Center for Electronic Correlations and Magnetism
University of Augsburg

Construction of exact ground states for correlated electron models

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Outline:

- Electronic correlations

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

- Diamond Hubbard chains
  → e.g., correlation-induced half-metal

  Triangle Hubbard chains/1D periodic Anderson model
  → ferromagnetism in $CeRh_3B_2$

  Pentagon Hubbard chains
  → route to ferromagnetism in organic polymers

In collaboration with

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

Correlations

Correlation [lat.]: *con* + *relatio* *("with relation")*

Grammar: *either ... or*

Correlations in mathematics, natural sciences:

$$\boxed{\langle AB \rangle \neq \langle A \rangle \langle B \rangle}$$

e.g., densities

$$\boxed{\langle \rho(\mathbf{r}) \rho(\mathbf{r}') \rangle \neq \langle \rho(\mathbf{r}) \rangle \langle \rho(\mathbf{r}') \rangle}$$

Correlations (I):

Effects beyond factorization approximations (e.g., Hartree-Fock)

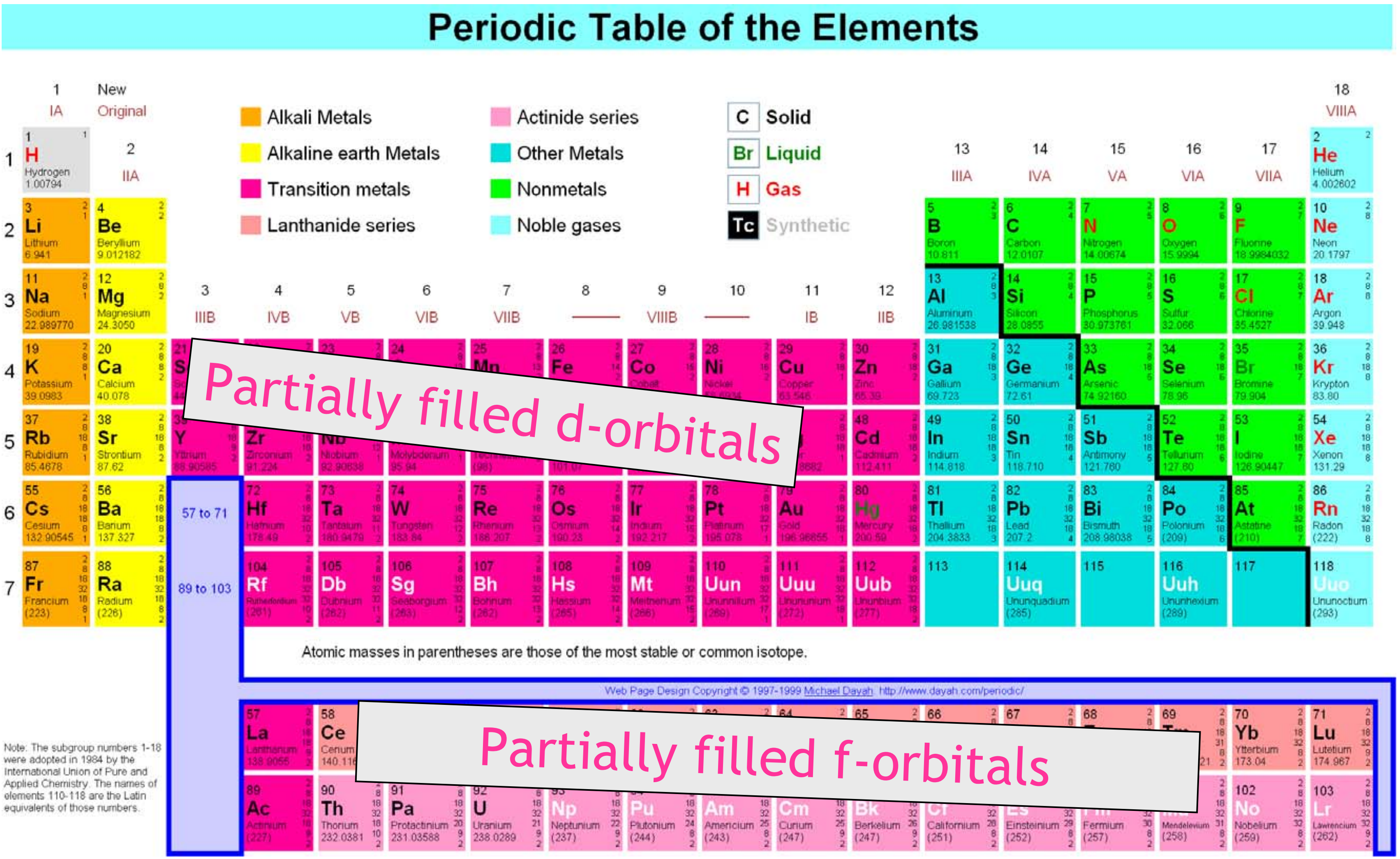
Temporal/spatial correlations in everyday life

