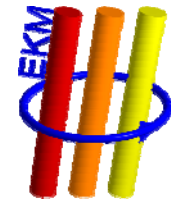




Center for Electronic Correlations and Magnetism
University of Augsburg



Construction of exact ground states for correlated lattice fermion models

Dieter Vollhardt

Supported by **DFG**

TRR 80 (Augsburg-Munich)



Stanford; January 6, 2011

Outline:

- Three-step strategy for the construction of exact many-electron ground states
- **Diamond** Hubbard chains
→ e.g., correlation-induced half-metal
- **Triangle** Hubbard chains
→ ferromagnetism in CeRh_3B_2
- **Pentagon** Hubbard chains
→ route to ferromagnetism in organic polymers



In collaboration with

Zsolt Gulacsi (Debrecen, Hungary)
Arno Kampf (Augsburg)



Correlated electron materials

High sensitivity to small changes of microscopic parameters

- large resistivity changes
- huge volume changes
- high T_c superconductivity
- strong thermoelectric response
- colossal magnetoresistance

with

Technological applications:

- sensors, switches
- magnetic storage
- thermoelectrics
- functional materials, ...

Wanted:

Exact results
for correlated electron models

(especially with experimental relevance)

Construction of exact many-electron ground states

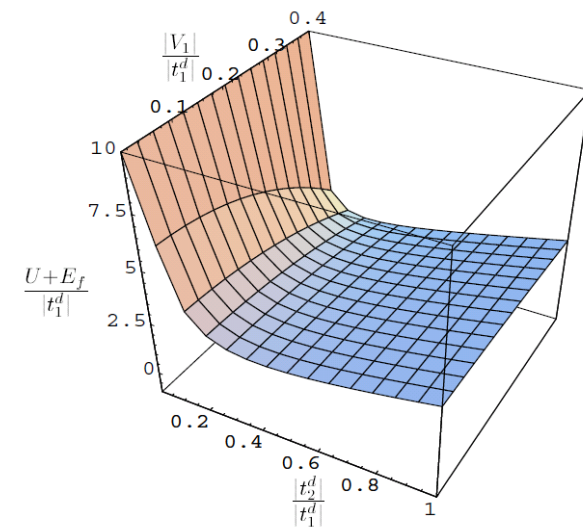
Strategy

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

Step 2: Construct a ground state

Step 3: Prove the uniqueness of the ground state

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



Hypersurface in parameter space

Construction of exact many-electron ground states

Strategy

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

Step 2: Construct a ground state

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)
Superconductivity in the extended Hubbard model	Montorsi, Campbell (1996)
Composite operators defined on the entire unit cell	Orlik, Gulacsi (1998, 2001)
PAM on regular lattices in $d=2,3$ at $U < \infty$	Gurin, Gulacsi (2001, 2002)
Application to $d=1$	Sarasua, Continentino (2002)
Optimal ground state of quantum spin models	Ahrens, Schadschneider, Zittartz (2005)
Gossamer Hamiltonian	Laughlin (2002/2006); Bernevig <i>et al.</i> 2003, 2006)

Construction of exact many-electron ground states

Strategy

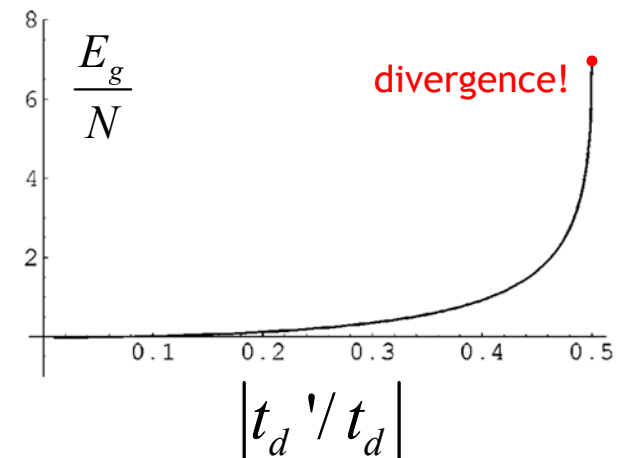
Step 1: Transform the many-electron Hamiltonian into positive semidefinite form

Step 2: Construct a ground state

Step 3: Prove the uniqueness of the ground state

PAM in $d=3$

- Exact insulating and itinerant (non-Fermi liquid) ground states at $\frac{1}{4}$ and $\frac{3}{4}$ filling
- Proof of ferromagnetism in the PAM in $d=3$



Gulacsi, DV (2003, 2005)

High sensitivity to small changes of microscopic parameters found

Construction of exact many-electron ground states: **Details**

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

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

→ spectrum has a well-defined lower bound

Transformation is feasible (if at all)

- in several different ways
- on a hypersurface in the full parameter space

Construction of exact many-electron ground states: **Details**

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

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

Step 2: Construct a 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 $\{\Omega, O^\dagger\} = 0$

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

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

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

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

Construction of exact many-electron ground states: **Details**

$$\hat{H} = \hat{H}_0 + \hat{H}_U \stackrel{!}{=} \sum_n \hat{P}_n + E_g \equiv \hat{H}' + E_g, \quad \hat{P}_n : \text{positive semidefinite}$$
$$\langle \psi | \hat{P}_n | \psi \rangle \geq 0$$

Step 3: Prove the uniqueness of the ground state:

$|\Psi_g\rangle$ has to span $\ker(\hat{H}') := \{|\phi\rangle \mid \hat{H}'|\phi\rangle = 0\}$

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

→ 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 $|\Psi_g\rangle$.

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)

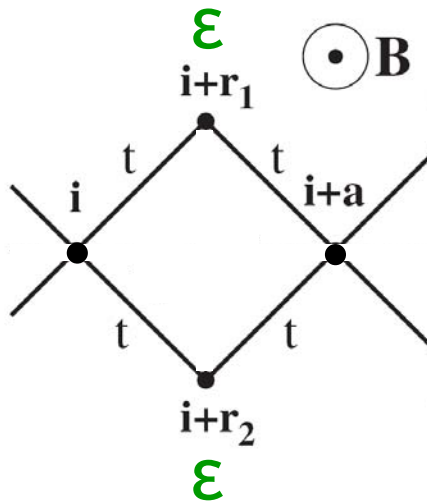
→ First step:

Find exact solutions of correlation models with flat bands

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)



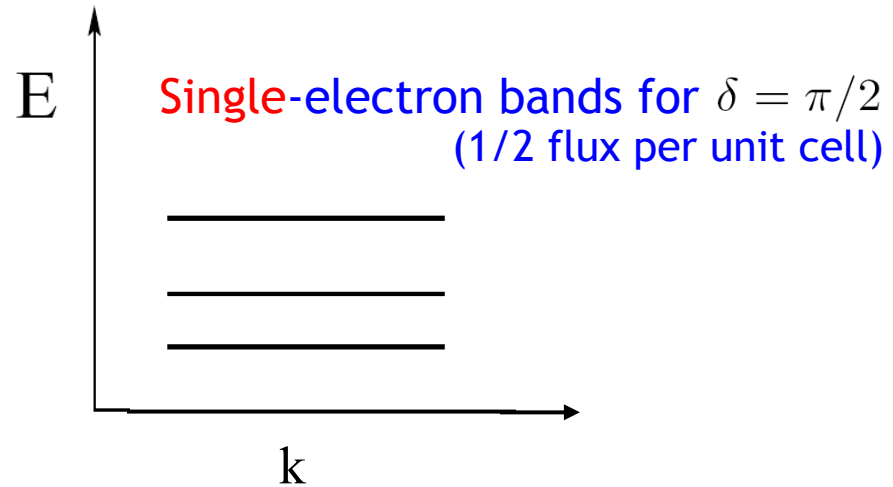
“Aharonov-Bohm cage”

