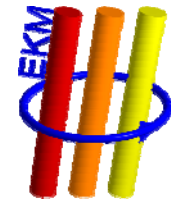




Center for Electronic Correlations and Magnetism  
University of Augsburg



# Construction of exact ground states for non-integrable lattice fermion models

WE-Heraeus-Seminar

*"Analytische und numerische Methoden korrelierter Elektronen"*

Physikzentrum Bad Honnef, 29. 9. 2010

Dieter Vollhardt

Supported by **DFG**

TRR 80 (Augsburg-Munich)



## Outline:

- Transformation of a Hamiltonian into positive semidefinite form
- Construction of exact many-electron ground states
- **Diamond** Hubbard chains  
**Triangle** Hubbard chains  
→ application to  $\text{CeRh}_3\text{B}_2$   
**Pentagon** Hubbard chains  
→ application to organic polymers

In collaboration with

Zsolt Gulacsi (Univ. Debrecen, Hungary)

Arno Kampf (Augsburg)

Highly desirable:  
Exact solutions of correlation models

# Construction of exact many-electron ground states from positive semidefinite Hamiltonians

## Strategy

Step 1: Transform many-electron Hamiltonian into positive semidefinite form

$$\hat{H} = \hat{H}_0 + \hat{H}_U = \sum_n \hat{P}_n + E_g \equiv \hat{H}' + E_g, \quad \hat{P}_n : \text{positive semidefinite operators}$$
$$\langle \psi | \hat{P}_n | \psi \rangle \geq 0$$
$$\text{e.g., } \hat{P}_n = \Omega^\dagger \Omega, \quad \Omega \Omega^\dagger$$

→ well-defined lower bound of spectrum

Transformation feasible

- in several different ways
- on a subspace of the full parameter space

# Construction of exact many-electron ground states from positive semidefinite Hamiltonians

**Strategy**

$$\hat{H} = \hat{H}_0 + \hat{H}_U = \sum_n \hat{P}_n + E_g \equiv \hat{H}' + E_g, \quad \hat{P}_n : \text{positive semidefinite}$$

$$\langle \psi | \hat{P}_n | \psi \rangle \geq 0$$

**Step 2: Construct many-electron ground state**

$$\hat{P}_n | \Psi_g \rangle = 0 \Rightarrow \hat{H} | \Psi_g \rangle = E_g | \Psi_g \rangle$$

ground state

ground-state energy

Construction of  $|\Psi_g\rangle$  depends on the structure of  $P_n$

**Guideline:**

a)  $P_n = \Omega^\dagger \Omega$

Ground state can have the form  $|\varphi_g\rangle = O^\dagger |0\rangle$ , with  $\{\Omega, O^\dagger\} = 0$

$\rightarrow P_n |\varphi_g\rangle = \Omega^\dagger \Omega O^\dagger |0\rangle = -\Omega^\dagger O^\dagger \Omega |0\rangle = 0$ ; then extend this property to all  $P_n$

b)  $P_n = \Omega \Omega^\dagger$

Use  $(\Omega^\dagger)^2 = 0$  and construct states  $|\psi_g\rangle = \Omega^\dagger |0\rangle$

$\rightarrow P_n |\psi_g\rangle = \Omega \Omega^\dagger \Omega^\dagger |0\rangle = 0$ ; then extend this property to all  $P_n$

## Construction of exact many-electron ground states from positive semidefinite Hamiltonians

**Strategy**

$$\hat{H} = \hat{H}_0 + \hat{H}_U = \sum_n \hat{P}_n + E_g \equiv \hat{H}' + E_g, \quad \hat{P}_n : \text{positive semidefinite}$$

**Step 3: Prove uniqueness of many-electron ground state:**

$$|\Psi_g\rangle \text{ spans } \ker(\hat{H}') := \{|\phi\rangle \mid \hat{H}'|\phi\rangle = 0\}$$

$$\langle \psi | \hat{P}_n | \psi \rangle \geq 0$$

$$\hat{H}' = \sum_{n=1}^L \hat{P}_n \rightarrow \ker(\hat{H}') = \bigcap_{n=1}^L \ker(\hat{P}_n)$$

→ Necessary and sufficient to prove that:

(i)  $|\Psi_g\rangle \in \ker(\hat{H}')$

(ii) all states  $|\Psi\rangle \in \bigcap_{n=1}^L \ker(\hat{P}_n)$  can be written in terms of the constructed ground state  $|\Psi_g\rangle$ .

- Works in any dimension
- No integrability required
- Applicable to any Hamiltonian with sufficiently many microscopic parameters (so far not possible for Hamiltonians with too simple structure)

In particular: Exact ground states with flat bands

Condensed matter systems with macroscopic degeneracies

- very sensitive reaction to perturbations
- emergent behavior

Examples:

- Electrons in a magnetic field in 2D Landau (1930)
- Spins on lattices with geometric frustration Moessner, Ramirez (2006)
- Dispersionless (“flat“) bands in solids Mielke (1991)  
Mielke, Tasaki (1993)  
Arita, Suwa Kuroki, Aoki (2002)

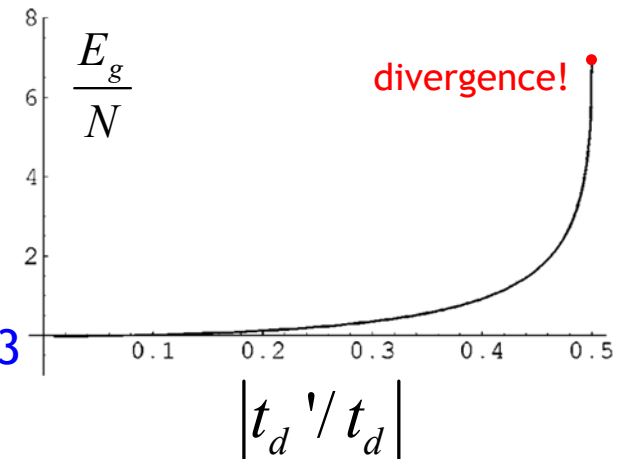
→ Find exact solutions of correlation models with flat bands

# Construction of exact many-electron ground states with flat bands from positive semidefinite Hamiltonians

|   |   |
|---|---|
| Hubbard model and PAM on decorated lattices in $d \geq 2$ at $U = \infty$ | Brandt, Gieseke (1992)                                    |
| PAM, Emery model in $d=1,2$ on regular lattices                           | Strack (1993)   |
| Ferromagnetism in extended Hubbard models for arbitrary $d$               | Strack, DV (1993, 1994, 1995)                             |
|   | de Boer, Schadschneider (1995); Kollar, Strack, DV (1996) |
| Composite operators defined on the entire unit cell                       | Orlik, Gulacsi (1998, 2001)                               |
| → PAM on regular lattices in $d=2,3$ at $U = \infty$                      |   |
| Application to $d=1$  | Sarasua, Continentino (2002)                              |
| PAM on regular lattices in $d=2,3$ at $U < \infty$                        | Gurin, Gulacsi (2001, 2002), Gulacsi (2002)               |
| Superconductivity in the extended Hubbard model                           | Montorsi, Campbell (1996), Laughlin (2006)                |

## PAM in $d=3$

- Exact insulating and itinerant (non-Fermi liquid) ground states at  $1/4$  and  $3/4$  filling
- First exact proof of ferromagnetism in the PAM in  $d=3$



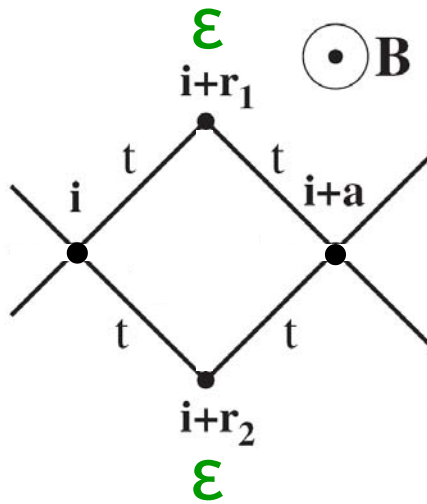
Gulacsi, DV (2003, 2005)

High sensitivity to small changes of microscopic parameters found

# 1. Exact many-electron ground states on diamond Hubbard chains

Flat bands in the single-electron band structure persist for  $U > 0$

Z. Gulacsi, A. Kampf, DV  
Phys. Rev. Lett. 99, 026404 (2007)



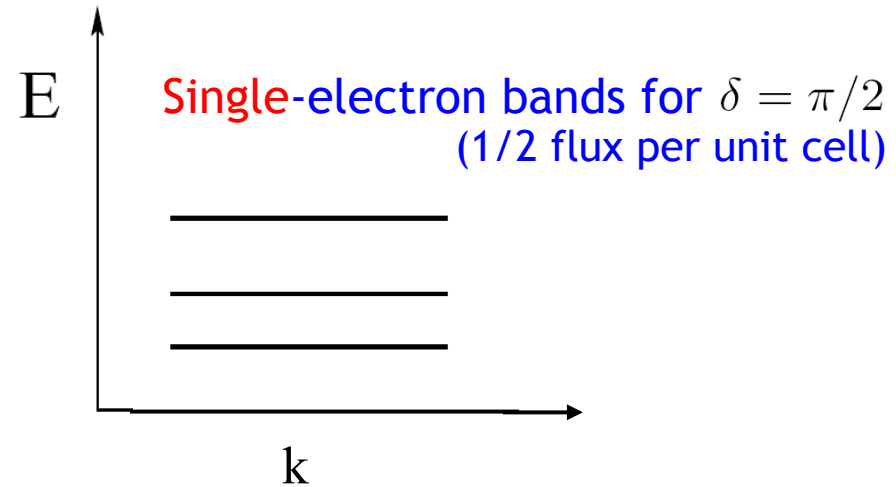
“Aharonov-Bohm cage”

Peierls phase factor

$$\delta = 2\pi\Phi/\Phi_0$$

$$\mathbf{A} \parallel \mathbf{a}$$

$$t_{j,j'}(\mathbf{B}) = t_{j,j'}(0) \exp[(i2\pi/\Phi_0) \int_j^{j'} \mathbf{A} \cdot d\mathbf{l}]$$



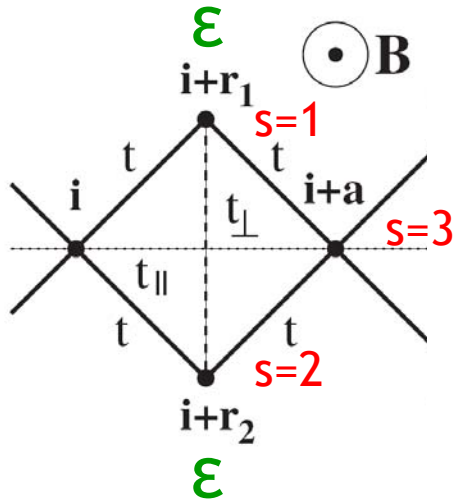
Vidal, Doucot, Mosseri, Butaud (2000):

$\epsilon=0$ ,  $\delta = \pi/2$ , 2 electrons: excited singlet eigenstates

- are localized for  $U=0$
- become delocalized for  $U>0$

→ Interaction  $U$  is able to induce subtle correlations leading to conducting states

Also valid for finite densities ?



