} \delta_{\sigma\sigma'}$$

# Partition Function

- „Grand Canonical Ensemble“: particles can be exchanged with a reservoir.

$$\text{partition function: } Z \equiv \text{Tr} \left[ e^{-\beta(H-\mu n)} \right]$$

$$\beta \equiv \frac{1}{kT} \quad \mu \equiv \text{"chemical potential"}$$

- Thermal expectation value of operator A:  $\langle A \rangle = \frac{1}{Z} \text{Tr} \left[ A e^{-\beta(H-\mu n)} \right]$
- Consider a single state with 0 or 1 electrons with energy  $\varepsilon$ :

$$H = \varepsilon c^\dagger c = \varepsilon n \quad \text{states: } \{|0\rangle, |1\rangle\}$$

$$Z = \langle 0 | e^{-\beta(H-\mu n)} | 0 \rangle + \langle 1 | e^{-\beta(H-\mu n)} | 1 \rangle = 1 + e^{-(\beta-\mu)}$$

- Average occupation:

$$\begin{aligned} \langle n \rangle &= \frac{1}{Z} \left[ \langle 0 | n e^{-\beta(H-\mu n)} | 0 \rangle + \langle 1 | n e^{-\beta(H-\mu n)} | 1 \rangle \right] = \frac{1}{Z} \left[ 0 + e^{-\beta(\varepsilon-\mu)} \right] = \frac{e^{-\beta(\varepsilon-\mu)}}{1 + e^{-\beta(\varepsilon-\mu)}} \\ &= \frac{1}{e^{\beta(\varepsilon-\mu)} + 1} = \text{Fermi - Dirac distribution} \end{aligned}$$

# Hubbard Model with t=0

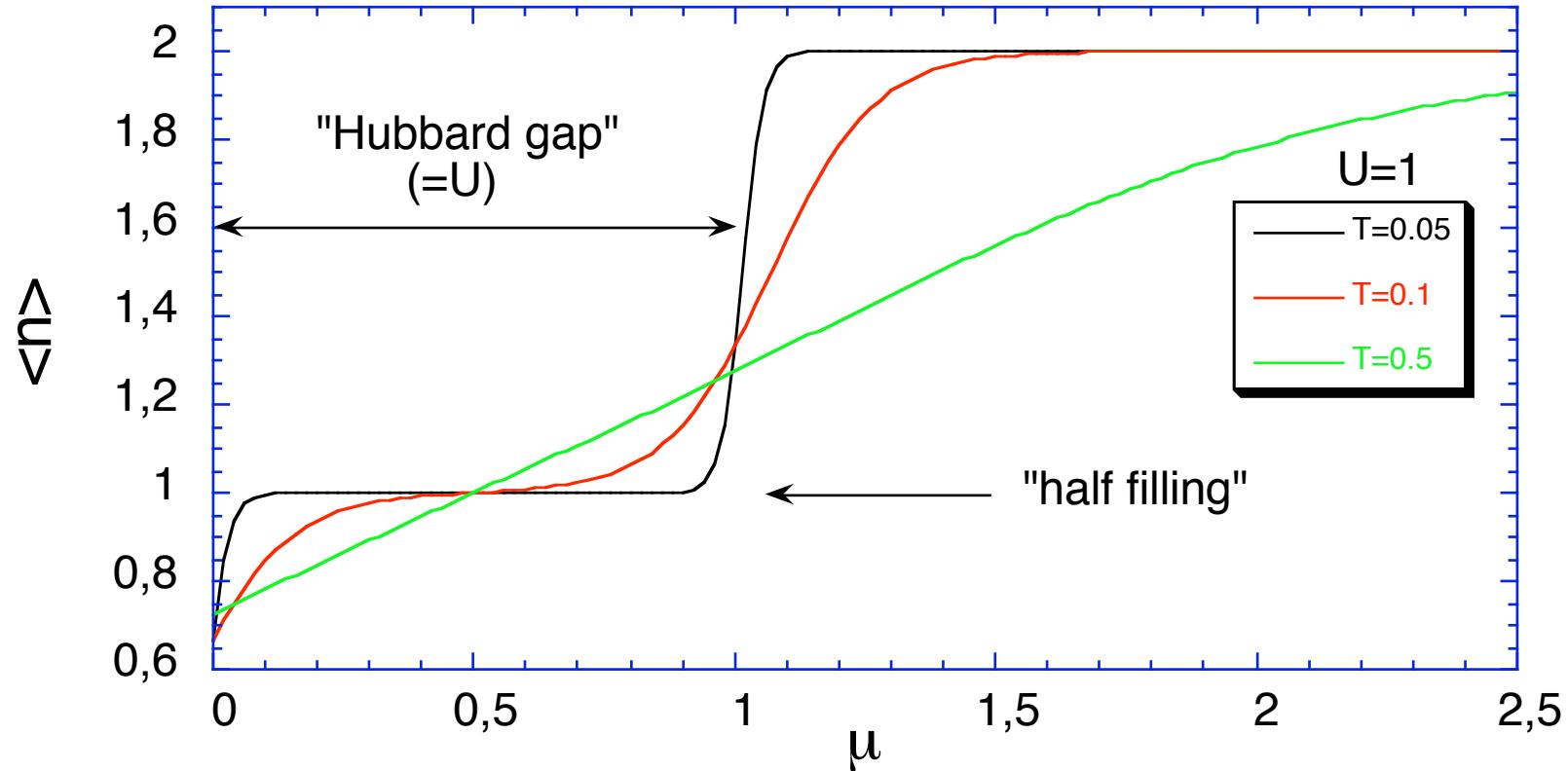
- No hopping implies independent sites. We thus consider a *single site* and calculate its average occupation.

$$\text{possible states} = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$$

$$H = U n_{\uparrow} n_{\downarrow}$$

$$Z = \sum_{\alpha} \langle \alpha | e^{-\beta(H - \mu n)} | \alpha \rangle = 1 + e^{\beta\mu} + e^{\beta\mu} + e^{-\beta U + 2\beta\mu}$$

$$\begin{aligned} \langle n \rangle &= \frac{1}{Z} \sum_{\alpha} \langle \alpha | (n_{\uparrow} + n_{\downarrow}) e^{-\beta(H - \mu n)} | \alpha \rangle = \frac{1}{Z} [0 + e^{\beta\mu} + e^{\beta\mu} + 2e^{-\beta U + 2\beta\mu}] \\ &= \frac{2(e^{\beta\mu} + e^{-\beta U + 2\beta\mu})}{1 + 2e^{\beta\mu} + e^{-\beta U + 2\beta\mu}} \end{aligned}$$



- Note: Since  $\mu = \frac{\partial E}{\partial n}$ , at half-filling, the energy to add another particle to the site jumps by  $U$ . This is the „Hubbard gap“.