Beware: External periodic potential

Temporal/spatial correlations in everyday life

Time/space average insufficient

Electronic Correlations in Solids



Narrow d,f-orbitals/bands → strong electronic correlations

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 a given correlated electron model

(with experimental relevance)

Construction of exact many-electron ground states

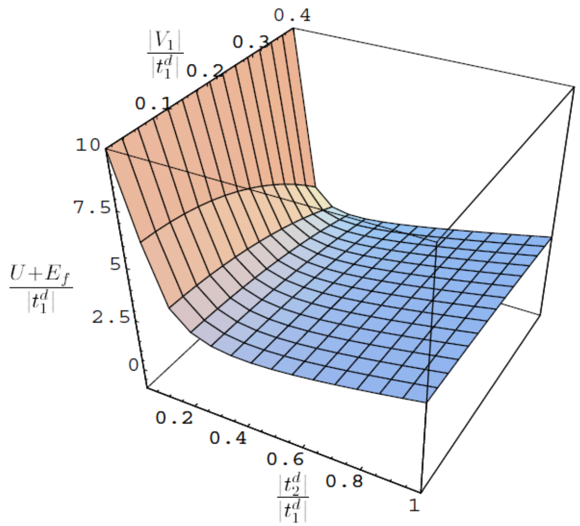
Strategy

Step 1: Transform a given many-electron Hamiltonian for a given lattice 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 a given many-electron Hamiltonian for a given lattice 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, Giesekus (1992)
PAM, Emery model in d=1,2 on regular lattices	Strack (1993)
Ferromagnetism in extended Hubbard models for arbitary 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 *et al*. 2003, 2006)

Construction of exact many-electron ground states

Strategy

Step 1: Transform a given many-electron Hamiltonian for a given lattice into positive semidefinite form

Step 2: Construct a ground state

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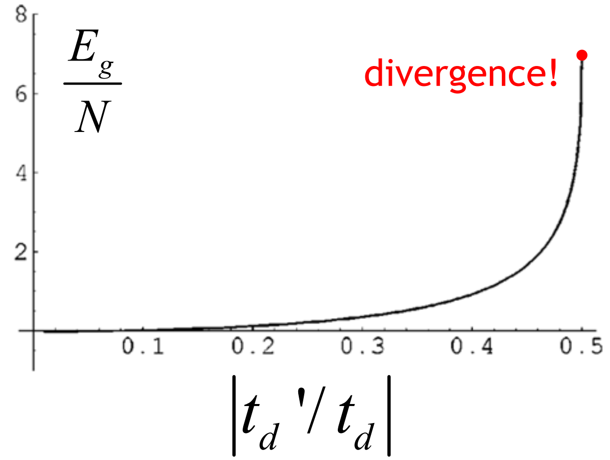
PAM in d=3

- Exact insulating and itinerant (non-Fermi liquid) ground states at ¼ and ¾ 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

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

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

e.g., $\hat{P}_n = \Omega^\dagger \Omega \ , \ \Omega \Omega^\dagger$

→ 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

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

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

Step 2: Construct a ground state

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

ground state ground-state energy

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

Construction of exact many-electron ground states: Details

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

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

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)

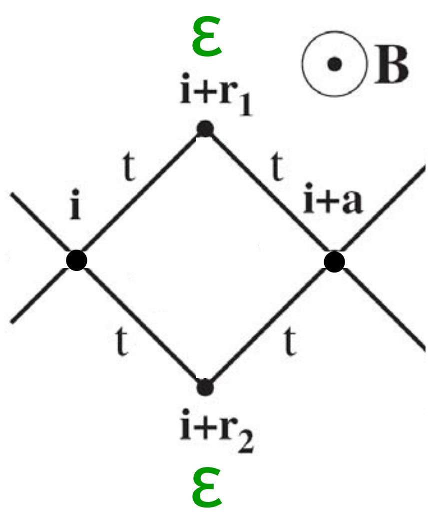
→ First step:

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)

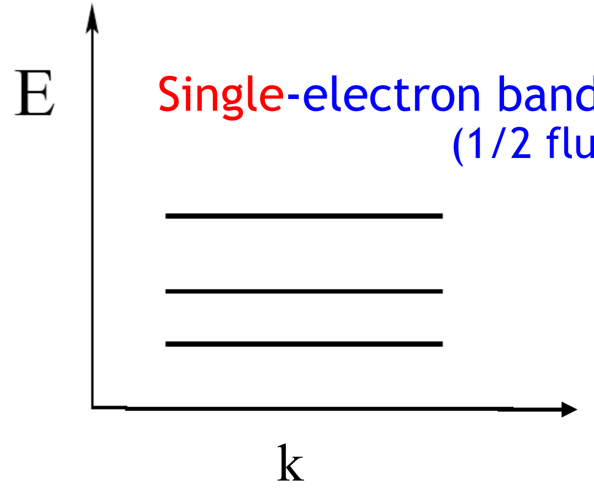


“Aharonov-Bohm cage”