3 sites per cell  $\rightarrow$  3 bands

$s=1,2,3$  sublattice index

$N_c$  = # cells

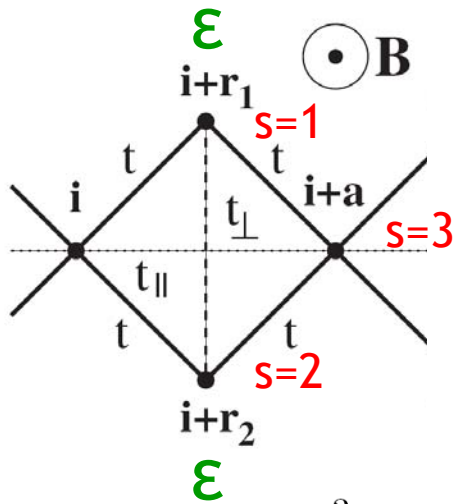
$N$  = # electrons

$n = \frac{N}{3N_c}$  electron density

$$\hat{H}_0 = \sum_{\sigma} \sum_{\mathbf{i}=1}^{N_c} \{ [t e^{i\frac{\delta}{2}} (\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma}^{\dagger} \hat{c}_{\mathbf{i},\sigma} + \hat{c}_{\mathbf{i}+\mathbf{a},\sigma}^{\dagger} \hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma} + \hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma}^{\dagger} \hat{c}_{\mathbf{i}+\mathbf{a},\sigma} + \hat{c}_{\mathbf{i},\sigma}^{\dagger} \hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma}) + t_{\perp} \hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma}^{\dagger} \hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma} + t_{\parallel} \hat{c}_{\mathbf{i}+\mathbf{a},\sigma}^{\dagger} \hat{c}_{\mathbf{i},\sigma} + H.c.] + \varepsilon \sum_{s=1,2} \hat{n}_{\mathbf{i}+\mathbf{r}_s,\sigma} \}$$

$$\hat{H}_U = U \sum_{\mathbf{i}=1}^{N_c} \sum_{s=1}^3 \hat{n}_{\mathbf{i}+\mathbf{r}_s,\uparrow} \hat{n}_{\mathbf{i}+\mathbf{r}_s,\downarrow}$$

$$\hat{H} = \hat{H}_0 + \hat{H}_U$$



3 sites per cell  $\rightarrow$  3 bands

$s=1,2,3$  sublattice index

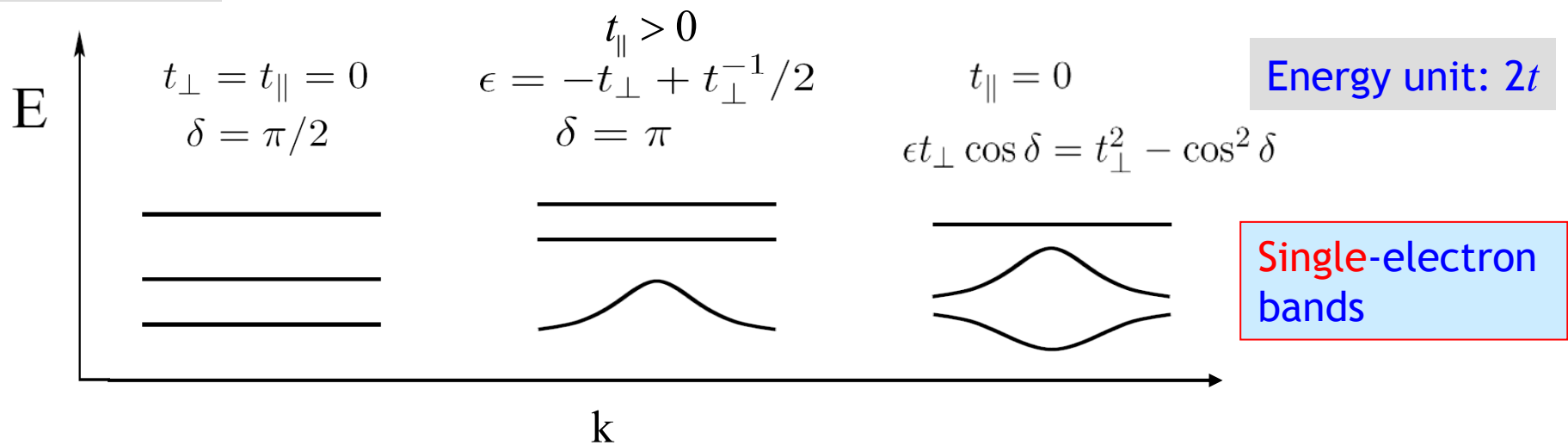
$N_c = \#$  cells

$N = \#$  electrons

$n = \frac{N}{3N_c}$  electron density

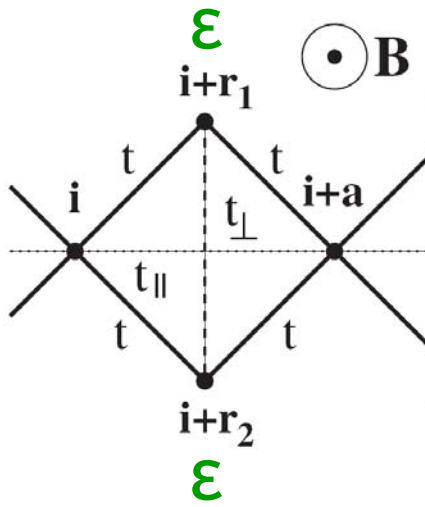
**FT** 
$$\hat{H}_0 = \sum_{\mathbf{k}, \sigma} \sum_{s, s'=1}^3 M_{s, s'}(\mathbf{k}) \hat{c}_{s, \mathbf{k}, \sigma}^\dagger \hat{c}_{s', \mathbf{k}, \sigma}$$

Examples:

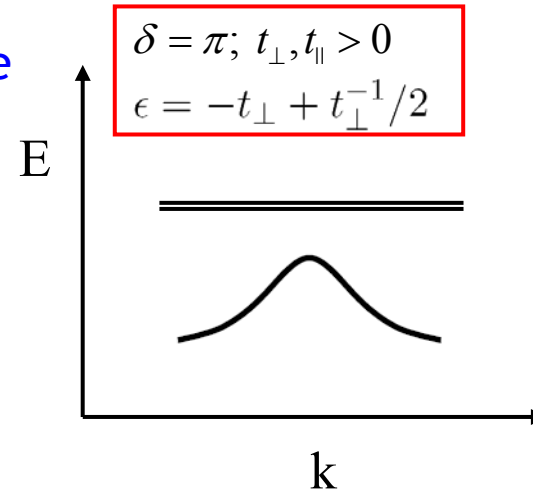


Solution I: Correlated half-metal

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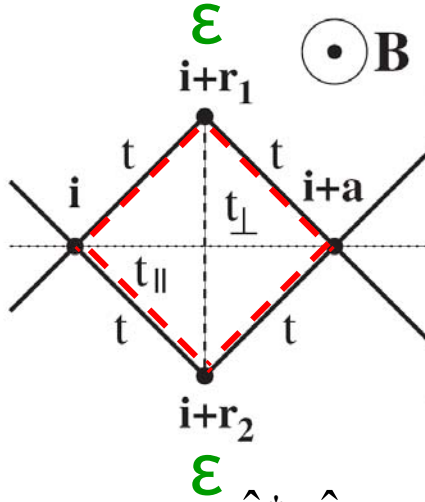


→ Investigate



Single-electron bands

## 1. Transformation of the Hamiltonian into positive semidefinite form



$\hat{H}_0$  Define non-canonical fermionic operators:  
One composite operator on each plaquette

$$\hat{A}_{i,\sigma} = a_1 \hat{c}_{i\sigma} + a_2 \hat{c}_{i+r_2\sigma} + a_3 \hat{c}_{i+a\sigma} + a_4 \hat{c}_{i+r_1\sigma}$$

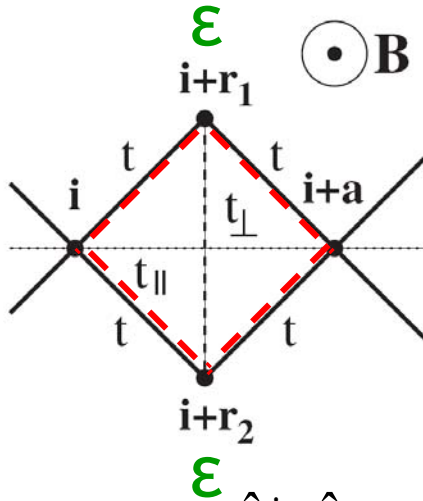
$$(\hat{A}_{i,\sigma})^2 = 0$$

$$\{\hat{A}_{i,\sigma}, \hat{A}_{j,\sigma}^\dagger\} \neq \delta_{i,j}$$

$$\begin{aligned} \Rightarrow \hat{A}_{i\sigma}^\dagger \hat{A}_{i\sigma} &= (a_2^* a_1 \hat{c}_{i+r_2\sigma}^\dagger \hat{c}_{i\sigma} + a_3^* a_2 \hat{c}_{i+a\sigma}^\dagger \hat{c}_{i+r_2\sigma} + a_4^* a_3 \hat{c}_{i+r_1\sigma}^\dagger \hat{c}_{i+a\sigma} + \\ & a_1^* a_4 \hat{c}_{i\sigma}^\dagger \hat{c}_{i+r_1\sigma} + a_2^* a_4 \hat{c}_{i+r_2\sigma}^\dagger \hat{c}_{i+r_1\sigma} + a_3^* a_1 \hat{c}_{i+a\sigma}^\dagger \hat{c}_{i\sigma} + \text{H.c.}) + \\ & |a_1|^2 n_{i\sigma} + |a_2|^2 n_{i+r_2\sigma} + |a_3|^2 n_{i+a\sigma} + |a_4|^2 n_{i+r_1\sigma} \end{aligned}$$

$$\begin{aligned} -\sum_{i\sigma} \hat{A}_{i\sigma}^\dagger \hat{A}_{i\sigma} &= \hat{H}_0 = \sum_{\sigma} \sum_{\mathbf{i}=1}^{N_c} \{ [t e^{i\frac{\delta}{2}} (\hat{c}_{\mathbf{i}+r_2,\sigma}^\dagger \hat{c}_{\mathbf{i},\sigma} + \hat{c}_{\mathbf{i}+a,\sigma}^\dagger \hat{c}_{\mathbf{i}+r_2,\sigma} + \\ & \hat{c}_{\mathbf{i}+r_1,\sigma}^\dagger \hat{c}_{\mathbf{i}+a,\sigma} + \hat{c}_{\mathbf{i},\sigma}^\dagger \hat{c}_{\mathbf{i}+r_1,\sigma}) + t_{\perp} \hat{c}_{\mathbf{i}+r_2,\sigma}^\dagger \hat{c}_{\mathbf{i}+r_1,\sigma} + \\ & t_{\parallel} \hat{c}_{\mathbf{i}+a,\sigma}^\dagger \hat{c}_{\mathbf{i},\sigma} + \text{H.c.}] + \epsilon \sum_{s=1,2} \hat{n}_{\mathbf{i}+r_s,\sigma} \} \end{aligned}$$