# Hubbard Model with U=0

- „Non-interacting“ limit: we go into reciprocal space:

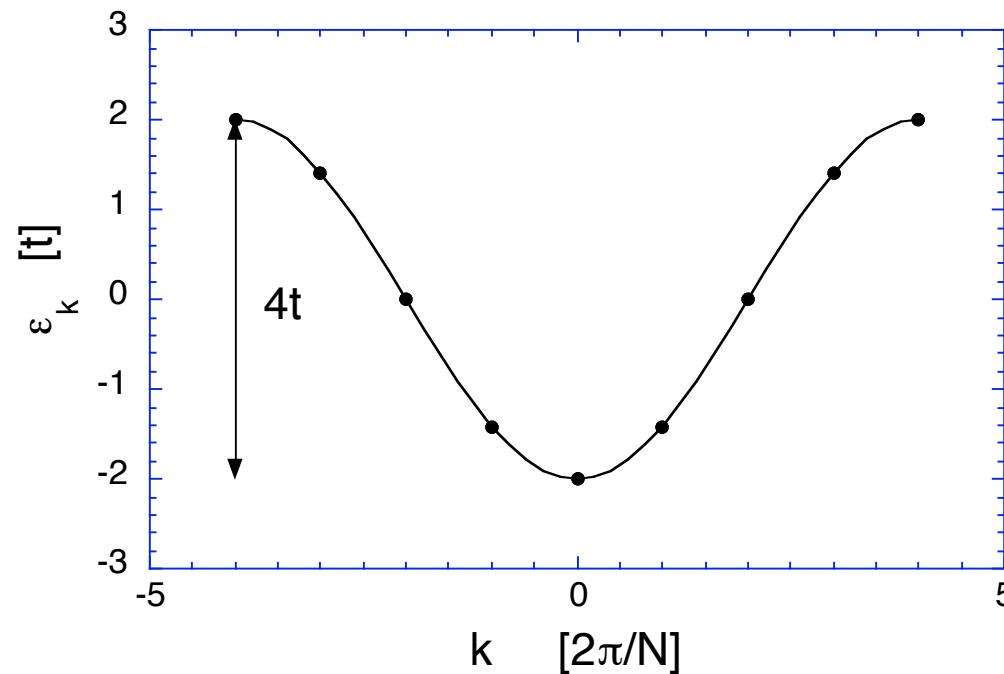
$$c_{k\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_l e^{ik \cdot l} c_{l\sigma}^\dagger$$

where  $k$  takes the values  $k_n = 2\pi n/N$ . (1-d, periodic boundary conditions)

$$\begin{aligned} H &= -t \sum_{\langle jl \rangle \sigma} c_{j\sigma}^\dagger c_{l\sigma} = \frac{-t}{N} \sum_{k,k'} \sum_{\langle jl \rangle \sigma} e^{ikj} e^{-ik'l} c_{k\sigma}^\dagger c_{k'\sigma} \\ &= \frac{-t}{N} \sum_{k,k',\sigma} c_{k\sigma}^\dagger c_{k'\sigma} \sum_j [e^{ikj} e^{-ik'(j+1)} + e^{ikj} e^{-ik'(j-1)}] = -t \sum_{k,k',\sigma} c_{k\sigma}^\dagger c_{k'\sigma} [e^{-ik'} + e^{ik'}] \frac{1}{N} \sum_j e^{i(k-k')j} \\ &= -t \sum_{k,k',\sigma} c_{k\sigma}^\dagger c_{k'\sigma} [2 \cos k'] \delta_{k,k'} = \sum_{k\sigma} \varepsilon_k n_{k\sigma} \quad \varepsilon_k = -2t \cos k \end{aligned}$$

- For  $U=0$ , the energy-eigenvalues of  $H$  are:

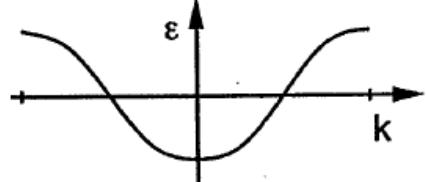
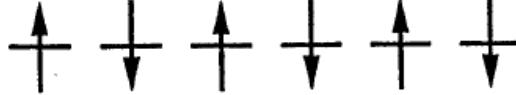
$$\varepsilon_k = -2t \cos k \quad k_n = \frac{2\pi n}{N} \quad n = 0, 1, 2, \dots N-1$$



- The „bandwidth“ is equal to  $4t$ .

- **The Mott Transition:**

- $U >> t$ : diagonalize  $H$  in real space – at half-filling we obtain a static (insulating) system.
- $t >> U$ : diagonalize  $H$  in reciprocal space – obtain itinerant electron band, width  $4t$ .

parameter range	physical picture	behavior
$t \gg U$ : band-limit		filling of a band ⇒ metal
$t \ll U$ : atomic limit		no hopping for integer filling ⇒ insulator

- At some intermediate value of  $U/t$ , there will be a „metal-to-insulator“ transition: the „Mott“ transition.

# Mean Field Theory

- We wish to treat the full Hubbard model (in 1-d):

$$H = -t \sum_{\langle jl \rangle \sigma} c_{j\sigma}^\dagger c_{l\sigma} + U \sum_l n_{l\uparrow} n_{l\downarrow}$$

Problem: the second term is proportional to  $c^4$ .

- „Mean field“ approximation: each electron feels an average interaction from all others.  
*This ignores possibly important electron correlations.*
- Write:

$$n_{l\uparrow} = \langle n_{\uparrow} \rangle + [n_{l\uparrow} - \langle n_{\uparrow} \rangle] = \langle n_{\uparrow} \rangle + \delta_{l\uparrow}$$

and assume  $\delta$  is small, and analogously for the down spins. Expand:

$$\begin{aligned} n_{l\uparrow} n_{l\downarrow} &\approx \langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle + \delta_{l\uparrow} \langle n_{\downarrow} \rangle + \delta_{l\downarrow} \langle n_{\uparrow} \rangle \\ &\approx n_{l\uparrow} \langle n_{\downarrow} \rangle + n_{l\downarrow} \langle n_{\uparrow} \rangle - \langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle \end{aligned}$$

- In reciprocal space:

$$c_{l\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-ikl} c_{k\sigma}^\dagger$$