Peierls phase factor

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

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

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



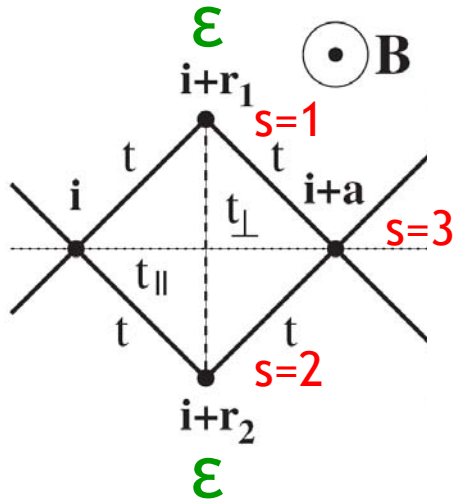
Vidal, Doucot, Mosseri, Butaud (2000):

$\epsilon=0$, $\delta = \pi/2$, 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? ✓



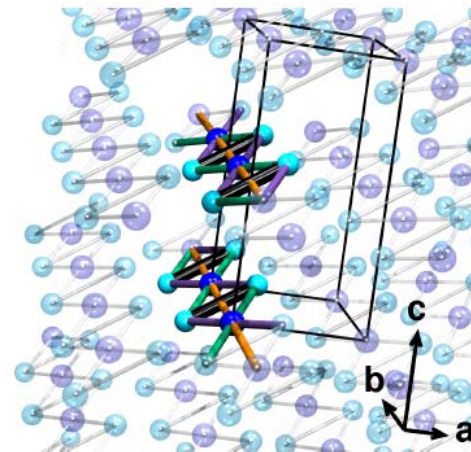
3 sites per cell \rightarrow 3 bands

$s=1,2,3$ sublattice index

$N_c = \# \text{ cells}$

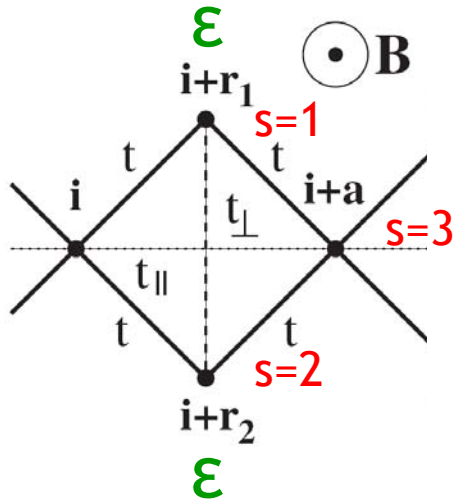
$N = \# \text{ electrons}$

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



Jeschke *et al.*,
arXiv:1012.1090

Azurite $\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$



3 sites per cell \rightarrow 3 bands

$s=1,2,3$ sublattice index

N_c = # cells

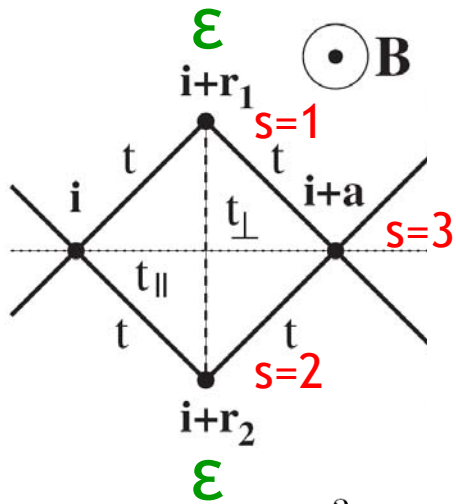
N = # electrons

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

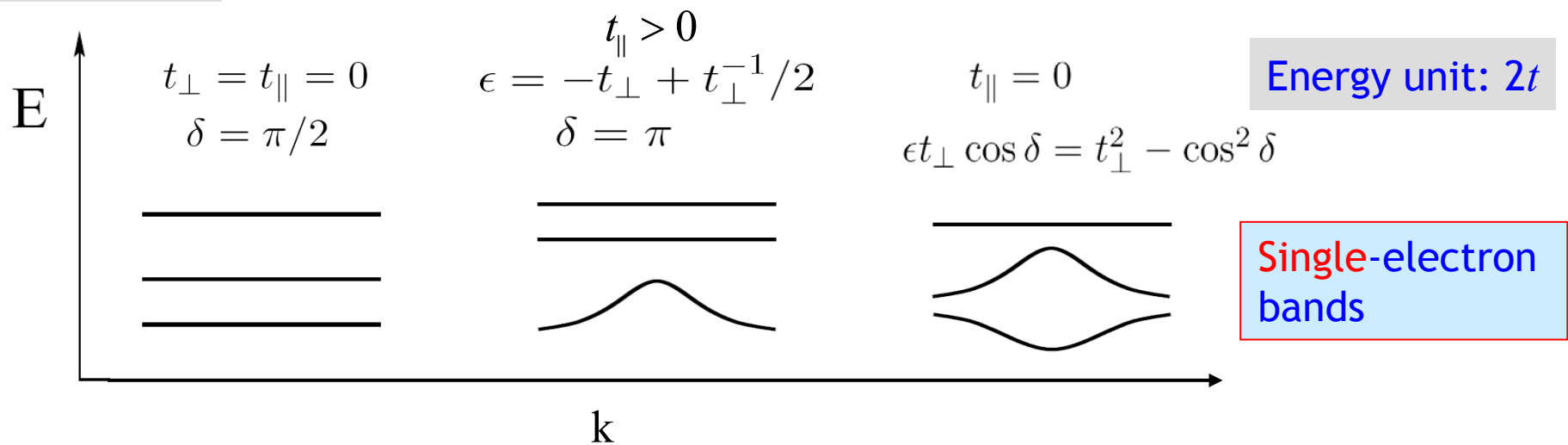
$N_c = \#$ cells

$N = \#$ electrons

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

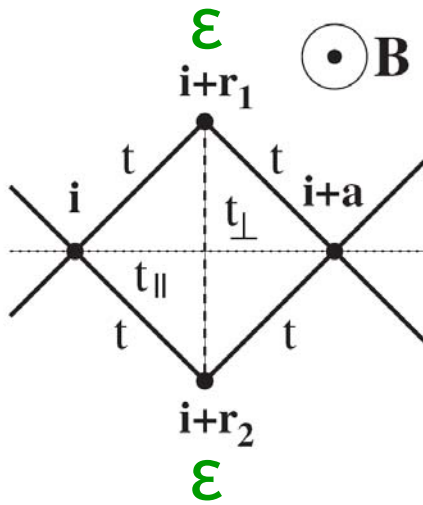
FT
$$\hat{H}_0 = \sum_{\mathbf{k}, \sigma} \sum_{s, s'=1}^3 M_{s, s'}(\mathbf{k}) \hat{C}_{s, \mathbf{k}, \sigma}^\dagger \hat{C}_{s', \mathbf{k}, \sigma}$$