# 1. Transformation of the Hamiltonian into positive semidefinite form



$\hat{H}_0$  Define non-canonical fermionic operators:  
One composite operator on each plaquette

$$\hat{A}_{i,\sigma} = a_1 \hat{c}_{i\sigma} + a_2 \hat{c}_{i+r_2\sigma} + a_3 \hat{c}_{i+a\sigma} + a_4 \hat{c}_{i+r_1\sigma}$$

$$(\hat{A}_{i,\sigma})^2 = 0$$

$$\{\hat{A}_{i,\sigma}, \hat{A}_{j,\sigma}^\dagger\} \neq \delta_{i,j}$$

$$\begin{aligned} \Rightarrow \hat{A}_{i\sigma}^\dagger \hat{A}_{i\sigma} &= (a_2^* a_1 \hat{c}_{i+r_2\sigma}^\dagger \hat{c}_{i\sigma} + a_3^* a_2 \hat{c}_{i+a\sigma}^\dagger \hat{c}_{i+r_2\sigma} + a_4^* a_3 \hat{c}_{i+r_1\sigma}^\dagger \hat{c}_{i+a\sigma} + \\ & a_1^* a_4 \hat{c}_{i\sigma}^\dagger \hat{c}_{i+r_1\sigma} + a_2^* a_4 \hat{c}_{i+r_2\sigma}^\dagger \hat{c}_{i+r_1\sigma} + a_3^* a_1 \hat{c}_{i+a\sigma}^\dagger \hat{c}_{i\sigma} + \text{H.c.}) + \\ & |a_1|^2 n_{i\sigma} + |a_2|^2 n_{i+r_2\sigma} + |a_3|^2 n_{i+a\sigma} + |a_4|^2 n_{i+r_1\sigma} \end{aligned}$$

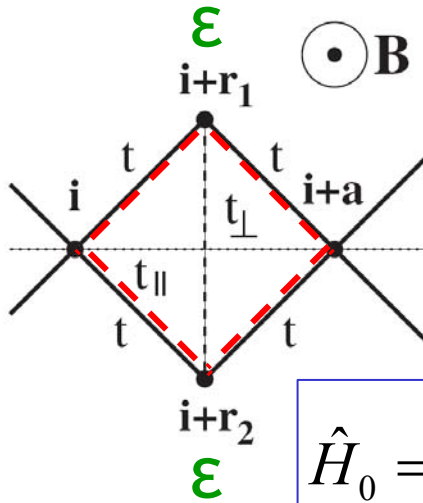
$$-\sum_{i\sigma} \hat{A}_{i\sigma}^\dagger \hat{A}_{i\sigma} \stackrel{!}{=} \hat{H}_0 \Rightarrow$$

$$\begin{aligned} a_2^* a_1 &= a_3^* a_2 = a_4^* a_3 = a_1^* a_4 = -te^{i\delta/2} \\ a_2^* a_4 &= -t_\perp \\ a_3^* a_1 &= -t_\parallel \\ |a_1|^2 + |a_3|^2 &= \varepsilon + |a_2|^2 = \varepsilon + |a_4|^2 \end{aligned}$$

$\Rightarrow$

$$\begin{aligned} \hat{A}_{i,\sigma} &= \sqrt{t_\parallel} [\hat{c}_{i,\sigma} - \hat{c}_{i+a,\sigma} \\ & - 2t_\perp e^{i\delta/2} (\hat{c}_{i+r_1,\sigma} - \hat{c}_{i+r_2,\sigma})] \end{aligned}$$

# 1. Transformation of the Hamiltonian into positive semidefinite form



$$\hat{H}_0 = -\sum_{i\sigma} \hat{A}_{i\sigma}^\dagger \hat{A}_{i\sigma} \quad \text{!} \quad + \sum_{i\sigma} \hat{A}_{i\sigma} \hat{A}_{i\sigma}^\dagger - 2N_c \sum_{m=1}^4 |a_m|^2$$

Positive semidefinite

$$\hat{H}_U$$

$$\hat{H}_U = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = U\hat{P} + U\hat{N} - UN_c$$

$N_c$ : # unit cells

$$\hat{P} = \sum_i \hat{P}_i, \quad \hat{P}_i = (\hat{n}_{i\uparrow} - 1)(\hat{n}_{i\downarrow} - 1) = \begin{cases} 1, & \text{unoccupied site} \\ 0, & \text{at least one electron} \end{cases}$$

$$\Rightarrow \hat{H} = \sum_{i,\sigma} \hat{A}_{i,\sigma} \hat{A}_{i,\sigma}^\dagger + U\hat{P} + E_g^I$$

positive semidefinite

$$E_g^I = (\epsilon + U + t_\perp)N - N_c[3U + 4t_\perp + 1/t_\perp]$$

## 2. Construction of the ground state

$$\hat{H} = \sum_{\mathbf{i}, \sigma} \hat{A}_{\mathbf{i}, \sigma} \hat{A}_{\mathbf{i}, \sigma}^\dagger + U \hat{P} + E_g^I$$

positive semidefinite

$$\hat{P} = \sum_{\mathbf{i}} \hat{P}_{\mathbf{i}}, \quad \hat{P}_{\mathbf{i}} = (\hat{n}_{\mathbf{i}\uparrow} - 1)(\hat{n}_{\mathbf{i}\downarrow} - 1) = \begin{cases} 1, & \text{unoccupied site} \\ 0, & \text{at least one electron} \end{cases}$$

Ground state for  $U > 0$ :  $\hat{A}_{i\sigma}^\dagger |\Psi_g\rangle = 0$  and  $\hat{P} |\Psi_g\rangle = 0 \Rightarrow \hat{H} |\Psi_g\rangle = E_g |\Psi_g\rangle$

$$\Rightarrow |\Psi_g^I(4N_c)\rangle \propto \prod_{\mathbf{i}} \hat{A}_{\mathbf{i}, -\sigma}^\dagger \hat{A}_{\mathbf{i}, \sigma}^\dagger |0\rangle$$

Creates one  $\sigma$  and one  $-\sigma$  electron in each unit cell

At least one electron required at each site

$$\hat{F}_\sigma^\dagger = \prod_{\mathbf{i}} [\hat{c}_{\mathbf{i}+\mathbf{r}_{s_{\mathbf{i},1}, \sigma}}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_{s_{\mathbf{i},2}, \sigma}}^\dagger]$$

Creates two more electrons with fixed spin  $\sigma$  on arbitrary sites of each unit cell

Ground state for

$$\delta = \pi; t_\perp, t_\parallel > 0$$

$$\epsilon = -t_\perp + t_\perp^{-1}/2$$

$$|\Psi_g^I(4N_c)\rangle = c \left[ \prod_{\mathbf{i}} \hat{A}_{\mathbf{i}, -\sigma}^\dagger \hat{A}_{\mathbf{i}, \sigma}^\dagger \right] \hat{F}_\sigma^\dagger |0\rangle$$

$$N = 4N_c \Leftrightarrow n = 4/3$$

$$n_\sigma = 1, n_{-\sigma} = 1/3$$

3. Proof of the uniqueness of the ground state  $|\Psi_g^I(4N_c)\rangle$ 

Prove  $|\Psi_g^I(4N_c)\rangle$  spans  $\ker(\hat{H}') := \{|\phi\rangle \mid \hat{H}'|\phi\rangle = 0\}$ ,  $\hat{H}' \equiv \hat{H} - E_g$

$$\Leftrightarrow \text{a) } |\Psi_g^I(4N_c)\rangle \in \ker(\hat{H}')$$

b) all states  $|\psi\rangle \in \ker(\hat{H}')$  can be written in the form

$$|\Psi_g^I(4N_c)\rangle = c \left[ \prod_{\mathbf{i}} \hat{A}_{\mathbf{i},-\sigma}^\dagger \hat{A}_{\mathbf{i},\sigma}^\dagger \right] \hat{F}_\sigma^\dagger |0\rangle$$

$$\hat{H}' = \sum_{n=1}^L \hat{P}_n \Rightarrow \ker(\hat{H}') = \bigcap_{n=1}^L \ker(\hat{P}_n)$$

Here: 
$$\hat{H}' = \sum_{\sigma} \sum_{\mathbf{i}=1}^{N_c} \hat{A}_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma}^\dagger + U \hat{P}$$

$$\Rightarrow \ker(\hat{H}') = \bigcap_{\sigma=\uparrow,\downarrow} \bigcap_{\mathbf{i}=1}^{N_c} \ker(\hat{A}_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma}^\dagger) \cap \ker(\hat{P})$$

**Theorem 1:**  $\ker(\hat{A}_{i\sigma}\hat{A}_{i\sigma}^\dagger)$  is spanned by vectors of the form  $|\Psi\rangle = \hat{A}_{i\sigma}^\dagger \hat{W} |0\rangle$ ,  
where  $\hat{W}$  is an arbitrary operator, as long as  $\langle \Psi | \Psi \rangle \neq 0$ .