$H$  is now diagonal:

$$\begin{aligned} H &= \sum_k \left[ -2t \cos k (n_{k\uparrow} + n_{k\downarrow}) + U(n_{k\uparrow}\langle n_\downarrow \rangle + n_{k\downarrow}\langle n_\uparrow \rangle) \right] - UN\langle n_\uparrow \rangle\langle n_\downarrow \rangle \\ &= \sum_k [\varepsilon_{k\uparrow} n_{k\uparrow} + \varepsilon_{k\downarrow} n_{k\downarrow}] - UN\langle n_\uparrow \rangle\langle n_\downarrow \rangle \quad \varepsilon_{k\uparrow} \equiv -2t \cos k + U\langle n_\downarrow \rangle \end{aligned}$$

- We define spin-dependent Fermi wavevectors:

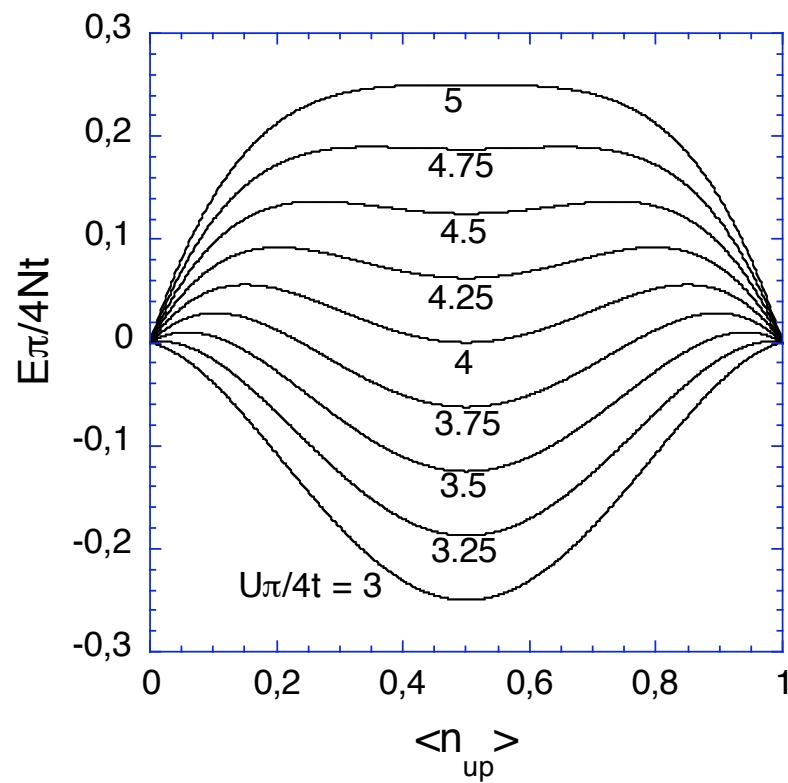
$$\sum_{k\uparrow} = \frac{N}{\pi} \int_0^{k_F \uparrow} dk \quad k_F \uparrow = \frac{\pi \langle n_\uparrow \rangle}{N}$$

- After integrating, we obtain for the total energy:

$$E_{tot} = \frac{-2Nt}{\pi} [\sin \pi \langle n_\uparrow \rangle + \sin \pi \langle n_\downarrow \rangle] + UN\langle n_\uparrow \rangle\langle n_\downarrow \rangle$$

- For half-filling:  $\langle n_{\uparrow} \rangle + \langle n_{\downarrow} \rangle = 1$  write  $E_{\text{tot}}$  as a function of  $\langle n_{\uparrow} \rangle$

$$\frac{\pi E_{\text{tot}}(\langle n_{\uparrow} \rangle)}{4Nt} = -\sin \pi \langle n_{\uparrow} \rangle + \frac{U\pi}{4t} \langle n_{\uparrow} \rangle (1 - \langle n_{\uparrow} \rangle)$$



small  $U \Rightarrow$  a paramagnet

large  $U \Rightarrow$  a ferromagnet

***This is completely wrong!***

The 1-dimensional Hubbard model has been exactly solved by Lieb and Wu, PRL 20, 1445 (1998). At *infinitesimal*  $U/t$  an *antiferromagnetic* state forms.

# Hubbard Model in Matrix Notation

„Toy Model“  
(simplified H<sub>2</sub> molecule)

- Two orthonormal orbitals separated by some distance:

$$\phi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \phi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{schematically: } \phi_1 = |\uparrow, \cdot\rangle, \quad \phi_2 = |\cdot, \uparrow\rangle$$

- Add a single electron, which moves with an amplitude  $-t$ .  
⇒ “Tight-binding” Hamiltonian:

$$H = \begin{pmatrix} 0 & -t \\ -t & 0 \end{pmatrix}$$

- Eigenvectors:  $\phi_{\pm} = \frac{1}{\sqrt{2}}(\phi_1 \pm \phi_2) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$
- Energy eigenvalues:  $\epsilon_{\pm} = \mp t$  Note:  $\phi_+$  is the ground state.

- We now consider ***two*** electrons:

$$|\uparrow, \downarrow\rangle = c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle \quad \text{„covalent states“}$$

$$|\downarrow, \uparrow\rangle = c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle$$

$$|\uparrow \downarrow, \cdot\rangle = c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle \quad \text{„ionic states“}$$

$$|\cdot, \uparrow \downarrow\rangle = c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle$$

- Hamiltonian

$$H = \begin{pmatrix} 0 & 0 & -t & -t \\ 0 & 0 & +t & +t \\ -t & +t & U & 0 \\ -t & +t & 0 & U \end{pmatrix} \quad \begin{matrix} |\uparrow, \downarrow\rangle \\ |\downarrow, \uparrow\rangle \\ |\uparrow \downarrow, \cdot\rangle \\ |\cdot, \uparrow \downarrow\rangle \end{matrix}$$

Note: „+t“ due to fermion transposition

- Diagonalize  $H$ :