Examples:

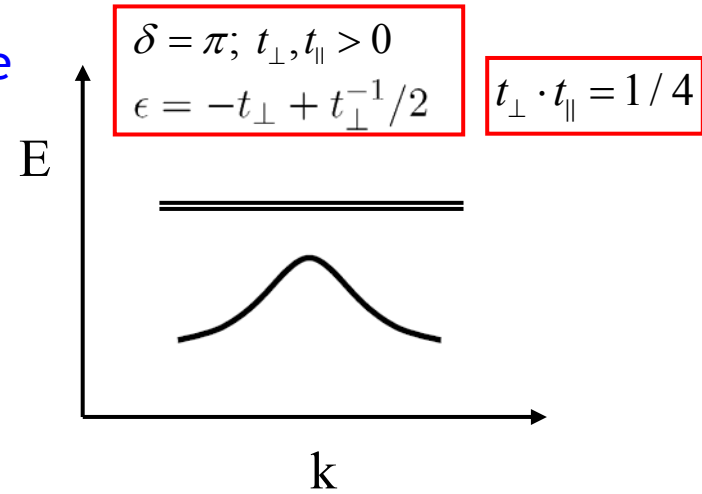


Solution I: Correlated half-metal

Solution I: Correlated half-metal

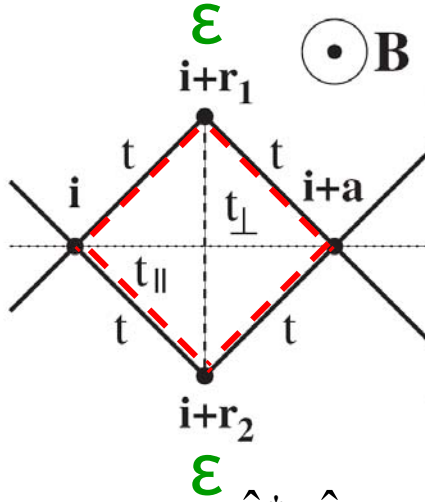


→ Investigate



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

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

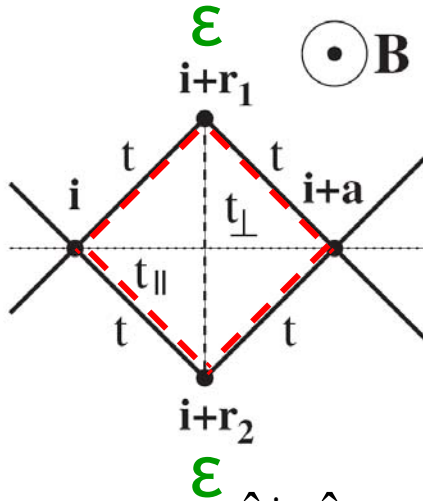
$$(\hat{A}_{i,\sigma})^2 = 0$$

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

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

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

1. Transformation of the Hamiltonian into positive semidefinite form



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

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

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

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

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

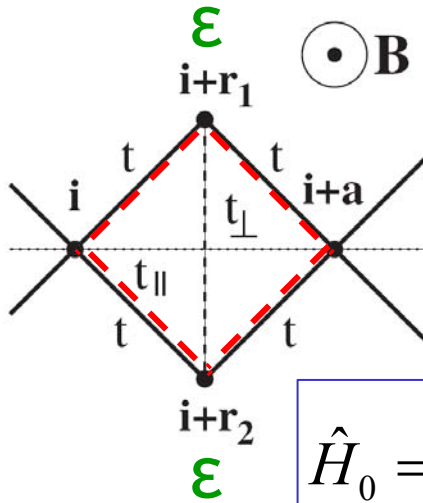
$$-\sum_{i\sigma} \hat{A}_{i\sigma}^\dagger \hat{A}_{i\sigma} \stackrel{!}{=} \hat{H}_0 \Rightarrow$$

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

\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 σ 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 σ on arbitrary sites of each unit cell

Ground state for

$$\begin{aligned} \delta &= \pi; t_\perp, t_\parallel > 0 \\ \epsilon &= -t_\perp + t_\perp^{-1}/2 \\ t_\perp \cdot t_\parallel &= 1/4 \end{aligned}$$

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

$$\begin{aligned} N &= 4N_c \Leftrightarrow n = 4/3 \\ n_\sigma &= 1, n_{-\sigma} = 1/3 \end{aligned}$$

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:

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 $N=4N_c$, $\hat{W} = \hat{F}_\sigma^\dagger = \prod_{\mathbf{i}} [\hat{c}_{\mathbf{i}+\mathbf{r}_{s_{i,1},\sigma}}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_{s_{i,2},\sigma}}^\dagger]$

↑
Creates two electrons with fixed spin σ
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 $\delta = \pi; t_{\perp}, t_{\parallel} > 0$

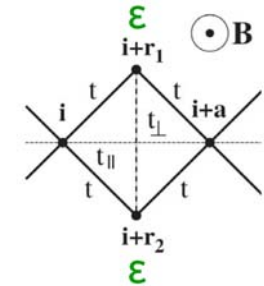
$$\epsilon = -t_{\perp} + t_{\perp}^{-1}/2$$

$$t_{\perp} \cdot t_{\parallel} = 1/4$$

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

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

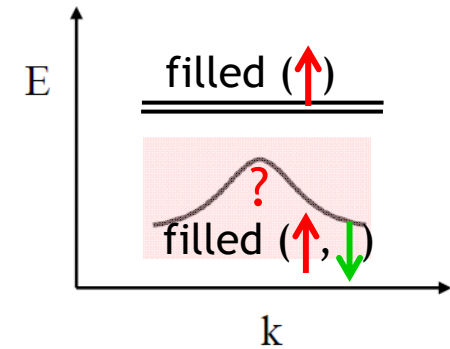
is the **unique** ground state



Physical properties:

One σ electron on every lattice site \rightarrow localized

$-\sigma$ electrons:



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

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

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

N_c : # unit cells

Solution I: Correlated half-metal

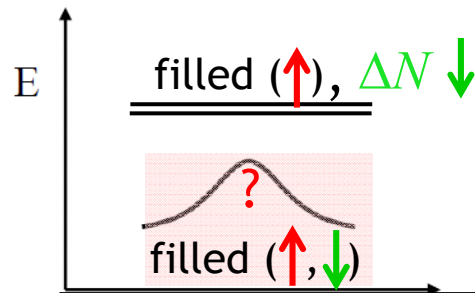
Add ΔN many $-\sigma$ electrons \rightarrow $n_\sigma = 1, n_{-\sigma} = \frac{1}{3} + \frac{\Delta N}{3N_c}$

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 $\Delta\mu = E_g(N) - 2E_g(N-1) + E_g(N-2) = 0$
 $\rightarrow \Delta N$ many $-\sigma$ electrons itinerant