**Proof:**

$$\text{a) } \hat{A}_{i\sigma}\hat{A}_{i\sigma}^\dagger |\Psi\rangle \stackrel{(\hat{A}_{i\sigma}^\dagger)^2=0}{=} 0 \Rightarrow |\Psi\rangle \in \ker(\hat{A}_{i\sigma}\hat{A}_{i\sigma}^\dagger) \quad \checkmark$$

b) To show that all vectors  $|\Psi\rangle \in \ker(\hat{A}_{i\sigma}\hat{A}_{i\sigma}^\dagger)$  can be written  
in the form  $|\Psi\rangle = \hat{A}_{i\sigma}^\dagger \hat{W} |0\rangle$  we assume  $|\Phi\rangle = \hat{Y} |0\rangle \in \ker(\hat{A}_{i\sigma}\hat{A}_{i\sigma}^\dagger)$ , i.e.,  $\hat{A}_{i\sigma}\hat{A}_{i\sigma}^\dagger \hat{Y} |0\rangle = 0$ .

$$\Rightarrow |\Phi\rangle = \hat{Y} |0\rangle \stackrel{\{\hat{A}_{i\sigma}, \hat{A}_{i\sigma}^\dagger\} = a_{i\sigma} = \text{const}}{=} \frac{1}{a_{i\sigma}} (\cancel{\hat{A}_{i\sigma}\hat{A}_{i\sigma}^\dagger} + \hat{A}_{i\sigma}^\dagger \hat{A}_{i\sigma}) \hat{Y} |0\rangle = \hat{A}_{i\sigma}^\dagger \underbrace{\left( \frac{1}{a_{i\sigma}} \hat{A}_{i\sigma} \hat{Y} \right)}_{\hat{W}} |0\rangle = \hat{A}_{i\sigma}^\dagger \hat{W} |0\rangle \quad \text{q.e.d.}$$

**Theorem 2:**  $\ker\left(\sum_{\sigma} \sum_{i=1}^{N_c} \hat{A}_{i\sigma}\hat{A}_{i\sigma}^\dagger\right)$  is spanned by vectors of the form  $|\Psi\rangle = \left[\prod_{\sigma} \prod_{i=1}^{N_c} \hat{A}_{i\sigma}^\dagger\right] \hat{W} |0\rangle$ ,  
where  $\hat{W}$  is an arbitrary operator, as long as  $\langle \Psi | \Psi \rangle \neq 0$ .

**Proof:** simple (since  $\hat{A}_{i\sigma}$  are linearly independent)

q.e.d.

$$\ker(\hat{H}') = \bigcap_{\sigma=\uparrow,\downarrow} \bigcap_{i=1}^{N_c} \ker(\hat{A}_{i\sigma} \hat{A}_{i\sigma}^\dagger) \cap \ker(\hat{P})$$

↑  
Spanned by states which have  
at least one electron per site

$$\Rightarrow |\Psi\rangle = \left[ \prod_{\sigma} \prod_{i=1}^{N_c} \hat{A}_{i\sigma}^\dagger \right] \hat{W} |0\rangle \text{ spans } \ker(\hat{H}),$$

provided the form of  $\hat{W}$  is compatible with  $\ker(\hat{P})$ .

**Theorem 3:** For  $N=4N_c$ ,  $\hat{W} = \hat{F}_\sigma^\dagger = \prod_i [\hat{c}_{i+r_{s_{i,1}},\sigma}^\dagger \hat{c}_{i+r_{s_{i,2}},\sigma}^\dagger]$

↑  
Creates two electrons with fixed spin  $\sigma$   
on arbitrary sites of each unit cell

**Proof:**

(I)  $\hat{W} = \hat{F}_\sigma^\dagger$  is a possible choice (rather simple)

(II)  $\hat{W} = \hat{F}_\sigma^\dagger$  is the unique choice (a little more difficult)      q.e.d.

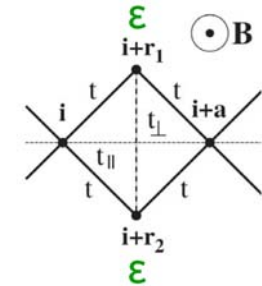
Solution I: Correlated half-metal

For  $\delta = \pi; t_{\perp}, t_{\parallel} > 0$   
 $\epsilon = -t_{\perp} + t_{\perp}^{-1}/2$

$n = 4/3: n_{\sigma} = 1, n_{-\sigma} = 1/3$

$$|\Psi_g^I(4N_c)\rangle = c \left[ \prod_{\mathbf{i}} \hat{A}_{\mathbf{i},-\sigma}^{\dagger} \hat{A}_{\mathbf{i},\sigma}^{\dagger} \right] \hat{F}_{\sigma}^{\dagger} |0\rangle$$

is the **unique** ground state



Physical properties:

One  $\sigma$  electron on every lattice site  $\rightarrow$  localized

$-\sigma$  electrons:

Expectation value of hopping term:  $\Gamma_{\mathbf{r},-\sigma} = \langle \hat{c}_{\mathbf{j},-\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r},-\sigma} + H.c. \rangle$

$$\Gamma_{m,-\sigma} \stackrel{N_c \rightarrow \infty}{=} \frac{(-1)^m}{\sqrt{1+1/t_{\perp}}} e^{-m/\xi_{-\sigma}} \quad , r/a = m$$

$\rightarrow$   $-\sigma$  electrons: spatially extended but localized for  $N_c \rightarrow \infty$

$N_c$ : # unit cells

Solution I: Correlated half-metal

Add  $\Delta N$  many  $-\sigma$  electrons  $\rightarrow n_\sigma = 1, n_{-\sigma} = 1/3 + \Delta N / N_c$

$N_c$ : # unit cells

Ground state

$$|\Psi_g^I(4N_c + \Delta N)\rangle = \prod_{\alpha=1}^{\Delta N} \hat{c}_{n_\alpha, \mathbf{k}_\alpha, -\sigma}^\dagger |\Psi_g^I(4N_c)\rangle \quad n_\alpha : s = 1, 2, 3$$

Physical properties:

- plane wave-type states due to  $-\sigma$  electrons
- charge gap  $\Delta\mu = E_g(N) - 2E_g(N-1) + E_g(N-2) = 0$   
 $\rightarrow \Delta N$   $-\sigma$  electrons **itinerant**

Conclusion:

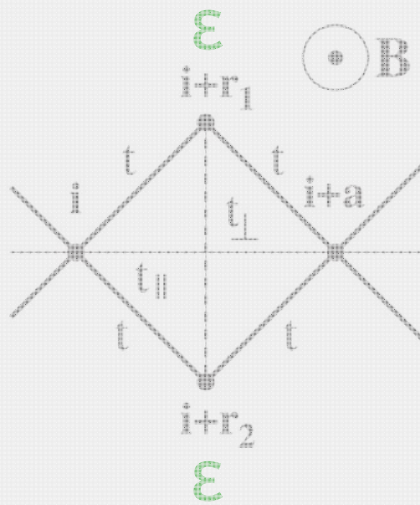
Ground state for  
 $4/3 < n < 5/3$

- $3N_c$  immobile  $\sigma$  electrons
- $N_c$   $-\sigma$  electrons confined to localized Wannier function  
 +  $\Delta N$  conducting  $-\sigma$  electrons
- Magnetization  $M \propto (1 - \Delta N / N_c) \xrightarrow{\Delta N \rightarrow N_c} 0$   
 $\rightarrow$  Low carrier-density metallic behavior

U=0: dispersionless, localized electrons  
 U>0: **correlation-induced half-metal**

Solution II:  
Exact ground states for general magnetic flux

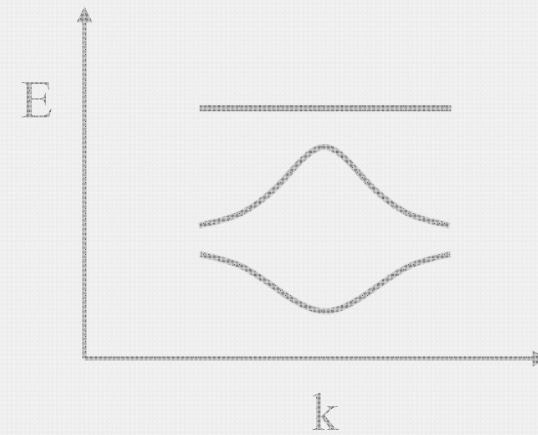
Solution II: Exact ground states for general magnetic flux



$$\delta \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$$

$$t_{\parallel} = 0, t_{\perp} < 0$$

$$b \equiv -\cos \delta / t_{\perp}, \quad \epsilon = b - b^{-1}$$



Single-electron bands

Ground states for  $n \geq 5/3$

$B = 0$ : localized  
non-magnetic  
ground state for  
 $n \geq 5/3$

$B \neq 0$

Non-saturated ferromagnet  
• insulating for  $n=5/3$   
• metallic for  $n > 5/3$

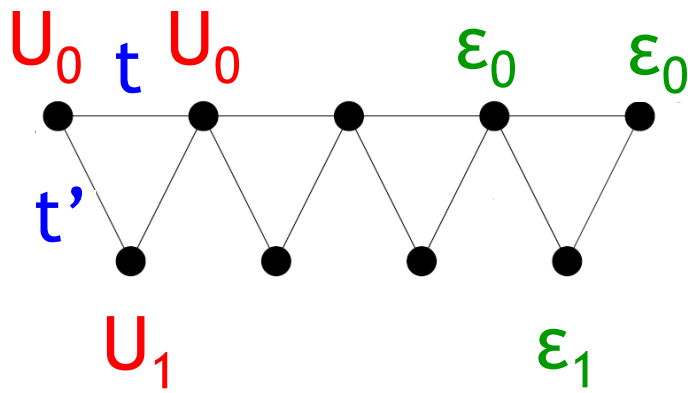
Conclusion

- Diamond Hubbard chain has remarkably complex properties
- Switch between different ground states by variation of  $B$ ,  $\epsilon$ ,  $n$

## 2. Exact many-electron ground states on triangle Hubbard chains

Flat bands in the single-electron band structure persist for  $U > 0$

Z. Gulacsi, A. Kampf, DV  
Prog. Theor. Phys. Suppl. 176, 1 (2008)



2 sites per cell  $\rightarrow$  2 bands

$N_c = \#$  cells

$N = \#$  electrons

$n = \frac{N}{2N_c}$  electron density

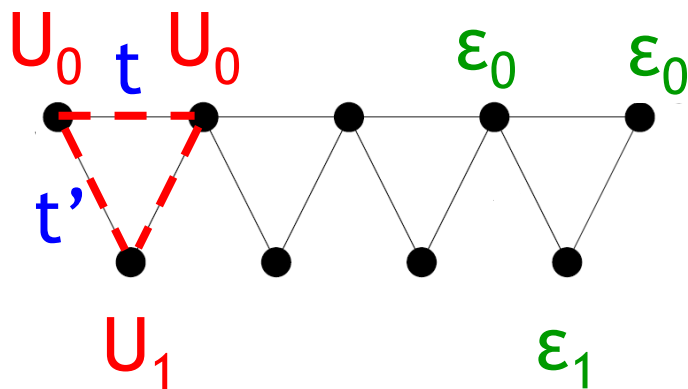
Müller-Hartmann (1995)

Penc, Shiba, Mila, Tsukagoshi (1996)

Fazekas (1997)

Derzho, Honecker, Richter (2007)

Derzho, Honecker, Richter, Maksymenko, Moessner (2010)