$$\varepsilon_{\pm} = \frac{U}{2} \pm \frac{\sqrt{U^2 + 16t^2}}{2}$$

$$\varepsilon_{\text{cov}} = 0$$

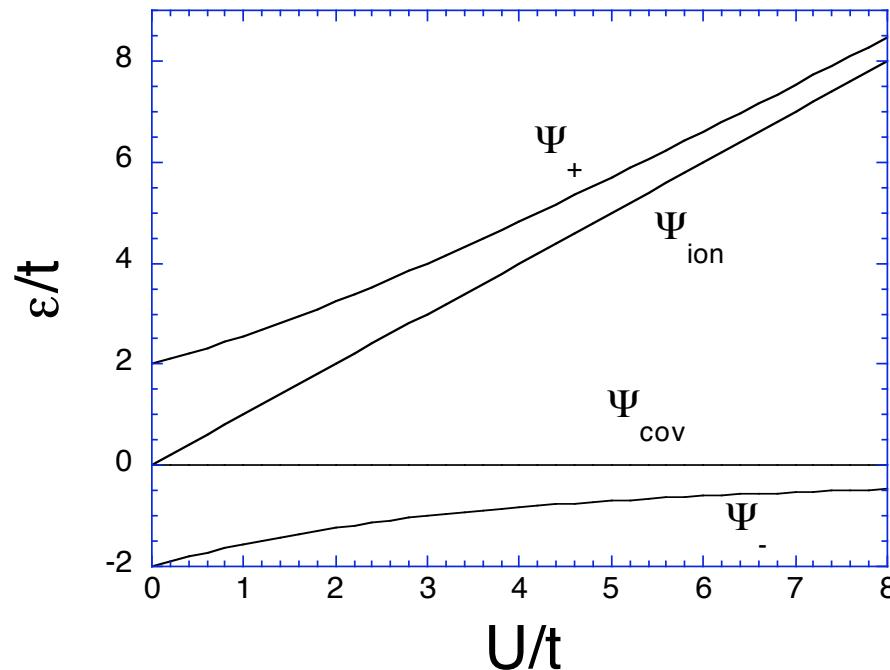
$$\varepsilon_{\text{ion}} = U$$

$$\psi_{\pm} = \frac{\left( |\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle - \frac{\varepsilon_{\pm}}{2t} [|\uparrow\downarrow,\cdot\rangle + |\cdot\uparrow\downarrow\rangle] \right)}{\sqrt{2 + \varepsilon_{\pm}^2 / (2t^2)}}$$

$$\psi_{\text{cov}} = \frac{1}{\sqrt{2}} (|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle)$$

$$\psi_{\text{ion}} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow,\cdot\rangle - |\cdot\uparrow\downarrow\rangle)$$

- Energy levels:



- Consider the limit of large  $U$ :

$$\varepsilon_{\text{cov}} = 0$$

$$\varepsilon_- \approx \frac{-4t^2}{U}$$

- $\Psi_-$  is now largely covalent, with a small ionic admixture.
- With „downfolding“, we will project out the interesting, low-energy, covalent-like part of Hilbert space.

- A note on matrix inversion by partitioning:

$$A = \begin{pmatrix} A_0 & A_1 \\ A_2 & A_3 \end{pmatrix}$$

We divide a matrix A into the blocks A0–A3.

$$A^{-1} = \begin{pmatrix} B_0 & B_1 \\ B_2 & B_3 \end{pmatrix}$$

The inverse can also be written in block form:

$$B_0 = \left( A_0 - A_1 \cdot A_3^{-1} \cdot A_2 \right)^{-1}$$

$$B_1 = -B_0 \cdot A_1 \cdot A_3^{-1}$$

$$B_2 = -A_3^{-1} \cdot A_2 \cdot B_0$$

$$B_3 = A_3^{-1} - B_2 \cdot A_1 \cdot A_3^{-1}$$

- Ref: Ch. 2.7, *Numerical Recipes*, 2nd Ed. (1992)

- We begin downfolding by partitioning  $H$  into blocks:

$$H = \begin{pmatrix} 0 & 0 & -t & -t \\ 0 & 0 & +t & +t \\ -t & +t & U & 0 \\ -t & +t & 0 & U \end{pmatrix} \equiv \begin{pmatrix} H_{00} & T_{01} \\ T_{10} & H_{11} \end{pmatrix}$$

$H_{00}$  = covalent Hamiltonian  
 $H_{11}$  = ionic Hamiltonian  
 $T_{ij}$  = covalent-ionic transitions

- The Green's function can also be partitioned:

$$G(\varepsilon) \equiv (\varepsilon - H)^{-1} = \begin{pmatrix} \varepsilon - H_{00} & -T_{01} \\ -T_{10} & \varepsilon - H_{11} \end{pmatrix}^{-1} \equiv \begin{pmatrix} G_{00} & G_{01} \\ G_{10} & G_{11} \end{pmatrix}$$

- and the (energy-dependent) covalent part  $G_{00}$  can be written:

$$G_{00}(\varepsilon) = \left( \varepsilon - \left[ H_{00} + T_{01}(\varepsilon - H_{11})^{-1} T_{10} \right] \right)^{-1}$$

- This looks like the Green's function for the effective Hamiltonian:

$$H_{eff}(\varepsilon) = H_{00} + T_{01}(\varepsilon - H_{11})^{-1} T_{10} \approx H_{eff}(\varepsilon_0) \quad \varepsilon_0 \text{ is a typical covalent energy.}$$

- We evaluate the effective Hamiltonian between the covalent states:

$$H_{\text{eff}}(\varepsilon_0) = H_{00} + T_{01}(\varepsilon_0 - H_{11})^{-1}T_{10} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} -t & -t \\ t & t \end{pmatrix} \begin{pmatrix} \varepsilon_0 - U & 0 \\ 0 & \varepsilon_0 - U \end{pmatrix}^{-1} \begin{pmatrix} -t & t \\ -t & t \end{pmatrix}$$

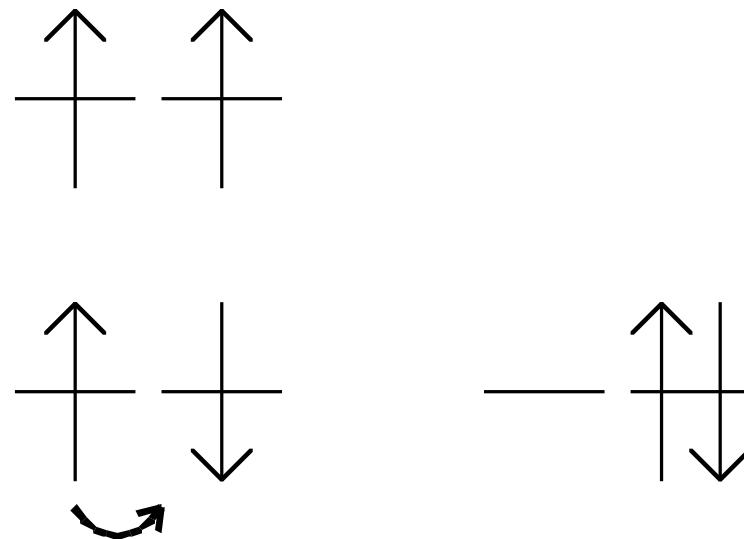
$$H_{\text{eff}}(0) = -\frac{2t^2}{U} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} |\uparrow,\downarrow\rangle \\ |\downarrow,\uparrow\rangle \end{pmatrix} \quad \text{Note that we choose } \varepsilon_0=0.$$

which diagonalizes to:

$$\begin{aligned} \varepsilon_s &= -\frac{4t^2}{U} & \psi_s &\approx \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle) \\ \varepsilon_t &= 0 & \psi_t &= \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle) \end{aligned} \quad \text{Recall that } \Psi_s \text{ includes a small ionic admixture.}$$

- These states correspond to singlet and triplet states of the  $\text{H}_2$  molecule.
- The other triplet states,  $|\uparrow,\uparrow\rangle$ ,  $|\downarrow,\downarrow\rangle$ , also have zero energy. (There is no Coulomb energy, and the electrons cannot hop, due to the Pauli principle.)