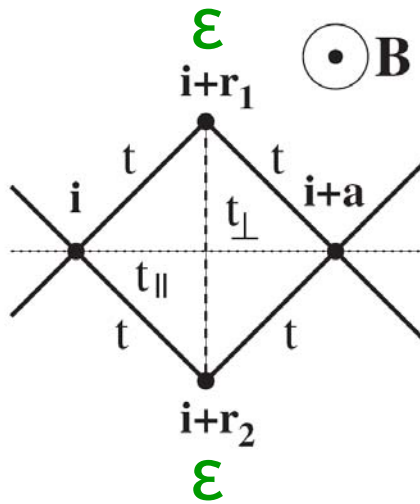
Ground state for $4/3 < n < 5/3$

- $3N_c$ immobile σ electrons
- N_c $-\sigma$ electrons confined to localized Wannier function + ΔN itinerant $-\sigma$ electrons
- Magnetization $M \propto (1 - \Delta N/N_c)$
 \rightarrow Low carrier-density metal due to $-\sigma$ electrons

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

Solution II:
Exact ground states for general magnetic flux

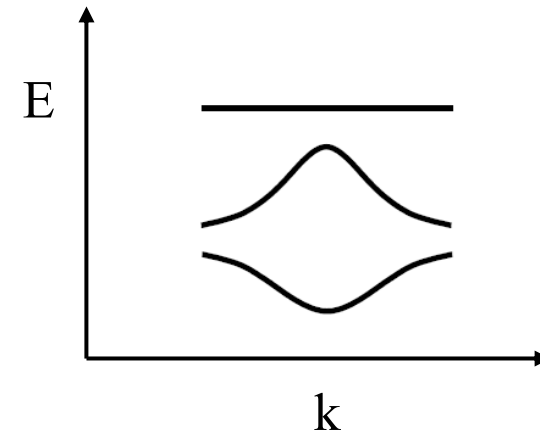
Solution II: Exact ground states for general magnetic flux



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

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

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



Single-electron bands

Ground states for $n \geq 5/3$

<p>$B = 0$: localized non-magnetic ground state for $n \geq 5/3$</p>	<p>$B \neq 0$</p> <p>→</p>	<p>Non-saturated ferromagnet</p> <ul style="list-style-type: none"> • insulating for $n=5/3$ • metallic for $n>5/3$
--	---------------------------------------	--

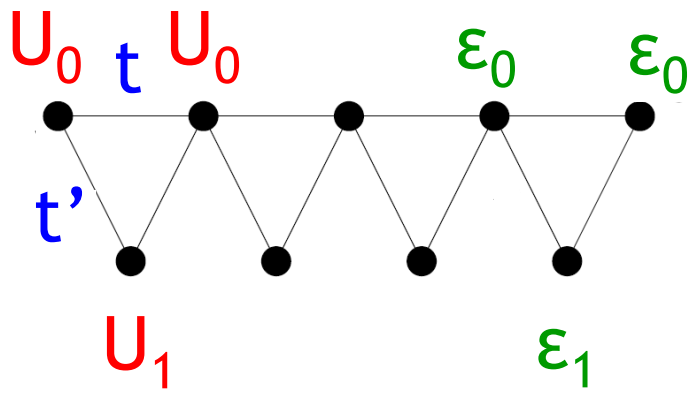
Conclusion

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

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

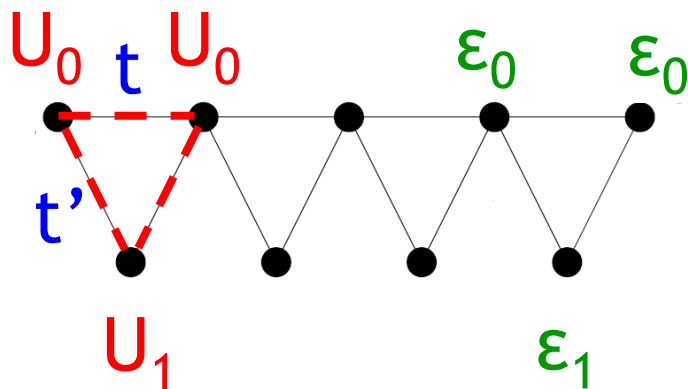
Müller-Hartmann (1995)

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

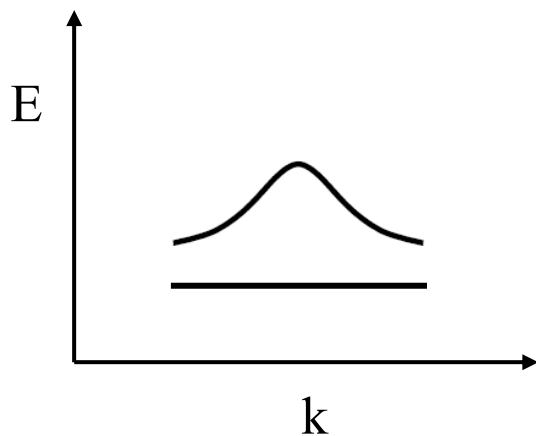
$n = \frac{N}{2N_c}$ electron density

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

Solution I:

$U_0, U_1 > 0$

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



Single-electron bands

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

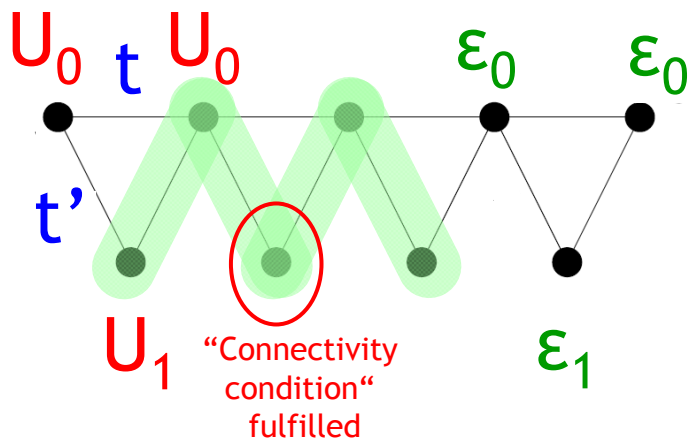
Positive semidefinite $\hat{H}^{tri} = \sum_{i,\sigma} \hat{A}_{i,\sigma}^\dagger \hat{A}_{i,\sigma} + K\hat{N} + H_U^{tri}$
 $K = \epsilon_0 - 2t$