2 sites per cell  $\rightarrow$  2 bands

$N_c = \#$  cells

$N = \#$  electrons

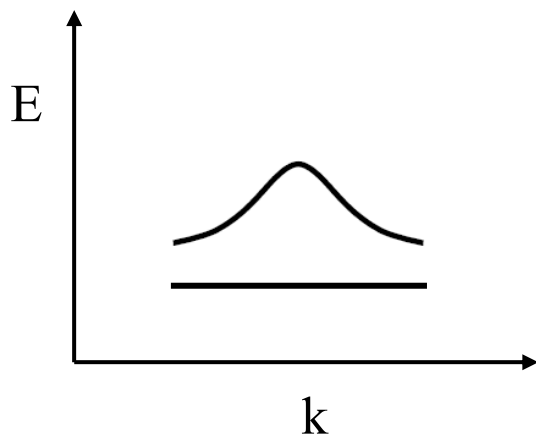
$n = \frac{N}{2N_c}$  electron density

$$\frac{(t')^2}{t} = \epsilon_1 - \epsilon_0 + 2t, \quad t > 0$$

**Solution I:**

$U_0, U_1 > 0$

$$\epsilon_1 - \epsilon_0 > -2t$$



Single-electron bands

Step 1  $\hat{A}_{i,\sigma} = \sqrt{t} [\hat{c}_{i,\sigma} + \hat{c}_{i+a,\sigma} + (t'/t)\hat{c}_{i+r,\sigma}]$

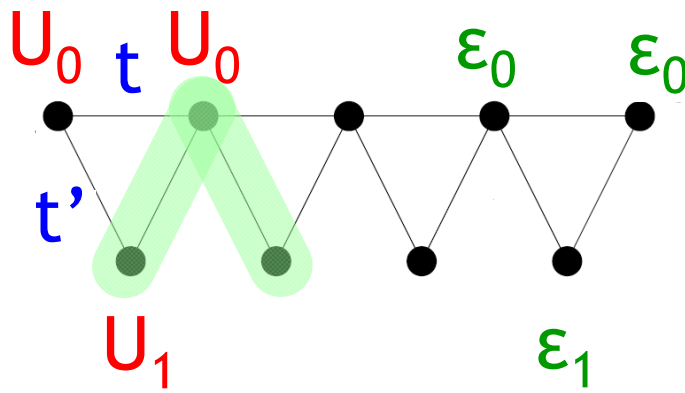
Positive semidefinite  $\hat{H}^{tri} = \sum_{i,\sigma} \hat{A}_{i,\sigma}^\dagger \hat{A}_{i,\sigma} + K\hat{N} + H_U^{tri}$   
 $K = \epsilon_0 - 2t$

Step 2

Construct operators  $B$  with  $\{\hat{A}_{i,\sigma}, \hat{B}_{i',\sigma'}^\dagger\} = 0$

$$\hat{B}_{i,\sigma}^\dagger = [\hat{c}_{i-a+r,\sigma}^\dagger + \hat{c}_{i+r,\sigma}^\dagger - (t'/t)\hat{c}_{i,\sigma}^\dagger]$$

Ground state  $|\Psi^{tri}(N)\rangle = \prod_i \hat{B}_{i,\sigma_i}^\dagger |0\rangle$



2 sites per cell  $\rightarrow$  2 bands

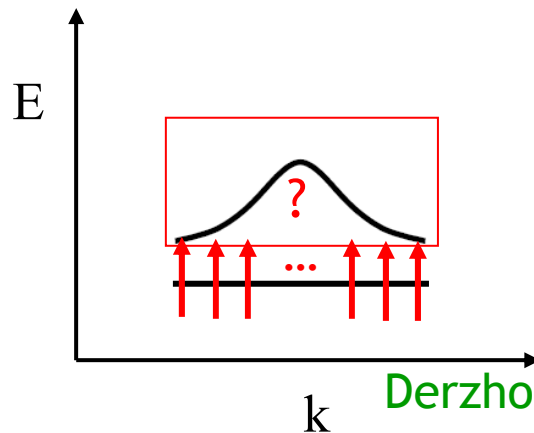
$N_c = \#$  cells

$N = \#$  electrons

$n = \frac{N}{2N_c}$  electron density

$$\frac{(t')^2}{t} = \epsilon_1 - \epsilon_0 + 2t, \quad t > 0$$

$$\epsilon_1 - \epsilon_0 > -2t$$



Derzho, Honecker, Richter, Maksymenko, Moessner (2010)

$$\hat{H} = \hat{H}_0 + \hat{H}_U$$

Solution I:

$$U_0, U_1 > 0$$

$n < 1/2$  : ferromagnetic clusters

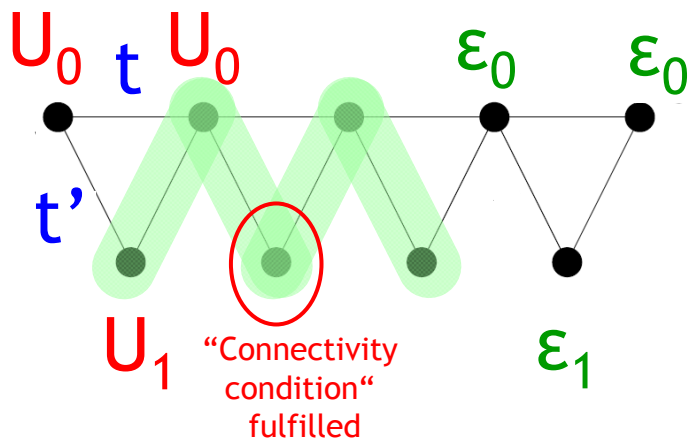
$n = 1/2$  : fully saturated ferromagnet

Mielke, Tasaki (1993)

Derzho, Honecker, Richter (2007)

$\rightarrow$  Flat-band ferromagnetism: Realizes ideas of Gutzwiller and Kanamori from 1963 about the origin of itinerant ferromagnetism

Not related to Stoner theory:  $\chi(\omega=0, \mathbf{q}=0) = \infty \rightarrow UN(E_F)=1$



2 sites per cell  $\rightarrow$  2 bands

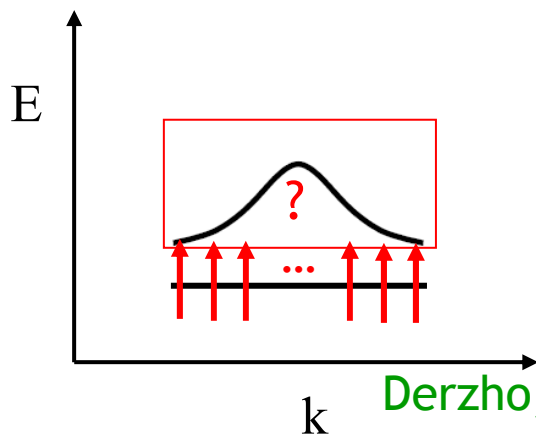
$N_c = \#$  cells

$N = \#$  electrons

$n = \frac{N}{2N_c}$  electron density

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Derzho, Honecker, Richter, Maksymenko, Moessner (2010)

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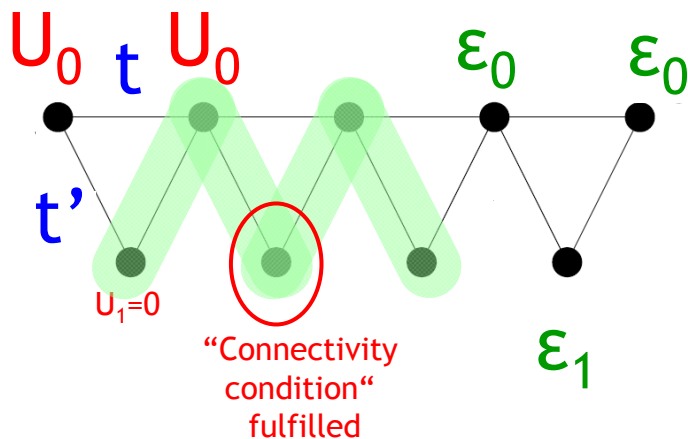
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2 sites per cell  $\rightarrow$  2 bands

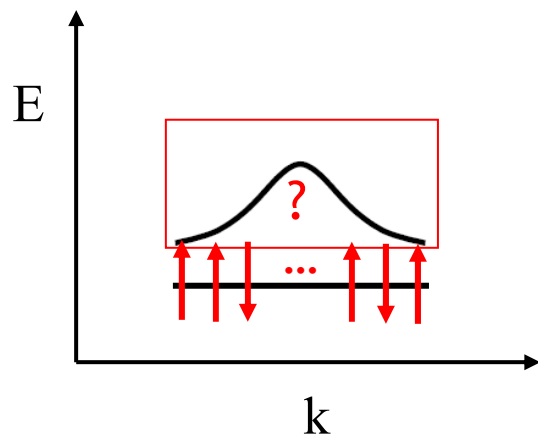
$$N_c = \# \text{ cells}$$

$$N = \# \text{ electrons}$$

$$n = \frac{N}{2N_c} \text{ electron density}$$

$$\frac{(t')^2}{t} = \epsilon_1 - \epsilon_0 + 2t, \quad t > 0$$

$$\epsilon_1 - \epsilon_0 > -2t$$



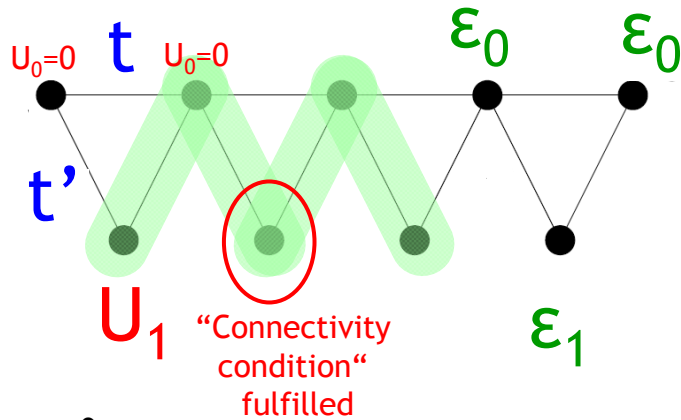
$$\hat{H} = \hat{H}_0 + \hat{H}_U$$

Solution II:

$$U_0 > 0, \quad U_1 = 0$$

$n=1/2$  : non-magnetic

$U_1=0$ : electrons uncorrelated on sites where Wannier functions connect



2 sites per cell  $\rightarrow$  2 bands

$N_c = \#$  cells

$N = \#$  electrons

$n = \frac{N}{2N_c}$  electron density

$$\frac{(t')^2}{t} = \epsilon_1 - \epsilon_0 + 2t, \quad t > 0$$

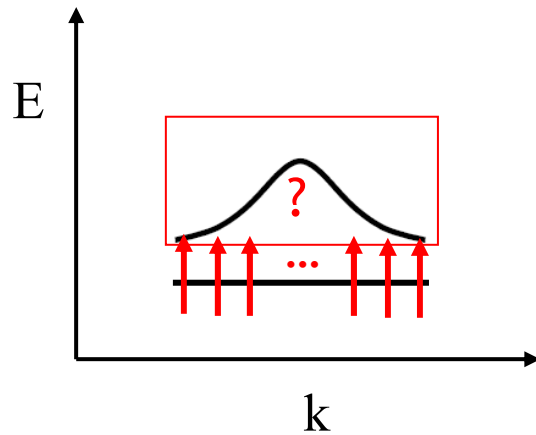
$$\epsilon_1 - \epsilon_0 > -2t$$

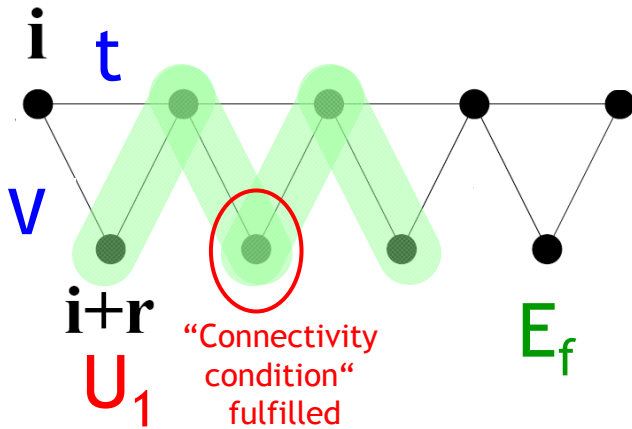
$$\hat{H} = \hat{H}_0 + \hat{H}_U$$

Solution III:

$$U_0 = 0, \quad U_1 > 0$$

$n=1/2$  : fully saturated ferromagnet





2 sites per cell  $\rightarrow$  2 bands

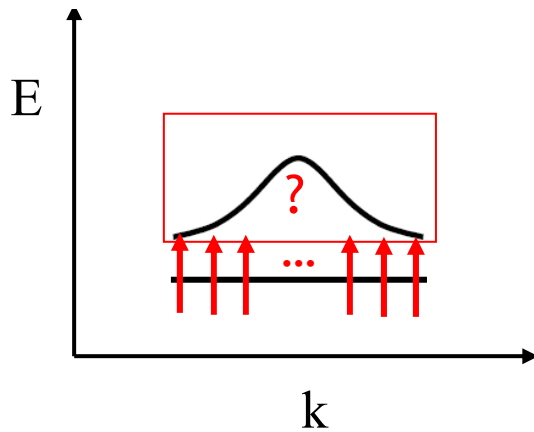
$$N_c = \# \text{ cells}$$

$$N = \# \text{ electrons}$$

$$n = \frac{N}{2N_c} \text{ electron density}$$

$$\frac{V^2}{t} = E_f + 2t, \quad t > 0$$

$$E_f > -2t$$



$$\hat{H} = \hat{H}_0 + \hat{H}_U$$

Solution III:

$$U_0 = 0, \quad U_1 > 0$$

$n=1/2$  : fully saturated ferromagnet

Change of notation:  $\hat{d}_{i,\sigma} \equiv \hat{c}_{i,\sigma}$ ,

$$\hat{f}_{i,\sigma} \equiv \hat{c}_{i+r,\sigma}, \quad V \equiv t', \quad E_f \equiv \epsilon_1, \quad \epsilon_0 = 0$$

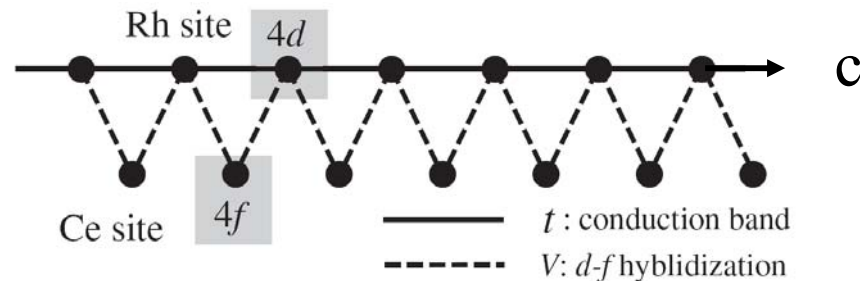
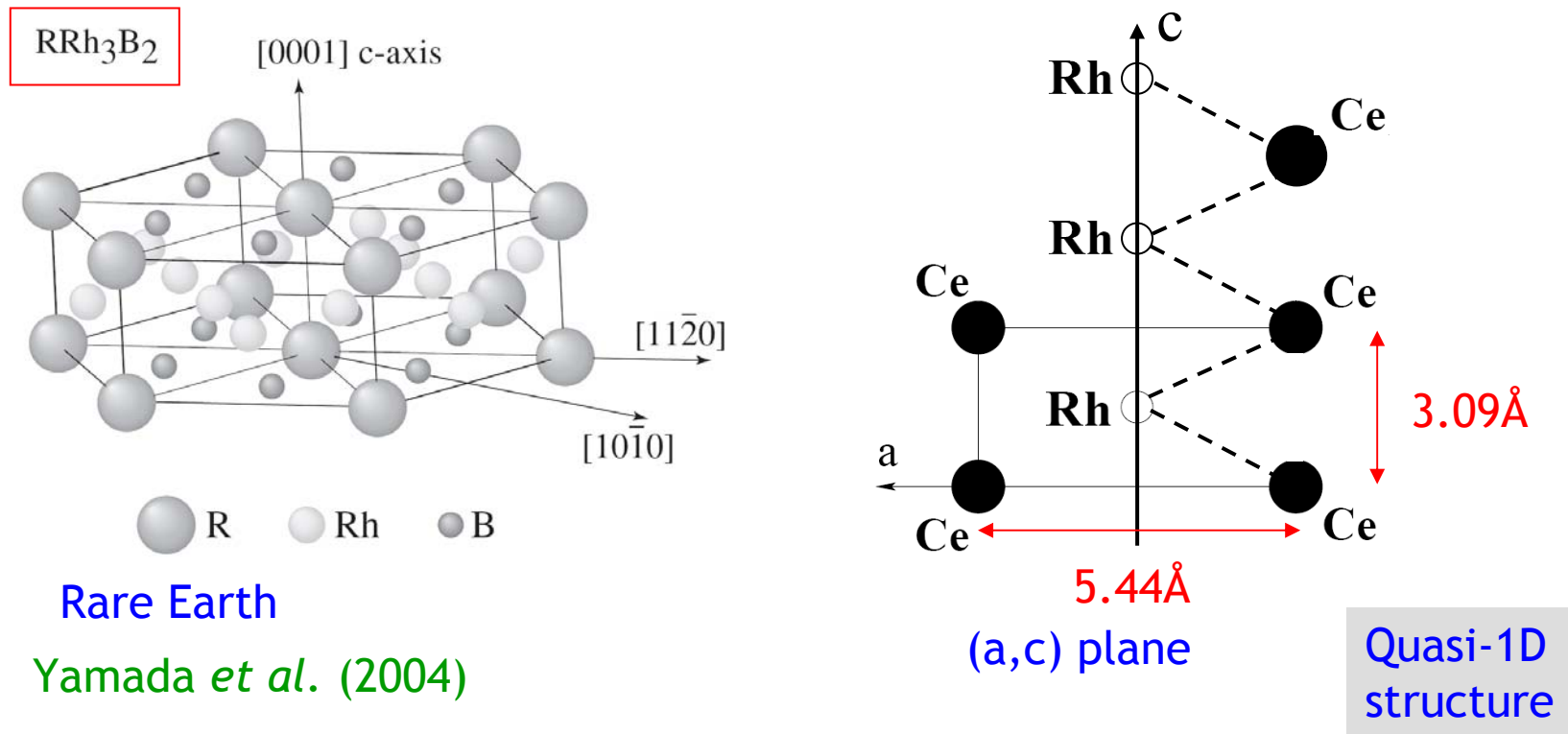
1D periodic Anderson model

## Application of the 1D periodic Anderson model to $\text{CeRh}_3\text{B}_2$

$\text{CeRh}_3\text{B}_2$  is an interesting  $4f$ -system because:

- RKKY interaction cannot explain ferromagnetism
- Small  $f$ -moment  $0.45 \mu_{\text{B}}$  (free  $\text{Ce}^{3+}$  ion:  $2.14 \mu_{\text{B}}$ )

# Application of the 1D periodic Anderson model to $\text{CeRh}_3\text{B}_2$



Kono, Kuramoto (2006)

## Mechanism for *f*-electron ferromagnetism in CeRh<sub>3</sub>B<sub>2</sub>?

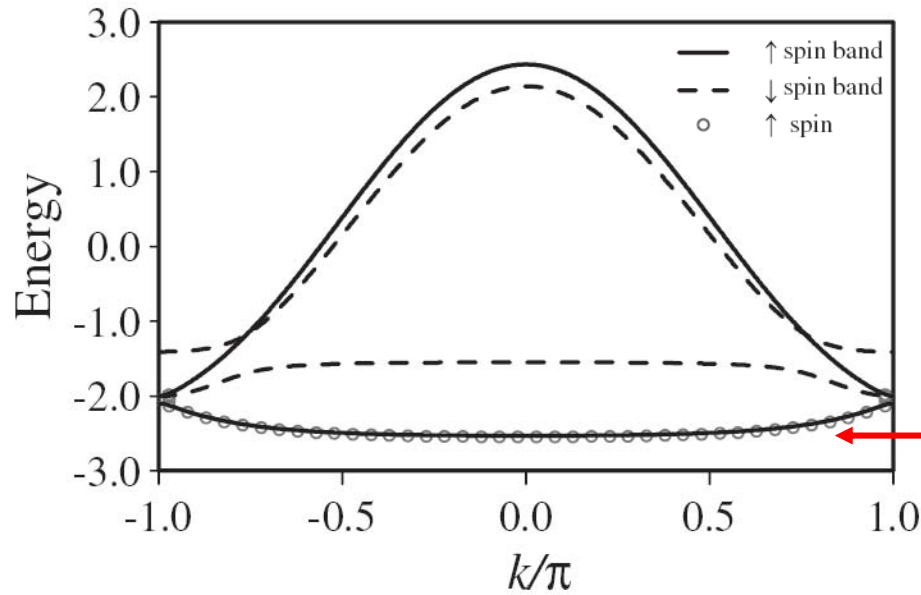
Gutzwiller projected variational wave function

$$|\Psi\rangle = P|\Phi\rangle$$

Evaluations by variational Monte Carlo (VMC)

Kono, Kuramoto (2006)