- „Kinetic Exchange“



- Anti-parallel alignment of the spins is favored, since it allows the electrons to hop to the neighboring site.

- We can write  $H_{\text{eff}}$  in terms of the fermion operators:

$$H_{\text{eff}} = -\frac{2t^2}{U} \left( c_{1\downarrow}^\dagger c_{1\downarrow} c_{2\uparrow}^\dagger c_{2\uparrow} - c_{1\uparrow}^\dagger c_{1\downarrow} c_{2\downarrow}^\dagger c_{2\uparrow} - c_{1\downarrow}^\dagger c_{1\uparrow} c_{2\uparrow}^\dagger c_{2\downarrow} + c_{1\uparrow}^\dagger c_{1\uparrow} c_{2\downarrow}^\dagger c_{2\downarrow} \right)$$

- Consider the properties of the Pauli spin matrices:

$$|\uparrow\rangle \equiv |+\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |\downarrow\rangle \equiv |-\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\vec{S} = \frac{1}{2} (\sigma_x \hat{x} + \sigma_y \hat{y} + \sigma_z \hat{z})$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_x |\pm\rangle = (c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow) |\pm\rangle = |\mp\rangle$$

$$\sigma_y |\pm\rangle = -i(c_\uparrow^\dagger c_\downarrow - c_\downarrow^\dagger c_\uparrow) |\pm\rangle = \pm i |\mp\rangle$$

$$\sigma_z |\pm\rangle = (c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow) |\pm\rangle = (n_\uparrow - n_\downarrow) |\pm\rangle = \pm |\pm\rangle$$

- We can therefore rewrite  $H_{\text{eff}}$ :

$$H_{\text{eff}} = \frac{4t^2}{U} \left( \vec{S}_1 \cdot \vec{S}_2 - \frac{n_1 n_2}{4} \right) \approx \text{Heisenberg Hamiltonian}$$

$$n_i \equiv n_{i\uparrow} + n_{i\downarrow}$$

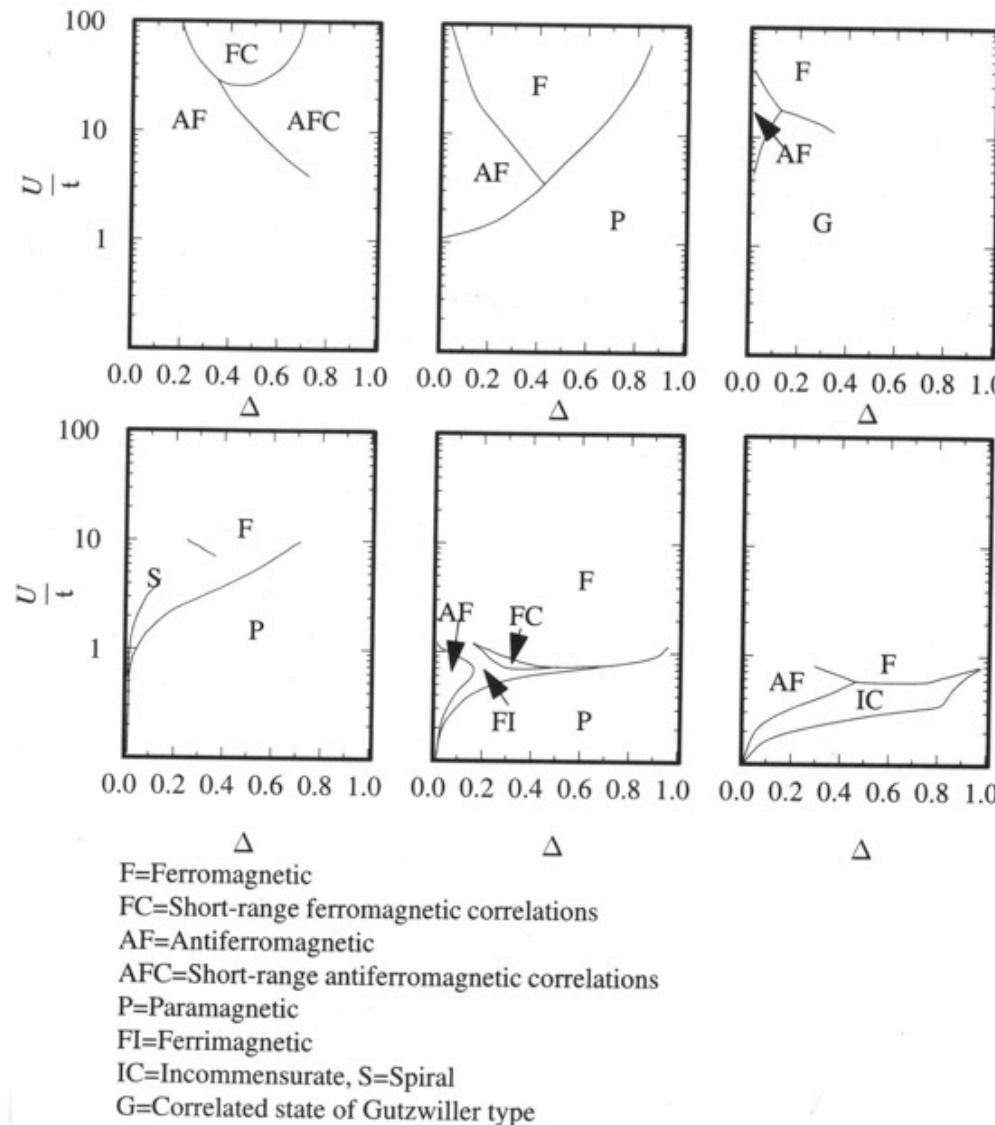
- The Hubbard Hamiltonian, for large  $U/t$ , has led us to an ***antiferromagnetic*** exchange coupling  $J=4t^2/U$ .
- This is the basis of the „t-J model“.

- We have solved the 4x4 Hubbard Hamiltonian by exact diagonalization. For larger systems, matrix expressions for H grow quickly in size. For N sites:

$$\text{dimension of Hilbert space} = \binom{N}{n_{\uparrow}} \times \binom{N}{n_{\downarrow}} \quad \binom{N}{n} \equiv \frac{N!}{n!(N-n)!} \quad \binom{2}{1} \times \binom{2}{1} = 4$$

- For 30 sites and 15 spins of each orientation, this dimension is  $2.4 \times 10^{16}$ .
- This is why we use 2<sup>nd</sup> quantization.
- No exact solution the Hubble model in >1 dimension is known.