Step 2

Construct operators \hat{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

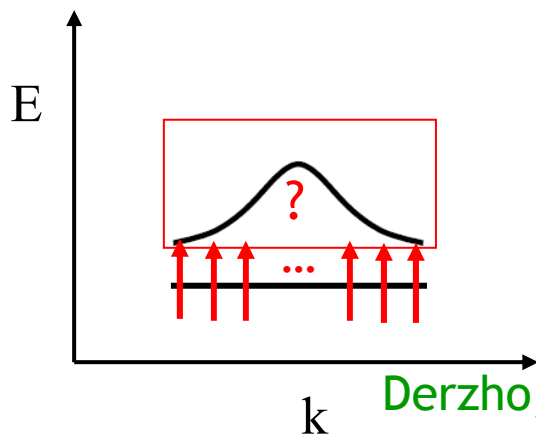
$N_c = \#$ cells

$N = \#$ 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

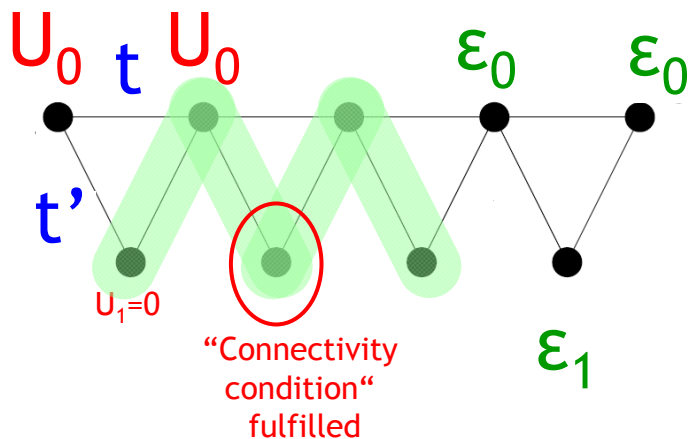
$n = 1/2$: fully saturated ferromagnet

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

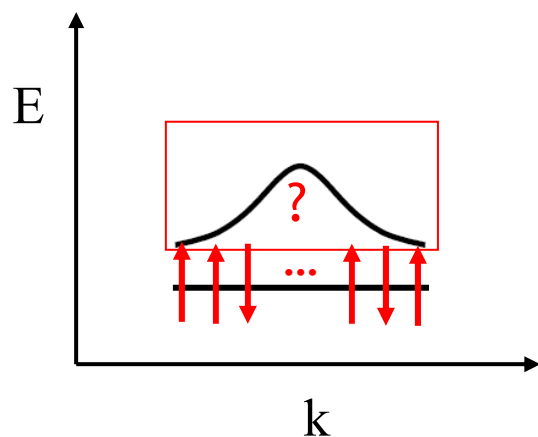
$$N_c = \# \text{ cells}$$

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

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

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

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



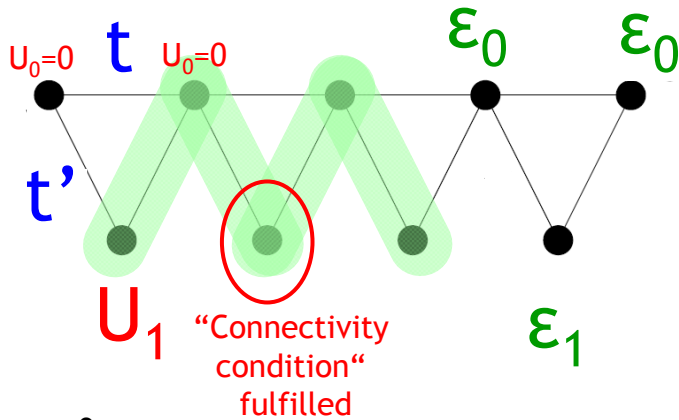
$$\hat{H} = \hat{H}_0 + \hat{H}_U$$

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

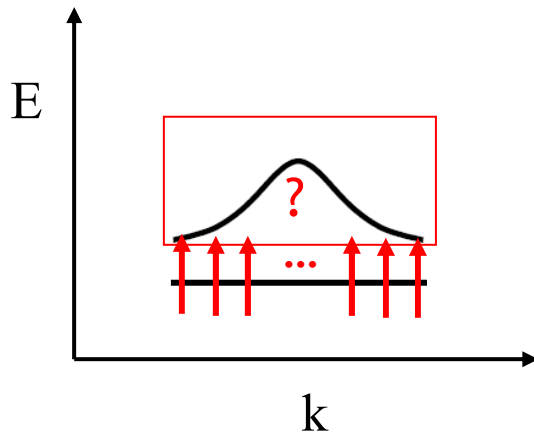
$N_c = \#$ cells

$N = \#$ electrons

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

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

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

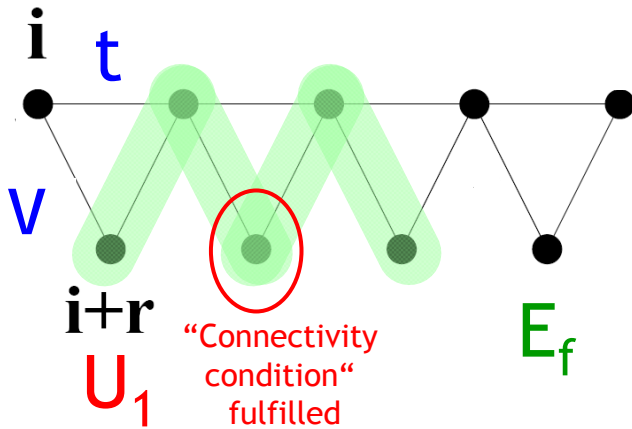


$$\hat{H} = \hat{H}_0 + \hat{H}_U$$

Solution III:

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

$n=1/2$: fully saturated ferromagnet



2 sites per cell \rightarrow 2 bands

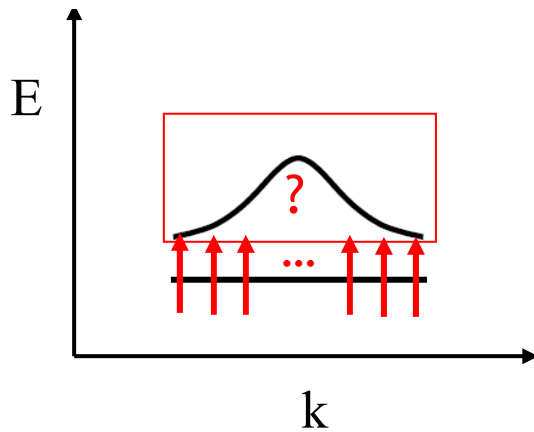
$N_c = \# \text{ cells}$

$N = \# \text{ electrons}$

$n = \frac{N}{2N_c}$ 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:

$$\hat{d}_{i,\sigma} \equiv \hat{c}_{i,\sigma},$$

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

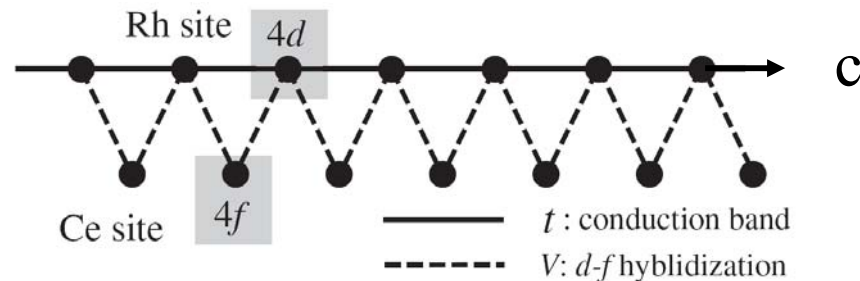
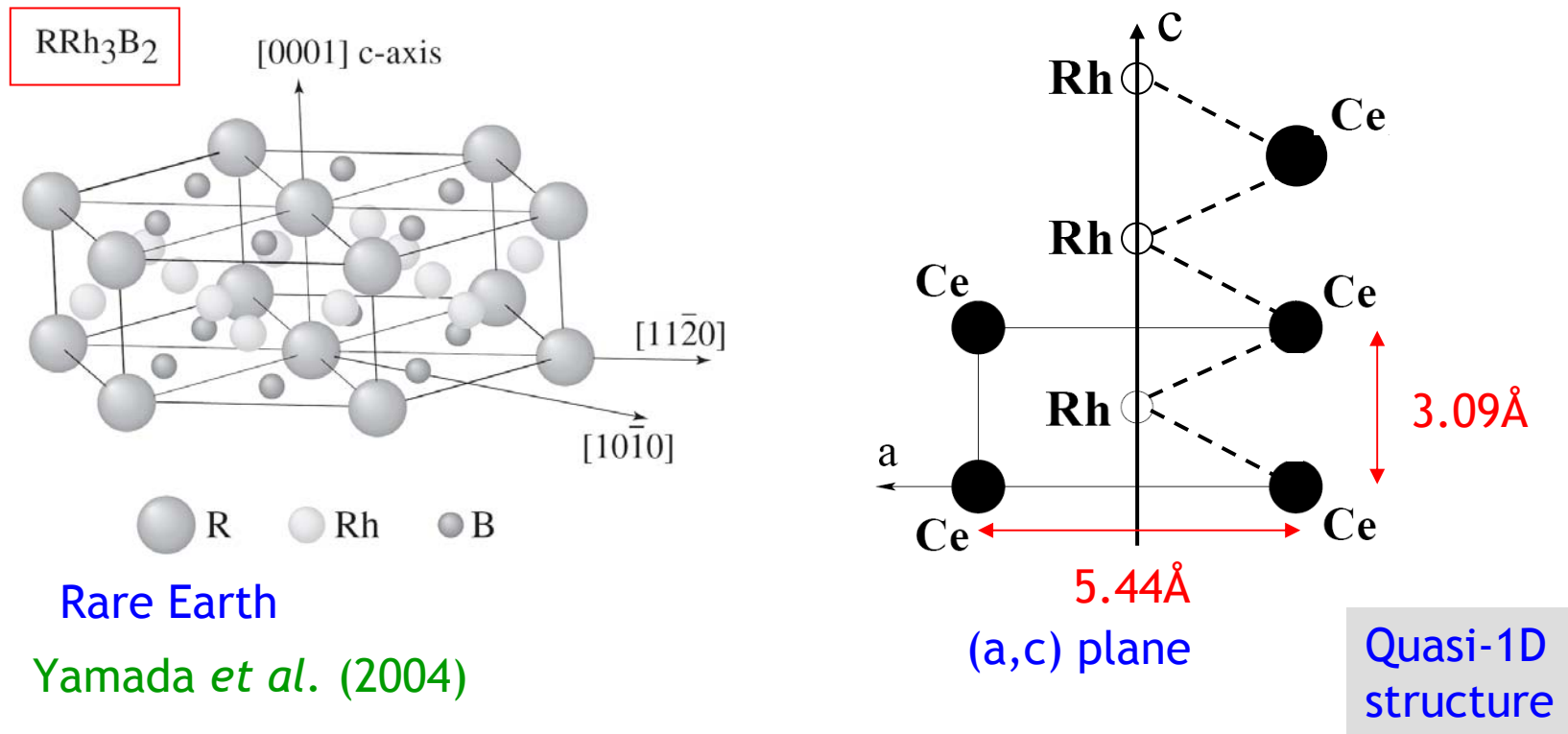
1D periodic Anderson model

Application of the 1D periodic Anderson model to CeRh_3B_2

CeRh_3B_2 is an interesting $4f$ -system because:

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

Application of the 1D periodic Anderson model to CeRh_3B_2



Kono, Kuramoto (2006)

Mechanism for *f*-electron ferromagnetism in CeRh₃B₂?

Gutzwiller projected variational wave function

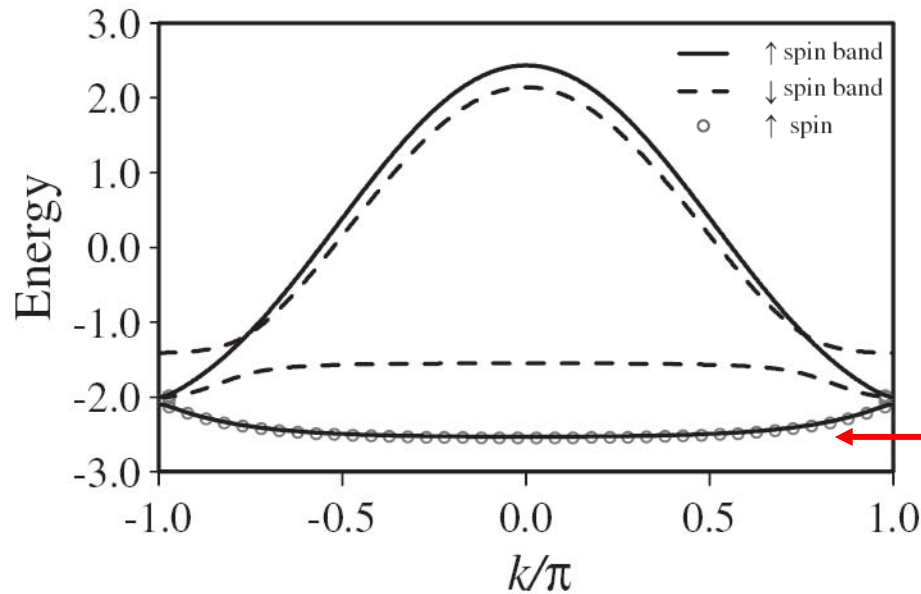
$$|\Psi\rangle = P|\Phi\rangle$$

Evaluations by variational Monte Carlo (VMC)

Kono, Kuramoto (2006)

f -electron ferromagnetism in CeRh_3B_2

VMC

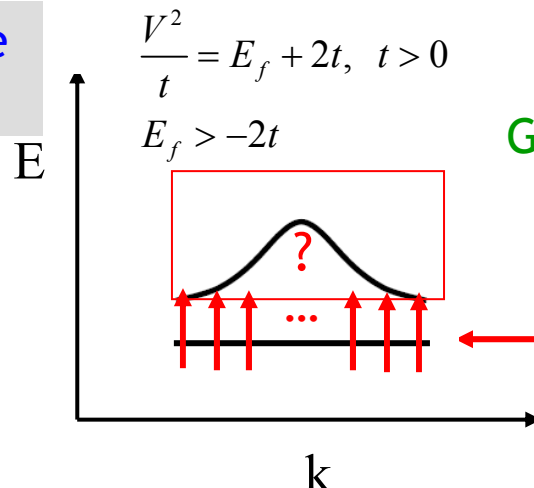


Kono, Kuramoto (2006)