VMC

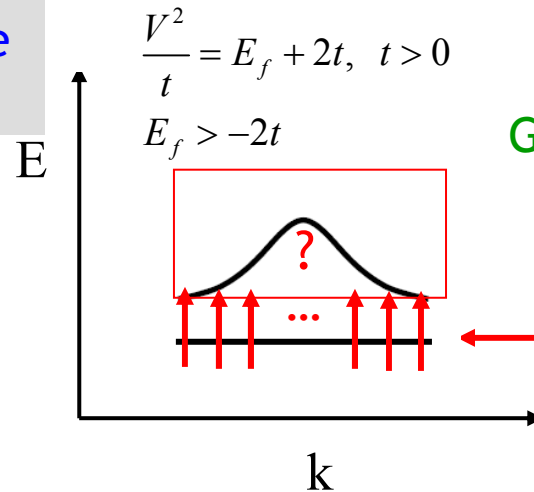


Kono, Kuramoto (2006)

almost flat band

$$t = 0.34 \text{ eV}, V = 0.24 \text{ eV}, E_f = -0.714 \text{ eV}, U = 7 \text{ eV}, n = 0.55$$

Exact ground state  
(Solution III)



Gulacsi, Kampf, DV (2008)

saturated ferromagnetism,  
bare flat band unchanged by U

$$\text{e.g., } t = 0.34 \text{ eV}, V = 0.23 \text{ eV}, E_f = -0.52 \text{ eV}, U > 0 \text{ arbitrary}, n = 0.5$$

## Magnetic moments

Free Ce<sup>3+</sup> ion

$$m_f = 2.14 \mu_B$$

Experiment:

$$m_f = 0.45 \mu_B$$

Galatanu *et al.* (2003)

VMC

$$t = 0.34 \text{ eV}, V = 0.24 \text{ eV}, E_f = -0.714 \text{ eV}, U = 7 \text{ eV}, n = 0.55$$

$$m_f = 0.94 \mu_B$$

Kono, Kuramoto (2006)

Exact ground state

$$\frac{V^2}{t} = E_f + 2t, \quad t > 0, \quad E_f > -2t$$

$$t = 0.34 \text{ eV}, V = 0.23 \text{ eV}, E_f = -0.52 \text{ eV}, U > 0 \text{ arbitrary}, n = 0.5$$

$$m_f = 0.68 \mu_B$$

Gulacsi, Kampf, DV (2008)

### III. Exact many-electron ground states on pentagon chain polymers

Exact dispersive band structure at  $U > 0$  can be tuned to become flat

Z. Gulacsi, A. Kampf, DV  
arXiv:1007.4994

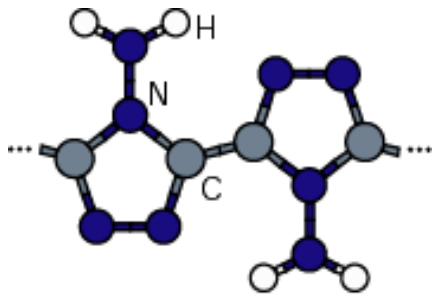
## Conducting polymers: wide range of applications in

- Nanoelectronics
- Nanooptics
- Medicine

Search for plastic ferromagnets and ferromagnetism in systems with non-magnetic elements

Candidate: **Flat-band ferromagnetism in organic polymers**

Polymethylaminotriazole



Spin-DFT

Suwa, Arita, Kuroki, Aoki (2003, arXiv:0907.2477)

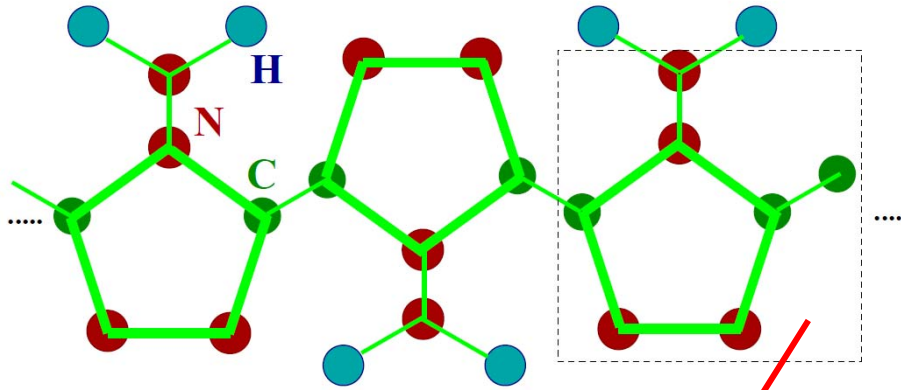
Arita, Suwa, Kuroki, Aoki (2002, 2003)

- Strong correlations in acene and thiophene organic molecular crystals
- stabilization of magnetic phases at high electron densities

Brocks, van den Brink, Morpurgo (2004)

# Polymethylaminotriazole

Gulacsi, Kampf, DV (arXiv:1007.4994)

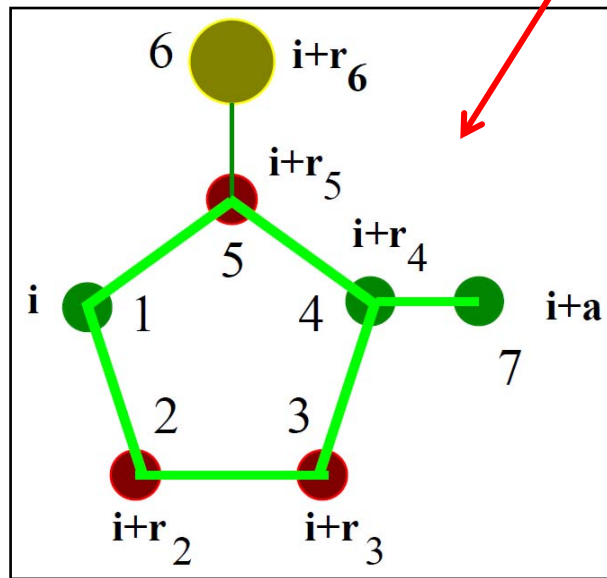


6 sites per cell  $\rightarrow$  6 bands

$N_c = \# \text{ cells}$

$N = \# \text{ electrons}$

$n = \frac{N}{6N_c}$  electron density



Arbitrary

- local interactions  $U_n > 0$
- on-site potentials  $\varepsilon_n$
- hopping amplitudes  $t_{n,n'}$

# Single-particle bands

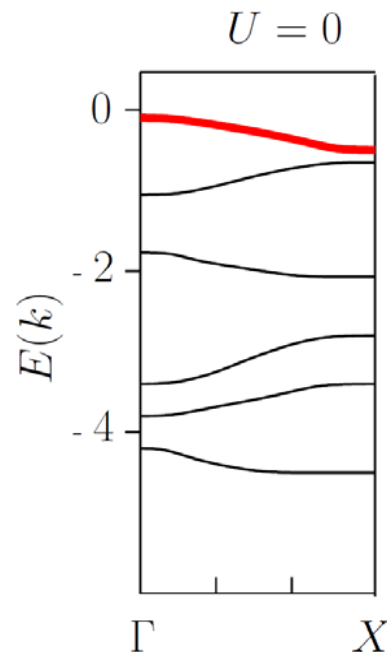
Gulacsi, Kampf, DV (arXiv:1007.4994)

Band dispersion

$$\epsilon = E_\nu(k), \nu \leq 6 \quad k = \mathbf{k} \cdot \mathbf{a}$$

$$2t_c t^2 [(\epsilon_6 - \epsilon)T_h - t_h T_f] \cos k + T_f \{t_h^2 t_c^2 - (\epsilon_2 - \epsilon)^2 t_c^2 + [(\epsilon_1 - \epsilon)(\epsilon_2 - \epsilon) - t^2]^2 - (\epsilon_1 - \epsilon)^2 t_h^2\} + 2(\epsilon_6 - \epsilon)t^2 \{t^2(\epsilon_2 + t_h - \epsilon) - (\epsilon_1 - \epsilon)T_h\} = 0,$$

with  $T_h = (\epsilon_2 - \epsilon)^2 - t_h^2$ ,  $T_f = (\epsilon_6 - \epsilon)(\epsilon_5 - \epsilon) - t_f^2$



$$t_c \equiv t_{4,7} = 0.5, \quad t_h \equiv t_{3,2} = -1.1, \quad t_f \equiv t_{5,6} = 1.2$$

$$\epsilon_1 = \epsilon_4 = -2.5, \quad \epsilon_2 = \epsilon_3 = -2.0, \quad \epsilon_5 = -2.1, \quad \epsilon_6 = -2.1$$

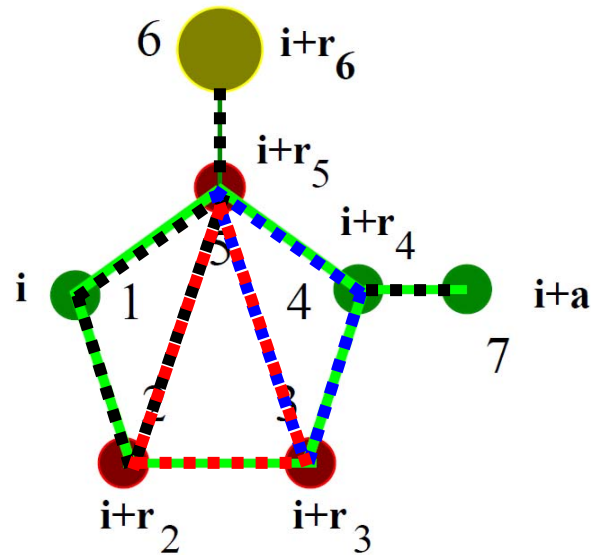
# Transform Hamiltonian in positive semidefinite form

Define operators acting on blocks  $\mathcal{B}_i$

$$\hat{G}_{\alpha, i, \sigma}^\dagger = \sum_{l \in \mathcal{B}_{i, \alpha}} a_{\alpha, l} \hat{c}_{i+r_l, \sigma}^\dagger \quad \alpha=1, \dots, 5$$

3 three-site blocks

2 two-site blocks



## Original form

$$\begin{aligned}\hat{H}_0 &= \sum_{\sigma, \mathbf{i}} \sum_{n, n' (n > n')} (t_{n, n'} \hat{c}_{\mathbf{i}+\mathbf{r}_n, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_{n'}, \sigma} + H.c.) + \\ &\quad + \sum_{\sigma, \mathbf{i}} \sum_{n=1}^m \epsilon_n \hat{n}_{\mathbf{i}+\mathbf{r}_n, \sigma}, \\ \hat{H}_U &= \sum_{\mathbf{i}} \sum_{n=1}^m U_n \hat{n}_{\mathbf{i}+\mathbf{r}_n, \uparrow} \hat{n}_{\mathbf{i}+\mathbf{r}_n, \downarrow}.\end{aligned}$$