- (mutually inconsistent) approximate solutions of the 2-D Hubbard Model



$$\Delta \equiv \langle n \rangle - 1$$

$\Delta = 0 \Rightarrow$  half - filling

Results of 6 groups,  
compiled by M.P. March,  
„Condensed Matter  
Physics“, Wiley, 2000.

# Extensions of the Hubbard Model

- „Three-Band“ Hubbard Model
- To describe the 2-d CuO<sub>2</sub> layers in superconducting cuprates, this model includes:

Cu(3dx<sup>2</sup>-y<sup>2</sup>) states ( $U_d$ )

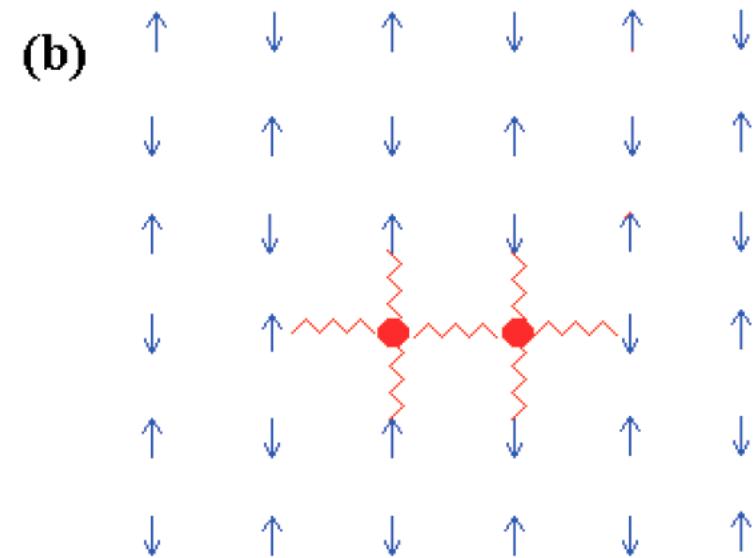
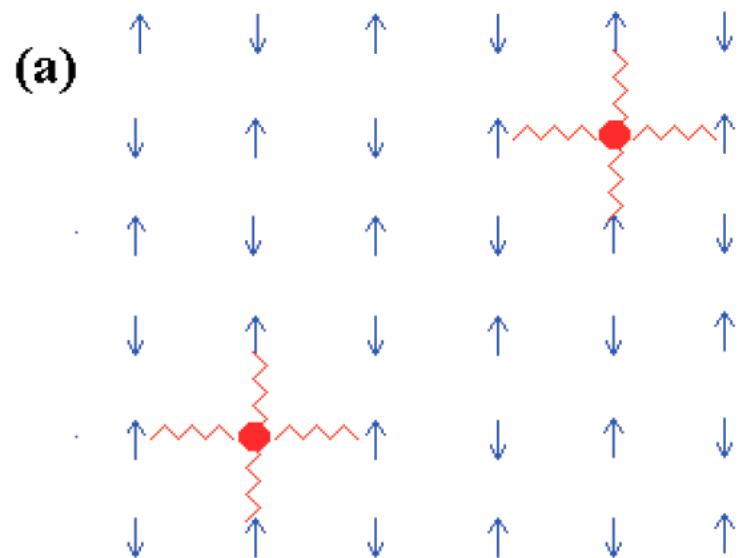
O(2px,y) states ( $U_p$ )

their nn interaction ( $U_{pd}$ )

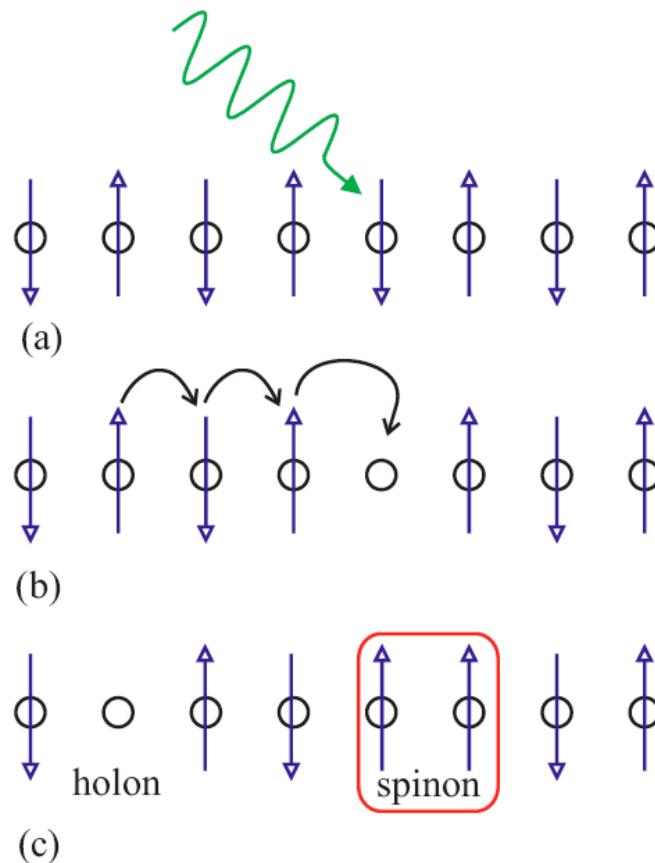
$$\begin{aligned} H = & \epsilon_d \sum_{i\sigma} d_{i,\sigma}^\dagger d_{i,\sigma} + \epsilon_p \sum_{l\sigma} p_{l,\sigma}^\dagger p_{l,\sigma} + U_d \sum_i d_{i,\uparrow}^\dagger d_{i,\uparrow} d_{i,\downarrow}^\dagger d_{i,\downarrow} \\ & + U_p \sum_l p_{l,\uparrow}^\dagger p_{l,\uparrow} p_{l,\downarrow}^\dagger p_{l,\downarrow} + U_{pd} \sum_{\langle i,l \rangle \sigma, \sigma'} d_{i,\sigma}^\dagger d_{i,\sigma} p_{l,\sigma'}^\dagger p_{l,\sigma'} \\ & - t_{pd} \sum_{\langle i,l \rangle \sigma} d_{i,\sigma}^\dagger p_{l,\sigma} + H.c., \end{aligned}$$

- For large  $U_{pd}$ , this Hamiltonian reduces to the t-J model.

- **2-d hole-pairing:**
- AF-coupling causes holes to form pairs.