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

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

f-electron ferromagnetism in CeRh₃B₂: Magnetic moments

Free Ce³⁺ 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

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

$$m_f = g\mu_B \frac{1}{2N_c} \sum_i \langle (\hat{n}_{i,\uparrow}^f - \hat{n}_{i,\downarrow}^f) \rangle$$

$$|\Psi_g\rangle = \prod_{i=1}^{N_c} \hat{B}_{i,\sigma}^\dagger |0\rangle$$

$$\hat{B}_{i,\sigma}^\dagger = \hat{f}_{i-a+r,\sigma}^\dagger + \hat{f}_{i+r,\sigma}^\dagger - (V/t) \hat{d}_{i,\sigma}^\dagger$$

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

$$m_f = 0.68 \mu_B$$

Gulacsi, Kampf, DV (2008)

Pentagon Hubbard chains

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

Z. Gulacsi, A. Kampf, DV
Phys. Rev.Lett. 105, 266403 (2010)

Conducting polymers: wide range of applications in

Heeger, Kivelson, Schrieffer, Su (1988)

- Nanoelectronics
- Nanooptics
- Medicine

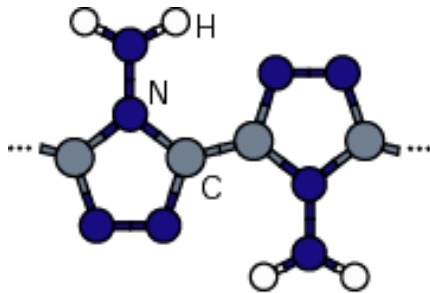
Search for **plastic** ferromagnets and ferromagnetism in systems with **non-magnetic** elements

Candidate: Flat-band ferromagnetism in organic polymers

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

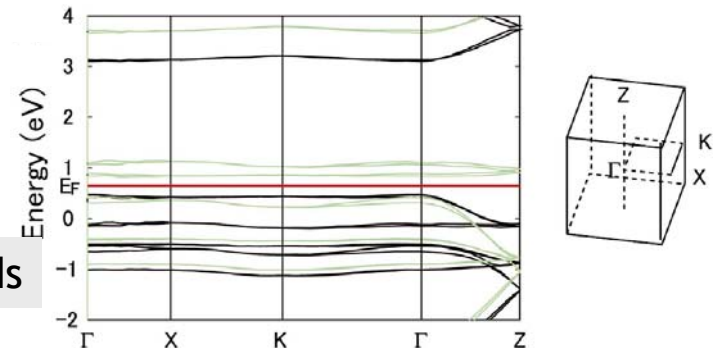
Arita, Suwa, Kuroki, Aoki (2002, 2003)

Polyaminotriazole



Spin-DFT

Single-particle bands

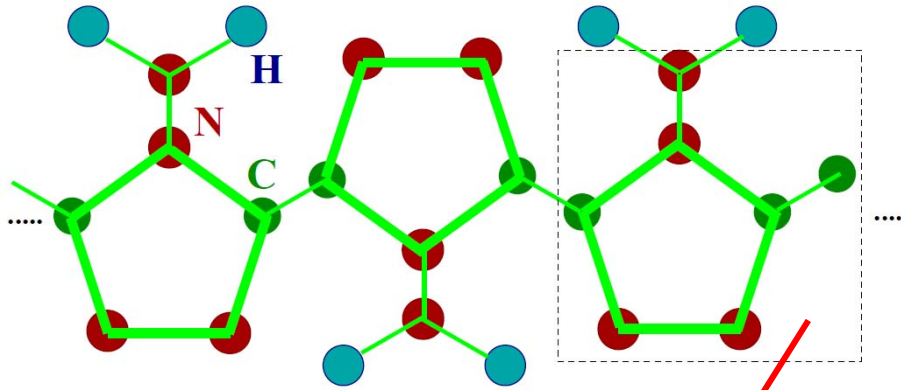


- Strong correlations in acene and thiophene organic molecular crystals
- stabilization of magnetic phases at high electron densities

Brocks, van den Brink, Morpurgo (2004)

Polyaminotriazole

Gulacsi, Kampf, DV (2010)

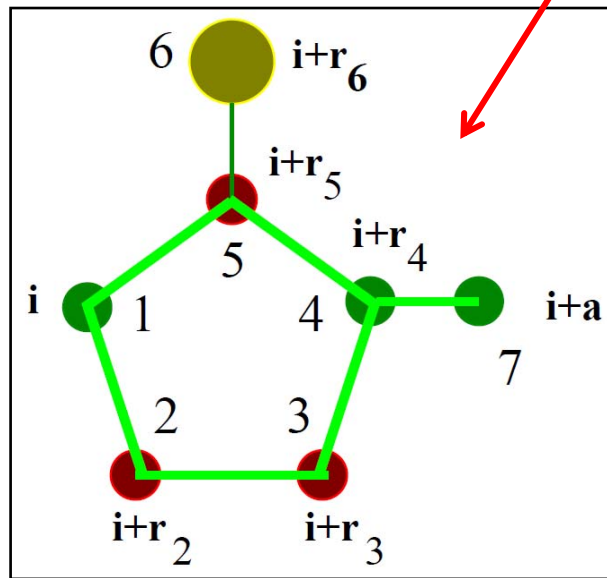


6 sites per cell \rightarrow 6 bands

$N_c = \# \text{ cells}$

$N = \# \text{ electrons}$

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



Arbitrary

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

Single-particle bands

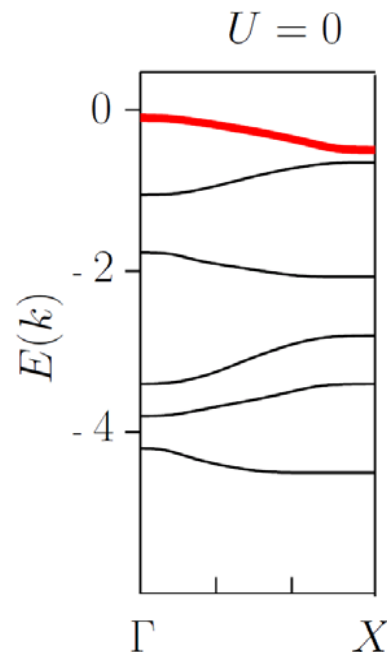
Gulacsi, Kampf, DV (2010)

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



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

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

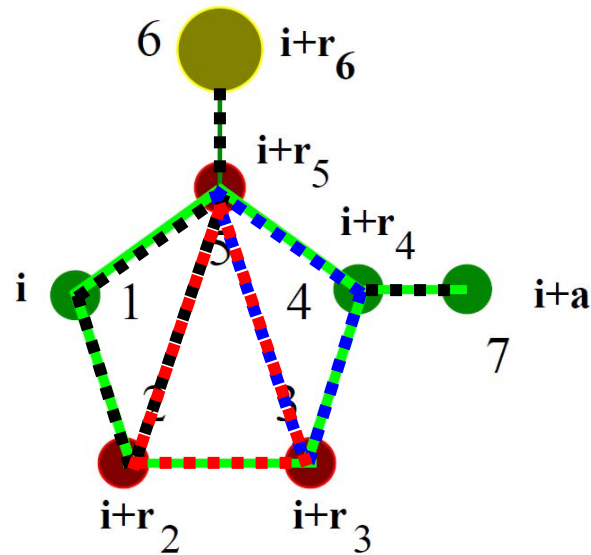
Transform Hamiltonian in positive semidefinite form