## Positive semidefinite form

$$\hat{H} - C_g = \hat{H}_G + \hat{H}_P$$

with  $\hat{H}_G = \sum_{\mathbf{i}, \sigma} \sum_{\alpha=1}^{m-1} \hat{G}_{\alpha, \mathbf{i}, \sigma} \hat{G}_{\alpha, \mathbf{i}, \sigma}^\dagger$ ,  $\hat{H}_P = \sum_{n=1}^m U_n \sum_{\mathbf{i}} \hat{P}_{\mathbf{i}+\mathbf{r}_n}$ ,  $\hat{P}_{\mathbf{j}} = \hat{n}_{\mathbf{j}, \uparrow} \hat{n}_{\mathbf{j}, \downarrow} - (\hat{n}_{\mathbf{j}, \uparrow} + \hat{n}_{\mathbf{j}, \downarrow}) + 1$

$$C_g = q_U N - N_c [\sum_{n=1}^m U_n + 2 \sum_{\alpha=1}^{m-1} z_\alpha], \quad z_\alpha = \sum_{\ell} |a_{\alpha, \ell}|^2$$

$$q_U = (1/2)[(U_1 + \epsilon_1 + |t_c|) + (U_2 + \epsilon_2 + |t_h|) + \{[(U_2 + \epsilon_2 + |t_h|) - (U_1 + \epsilon_1 + |t_c|)]^2 + 4t^2\}^{1/2}]$$

## Original form

$$\begin{aligned}\hat{H}_0 &= \sum_{\sigma, \mathbf{i}} \sum_{n, n' (n > n')} (t_{n, n'} \hat{c}_{\mathbf{i}+\mathbf{r}_n, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_{n'}, \sigma} + H.c.) + \\ &\quad + \sum_{\sigma, \mathbf{i}} \sum_{n=1}^m \epsilon_n \hat{n}_{\mathbf{i}+\mathbf{r}_n, \sigma}, \\ \hat{H}_U &= \sum_{\mathbf{i}} \sum_{n=1}^m U_n \hat{n}_{\mathbf{i}+\mathbf{r}_n, \uparrow} \hat{n}_{\mathbf{i}+\mathbf{r}_n, \downarrow}.\end{aligned}$$

## Positive semidefinite form

$$\hat{H} - C_g = \hat{H}_G + \hat{H}_P$$

with  $\hat{H}_G = \sum_{\mathbf{i}, \sigma} \sum_{\alpha=1}^{m-1} \hat{G}_{\alpha, \mathbf{i}, \sigma} \hat{G}_{\alpha, \mathbf{i}, \sigma}^\dagger$ ,  $\hat{H}_P = \sum_{n=1}^m U_n \sum_{\mathbf{i}} \hat{P}_{\mathbf{i}+\mathbf{r}_n}$

## Matching conditions:

$$\begin{aligned}\sum_{\alpha=1}^{m-1} z_\alpha &= 4Q_1 + Q_1^2/|t_h| + 2t^2/Q_1 + 2(|t_h| + |t_c|) + Q_3^2 + t_f^2/Q_3^2 \\ Q_1 &= q_U - U_2 - \epsilon_2 - |t_h|, \quad Q_2 = q_U - U_1 - \epsilon_1 - |t_c|, \\ Q_3 &= |t_f| \sqrt{|t_h|} / [ |t_h| (q_U - U_5 - \epsilon_5) - (q_U - U_2 - \epsilon_2)^2 + t_h^2 ]^{1/2}\end{aligned}$$

# free parameters in block operators < # matching conditions

## Parameter space for which the transformation holds

$$t_h < 0, \quad Z = (q_U - Q_3^2) > \epsilon_6,$$

$$W = q_U - [(q_U - U_2 - \epsilon_2)^2 - t_h^2]/|t_h| > \epsilon_5,$$

$$W - \epsilon_5 > U_5 > 0, \quad U_6 = Z - \epsilon_6.$$

No strong restrictions!

Explicit form of block operators:

$$\hat{G}_{1,i,\sigma} = q_S \hat{b}_{i,5,2} - t/q_S \hat{c}_{i+r_1,\sigma},$$

$$\hat{G}_{2,i,\sigma} = -t_S \hat{b}_{i,2,3} + Q_1 \hat{c}_{i+r_5,\sigma}/t_S,$$

$$\hat{G}_{3,i,\sigma} = q_S \hat{b}_{i,5,3} - t/q_S \hat{c}_{i+r_4,\sigma},$$

$$\hat{G}_{4,i,\sigma} = Q_3 \hat{c}_{i+r_6,\sigma} - t_f/Q_3 \hat{c}_{i+r_5,\sigma},$$

$$\hat{G}_{5,i,\sigma} = |t_c|^{1/2} [\hat{c}_{i+r_4,\sigma} - t_c \hat{c}_{i+a,\sigma}/|t_c|],$$

with  $q_S = Q_1^{1/2}$ ,  $t_S = |t_h|^{1/2}$ ,  $\hat{b}_{i,n,m} = \sum_{p=n,m} \hat{c}_{i+r_p,\sigma}$

# Effective band structure

$$\hat{H}_G = \hat{H}_{kin} + \text{const}$$

$$\hat{H}_{kin} = - \sum_{\mathbf{i}, \sigma} \sum_{\alpha=1}^{m-1} \hat{G}_{\alpha, \mathbf{i}, \sigma}^\dagger \hat{G}_{\alpha, \mathbf{i}, \sigma}$$

↑  
quadratic in the original c-operators

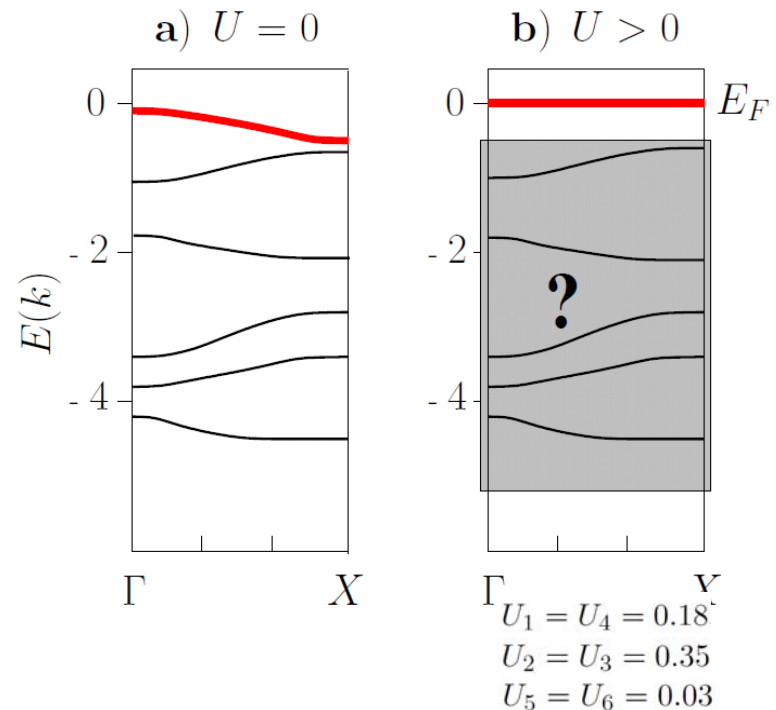
→ Effective, interaction dependent band structure:  
same as for  $H_0$  but with renormalizatic

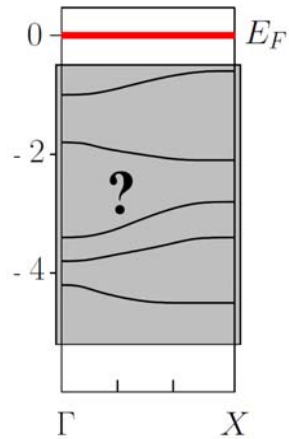
$$\epsilon_n \rightarrow \epsilon_n^R = \epsilon_n + U_n - qU$$

# free parameters in block operators  
< # matching conditions

→ exact effective band structure is  
in general **dispersive**

Upper band can be **tuned** to  
become flat due to interactions





Upper flat band half filled for  $N=N^*=11N_c \rightarrow$  density  $n=11/6$

Ground state for  $n=11/6$ :

$$|\Psi_g(N^*)\rangle = \left[ \prod_{\sigma} \hat{G}_{\sigma}^{\dagger} \right] \hat{F}^{\dagger} |0\rangle$$

$$\hat{G}_{\sigma}^{\dagger} = \prod_i \prod_{\alpha=1}^{m-1} \hat{G}_{m,i,\sigma}^{\dagger} \text{ creates } (m-1)N_c \text{ } \sigma\text{-electrons}$$

$$\hat{F}^{\dagger} = \prod_i \hat{c}_{i+r_{n_1},\sigma}^{\dagger} \text{ creates one } \sigma\text{-electrons in each unit cell}$$

one  $\sigma$ -electron per site  $\rightarrow$  localized  
 $-\sigma$ -electron are mobile (= Slater determinant)

### Physical properties

$$\Gamma_{\mathbf{i}}(\mathbf{r}) = \langle \Psi_g(N^*) | (\hat{c}_{\mathbf{i}+\mathbf{r}_n,-\sigma}^{\dagger} \hat{c}_{\mathbf{i}+\mathbf{r}_n+\mathbf{r},-\sigma} + H.c.) | \Psi_g(N^*) \rangle \xrightarrow{N_c \rightarrow \infty} e^{-r/\xi}$$

Ground state for  $n = 11/6$ : **localized ferromagnet**

Ground state for  $n > 11/6$  ( $S_{z,\max}$  sector)

charge gap  $\Delta\mu = E_g(N) - 2E_g(N-1) + E_g(N-2) = 0$ ,  $\xi = \infty \rightarrow$  **itinerant ferromagnet**

Matching conditions allow for parameters

$$n \geq 11/6, \quad W/t = 0.15, \quad \text{with } 0.2 \leq U_n/W \leq 2.3$$

Fulfills experimental conditions:

- Strong correlations in acene and thiophene organic molecular crystals
- stabilization of magnetic phases at high electron densities

Brocks, van den Brink, Morpurgo (2004)

Dispersive band may be tuned by interactions to become flat

→ new route for the design of ferromagnetic pentagon-chain polymers

## Conclusion 1:

### Strategy for the construction of exact many-electron ground states

**Step 1:** Transform many-electron Hamiltonian into positive semidefinite form

**Step 2:** Construct many-electron ground state

**Step 3:** Prove uniqueness of many-electron ground state:

- Works in any dimension
- No integrability required
- Applicable to any Hamiltonian with sufficiently many microscopic parameters

## Conclusion 2:

### Exact many-electron ground states on Hubbard chains

Hubbard chains have remarkably complex properties, e.g.,

#### Square Hubbard chain:

- **Lowest** flat-band ferromagnetism (general property)
- Correlated half-metal behavior
- Metal-insulator transitions
- Tune between different ground states by varying  $B$ ,  $\epsilon$ ,  $n$ ,  $U$ ,  $t$   
→ Design of new switches

#### Pentagon chain polymers:

Tune dispersive band structure by the interaction

→ design flat band structure with ferromagnetic or half metallic ground state