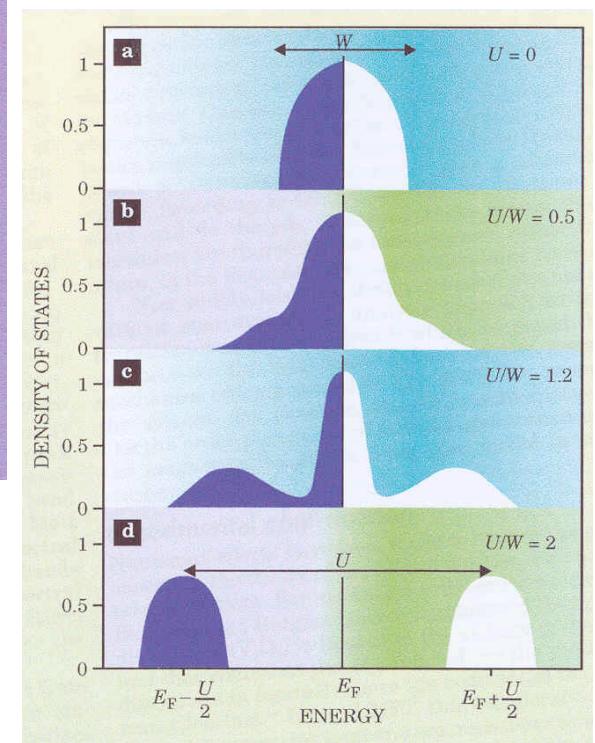
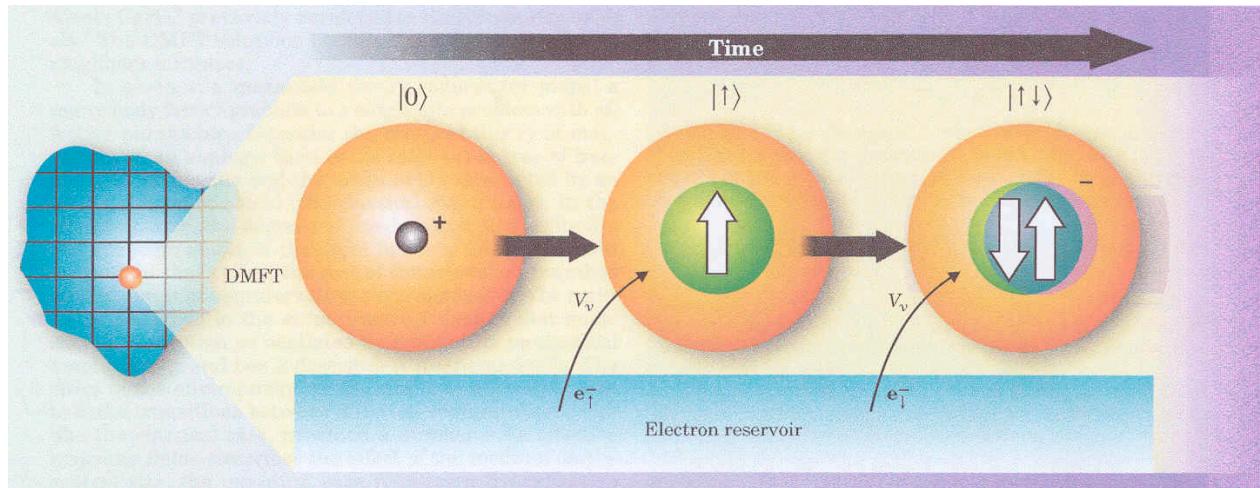


- **Charge-Spin separation:**
- In 1-d, Fermi liquid theory breaks down, due to the destruction of the Fermi surface (Fermi „points“) by an arbitrarily small perturbation. In this case, separate gapless charge (holon) and spin (spinon) excitations arise. This state is a „Luttinger liquid“.



Creation in photoemission  
of a holon and a spinon.

- **The Hubbard model with an infinite number of dimensions**
- Each site of the Hubbard model can then be treated as an isolated impurity interacting with an electron reservoir. This problem can be attacked with the „**dynamical mean-field theory**“.
- Ref: G. Kotliar and D. Vollhardt, Phys. Today March, 53 (2004).



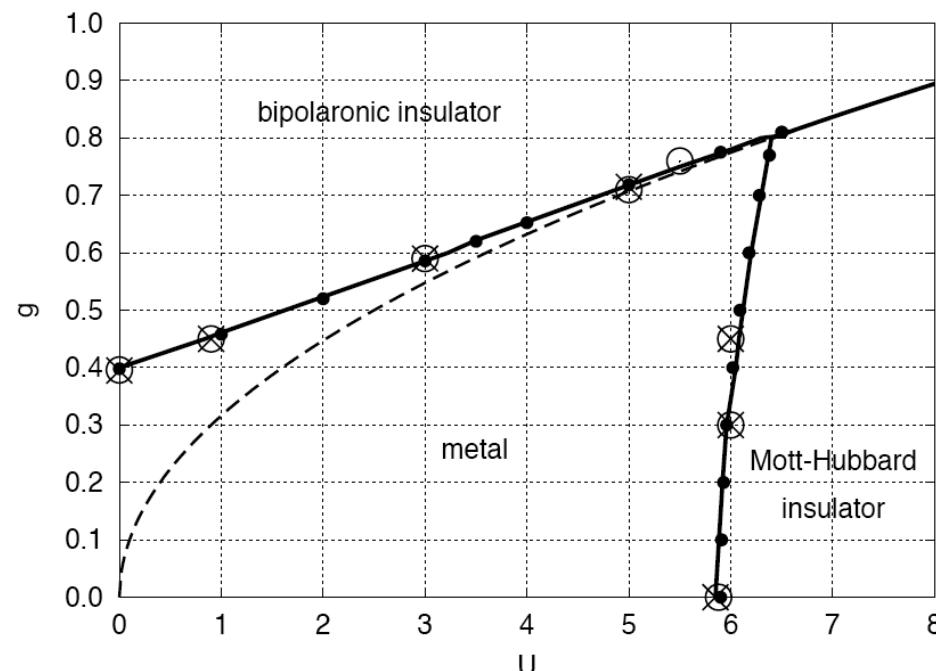
At intermediate  $U/W$  ( $=U/t$ ), we now see a sharp DOS peak at the Fermi level (Kondo resonance).