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

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

$$\begin{aligned} \hat{H}_0 &= \sum_{\sigma, \mathbf{i}} \sum_{n, n' (n > n')} (t_{n, n'} \hat{c}_{\mathbf{i}+\mathbf{r}_n, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_{n'}, \sigma} + H.c.) + \\ &\quad + \sum_{\sigma, \mathbf{i}} \sum_{n=1}^6 \epsilon_n \hat{n}_{\mathbf{i}+\mathbf{r}_n, \sigma}, \\ \hat{H}_U &= \sum_{\mathbf{i}} \sum_{n=1}^6 U_n \hat{n}_{\mathbf{i}+\mathbf{r}_n, \uparrow} \hat{n}_{\mathbf{i}+\mathbf{r}_n, \downarrow}. \end{aligned}$$

Positive semidefinite form

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

$$\text{with } \hat{H}_G = \sum_{\mathbf{i}, \sigma} \sum_{\alpha=1}^5 \hat{G}_{\alpha, \mathbf{i}, \sigma} \hat{G}_{\alpha, \mathbf{i}, \sigma}^\dagger, \quad \hat{H}_P = \sum_{n=1}^6 U_n \sum_{\mathbf{i}} \hat{P}_{\mathbf{i}+\mathbf{r}_n}, \quad \hat{P}_j = \hat{n}_{j, \uparrow} \hat{n}_{j, \downarrow} - (\hat{n}_{j, \uparrow} + \hat{n}_{j, \downarrow}) + 1$$

$$C_g = q_U N - N_c [\sum_{n=1}^6 U_n + 2 \sum_{\alpha=1}^5 z_\alpha], \quad z_\alpha = \sum_{\ell} |a_{\alpha, \ell}|^2$$

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

Original form

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

$$\begin{aligned}\hat{H}_0 &= \sum_{\sigma, \mathbf{i}} \sum_{n, n' (n > n')} (t_{n, n'} \hat{c}_{\mathbf{i}+\mathbf{r}_n, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_{n'}, \sigma} + H.c.) + \\ &\quad + \sum_{\sigma, \mathbf{i}} \sum_{n=1}^6 \epsilon_n \hat{n}_{\mathbf{i}+\mathbf{r}_n, \sigma}, \\ \hat{H}_U &= \sum_{\mathbf{i}} \sum_{n=1}^6 U_n \hat{n}_{\mathbf{i}+\mathbf{r}_n, \uparrow} \hat{n}_{\mathbf{i}+\mathbf{r}_n, \downarrow}.\end{aligned}$$

Positive semidefinite form

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

$$\text{with } \hat{H}_G = \sum_{\mathbf{i}, \sigma} \sum_{\alpha=1}^5 \hat{G}_{\alpha, \mathbf{i}, \sigma} \hat{G}_{\alpha, \mathbf{i}, \sigma}^\dagger, \quad \hat{H}_P = \sum_{n=1}^6 U_n \sum_{\mathbf{i}} \hat{P}_{\mathbf{i}+\mathbf{r}_n}$$

→ Matching conditions

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

$$\hat{H}_{kin} = - \sum_{\mathbf{i}, \sigma} \sum_{\alpha=1}^5 \hat{G}_{\alpha, \mathbf{i}, \sigma}^\dagger \hat{G}_{\alpha, \mathbf{i}, \sigma} + \text{const}$$

↑
quadratic in the original c-operators

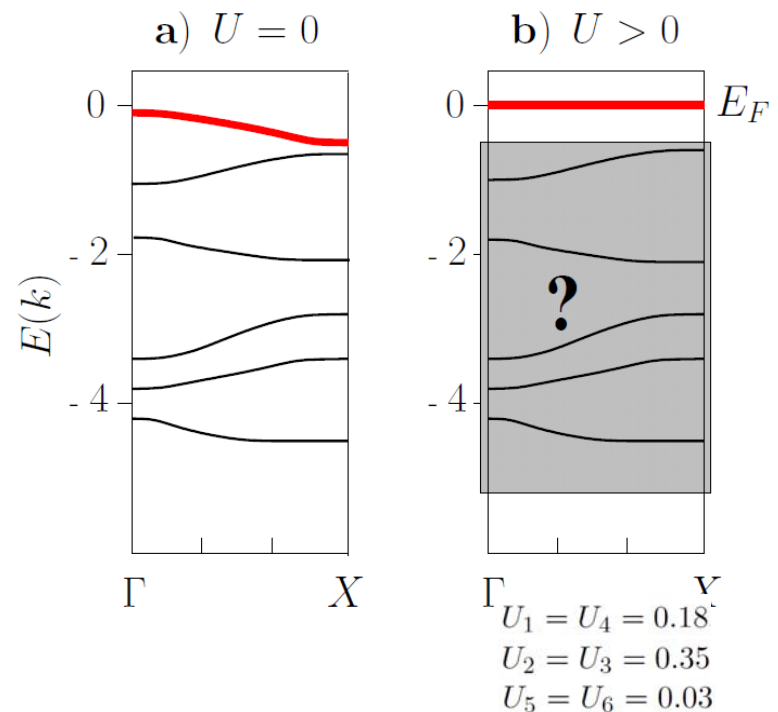
→ Effective, interaction dependent band structure:
same as for H_0 but with renormalization

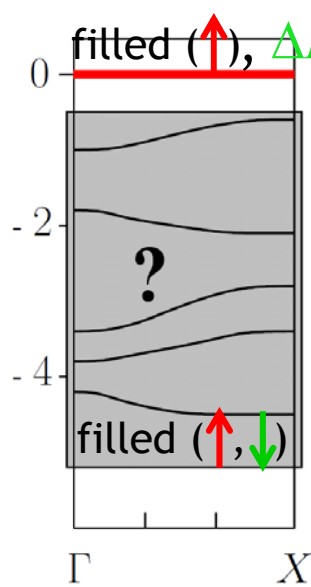
$$\epsilon_n \rightarrow \epsilon_n^R = \epsilon_n + U_n - qU$$

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 $n=11/6$:

$$|\Psi_g(N^*)\rangle = \prod_{\mathbf{i}} \left[\left(\prod_{n=1}^6 \hat{c}_{\mathbf{i}+\mathbf{r}_n, \sigma}^\dagger \right) \left(\prod_{\alpha=1}^5 \hat{G}_{\alpha, \mathbf{i}, -\sigma}^\dagger \right) \right] |0\rangle$$

creates $6N_c$
 σ electrons
 \rightarrow localized

creates $5N_c$
 $-\sigma$ electrons

Physical properties of $-\sigma$ electrons

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

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

Ground state for $n > 11/6$ ($S_{z, \max}$ sector) : add ΔN many $-\sigma$ electrons

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

\rightarrow **itinerant ferromagnet (half-metal)**

Matching conditions are valid for

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

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)

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 , ϵ , n , U , t

Pentagon chain polymers:

- Tune dispersive band structure by the interaction
→ **design of flat bands with ferromagnetic or half-metallic ground states**