- The Hubbard-Holstein model (with electron-phonon interaction)

$$H_{H-H} = -t \sum_{\langle ij \rangle \sigma} c_{j\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - g \sum_{i\sigma} (b_i^\dagger + b_i) n_{i\sigma} + \omega_0 \sum_i b_i^\dagger b_i$$

$b_i^\dagger$  = creation operator of the local phonon mode at site i

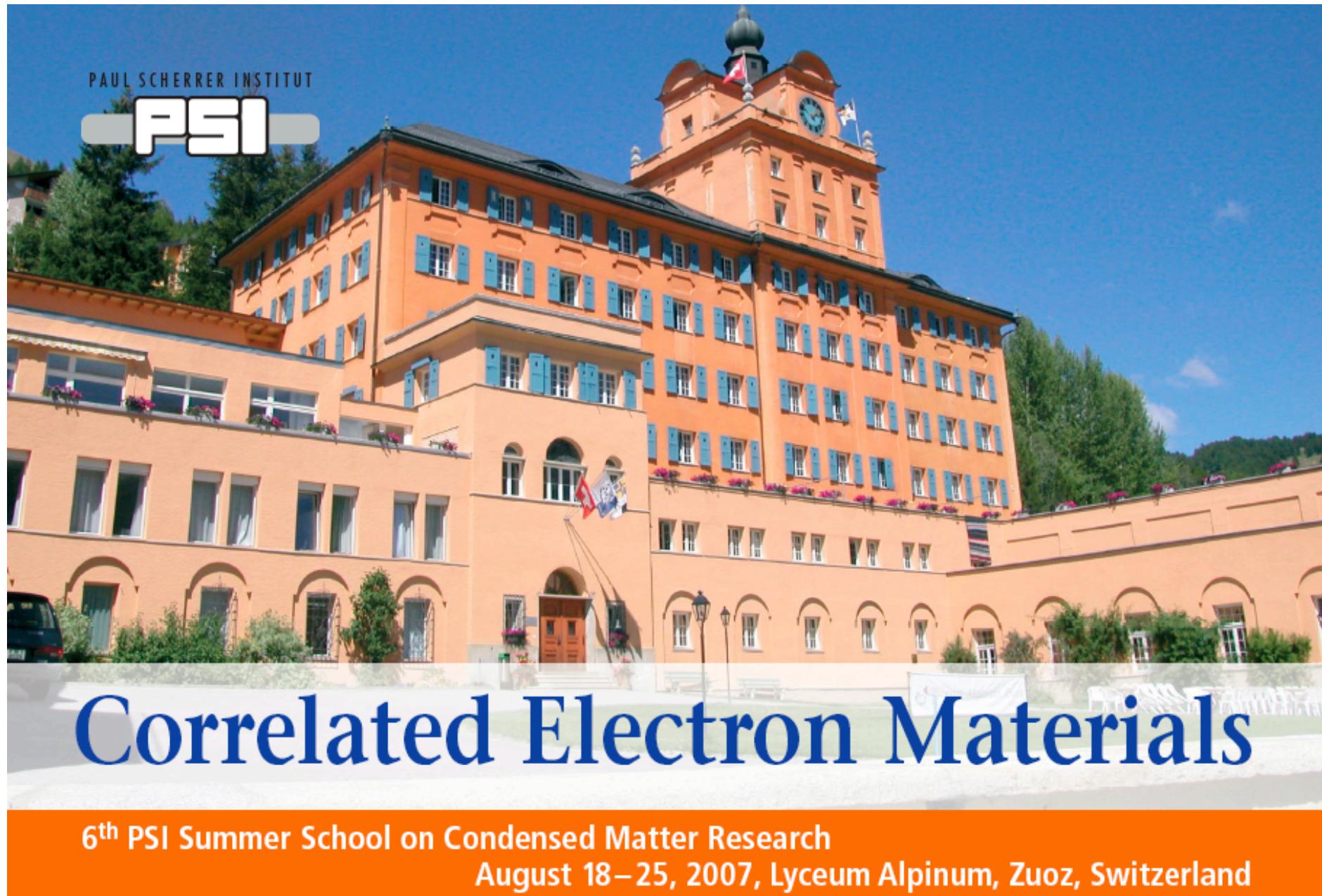
$g$  = electron - phonon coupling constant



In the limit of large  $\omega_0$ , the H-H model maps onto the Hubbard model with  $H_{\text{eff}} = U - 2g^2/\omega_0$ .

- Ref: W. Koller, et al, cond-mat/0312367v2 (2004).

- **Introductory References to the Hubbard Model**
- E. Koch, „Electronic Structure of Matter: Electron Correlations“, in „Probing the Nanoworld“, lecture manuscripts of the 38th Spring School, Jülich (2006).
- R.T. Scalettar, „Elementary Introduction to the Hubbard Model“, lecture notes, UC Davis,  
<http://leopard.physics.ucdavis.edu/rts/p210/hubbard7.pdf>
- M.P. March, „Condensed Matter Physics“, Wiley, 2000.



# Correlated Electron Materials

6<sup>th</sup> PSI Summer School on Condensed Matter Research

August 18–25, 2007, Lyceum Alpinum, Zuoz, Switzerland

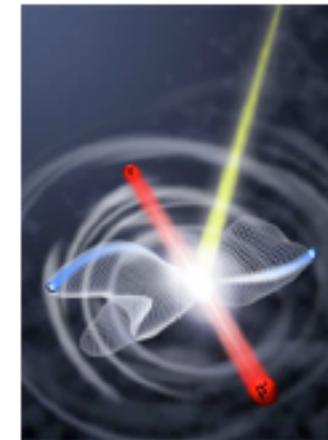
# Lectures on “Electron Correlations”

Proposal for a new lecture for Master and PhD students,  
2h Lecture +1h Exercises 5 (UZH) to 6 (ETHZ) Credit-Points

(English)

WS 07/08

By Bruce Patterson and Thomas Greber, UZH



- Some examples of 2-electron calculations:

$$c_{1\uparrow}^\dagger c_{2\uparrow} |\uparrow, \downarrow\rangle = c_{1\uparrow}^\dagger c_{2\uparrow} c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle = -c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger c_{2\uparrow} c_{1\uparrow}^\dagger |0\rangle = +c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger c_{2\uparrow} |0\rangle = 0$$

$$c_{1\downarrow}^\dagger c_{2\downarrow} |\cdot, \uparrow \downarrow\rangle = c_{1\downarrow}^\dagger c_{2\downarrow} c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle = c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle - c_{1\downarrow}^\dagger c_{2\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow}^\dagger |0\rangle = -c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle = -|\downarrow, \uparrow\rangle$$

$$c_{2\uparrow}^\dagger c_{1\uparrow} |\uparrow, \downarrow\rangle = c_{2\uparrow}^\dagger c_{1\uparrow} c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle = -c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger c_{1\uparrow} c_{1\uparrow}^\dagger |0\rangle = -c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle + c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger c_{1\uparrow} |0\rangle = c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle = |\cdot, \uparrow \downarrow\rangle$$