Peierls phase factor

$\delta = 2\pi\Phi/\Phi_0$ $\quad\quad\quad \mathbf{A} \parallel \mathbf{a}$

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



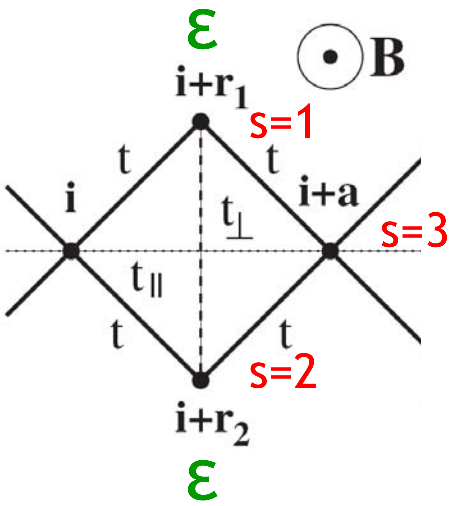
Vidal, Doucot, Mosseri, Butaud (2000):

ε=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

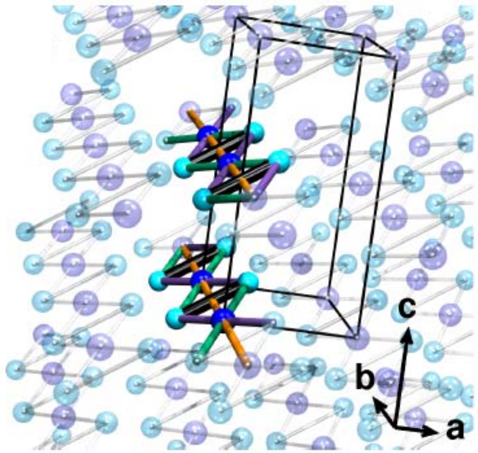
Also valid for finite densities ? $\surd$



3 sites per cell → 3 bands

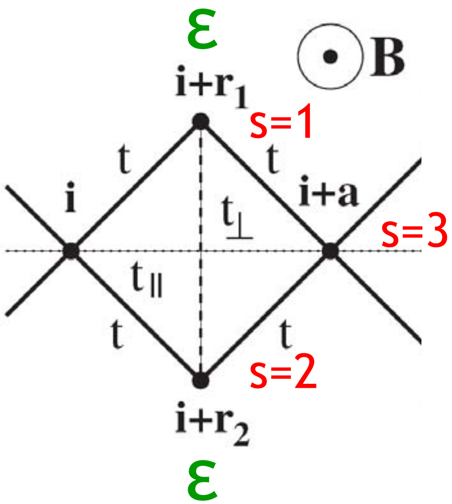
s=1,2,3 sublattice index

N_c = # cells
N = # electrons
$n = \dfrac{N}{3N_c}$ electron density

Jeschke *et al.*,
arXiv:1012.1090

Azurite $Cu_3(CO_3)_2(OH)_2$



3 sites per cell → 3 bands

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N_c = # cells
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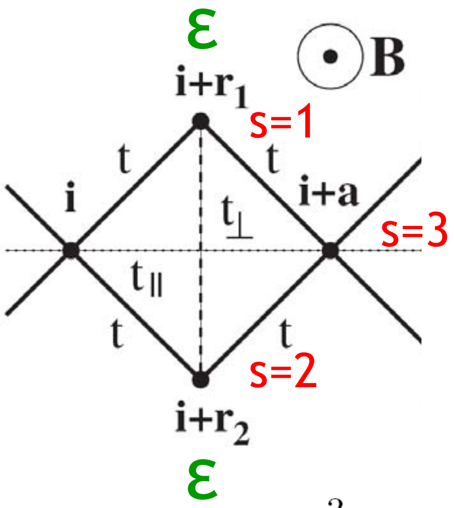
$$\hat{H}_0 = \sum_{\sigma}\sum_{\mathbf{i}=1}^{N_c}\{[te^{i\frac{\delta}{2}}(\hat{c}^{\dagger}_{\mathbf{i}+\mathbf{r}_2,\sigma}\hat{c}_{\mathbf{i},\sigma} + \hat{c}^{\dagger}_{\mathbf{i}+\mathbf{a},\sigma}\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma} +$$

$$\hat{c}^{\dagger}_{\mathbf{i}+\mathbf{r}_1,\sigma}\hat{c}_{\mathbf{i}+\mathbf{a},\sigma} + \hat{c}^{\dagger}_{\mathbf{i},\sigma}\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma}) + t_{\perp}\,\hat{c}^{\dagger}_{\mathbf{i}+\mathbf{r}_2,\sigma}\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma} +$$

$$t_{\parallel}\,\hat{c}^{\dagger}_{\mathbf{i}+\mathbf{a},\sigma}\hat{c}_{\mathbf{i},\sigma} + H.c.] + \varepsilon\sum_{s=1,2}\hat{n}_{\mathbf{i}+\mathbf{r}_s,\sigma}\}$$

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

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



3 sites per cell → 3 bands

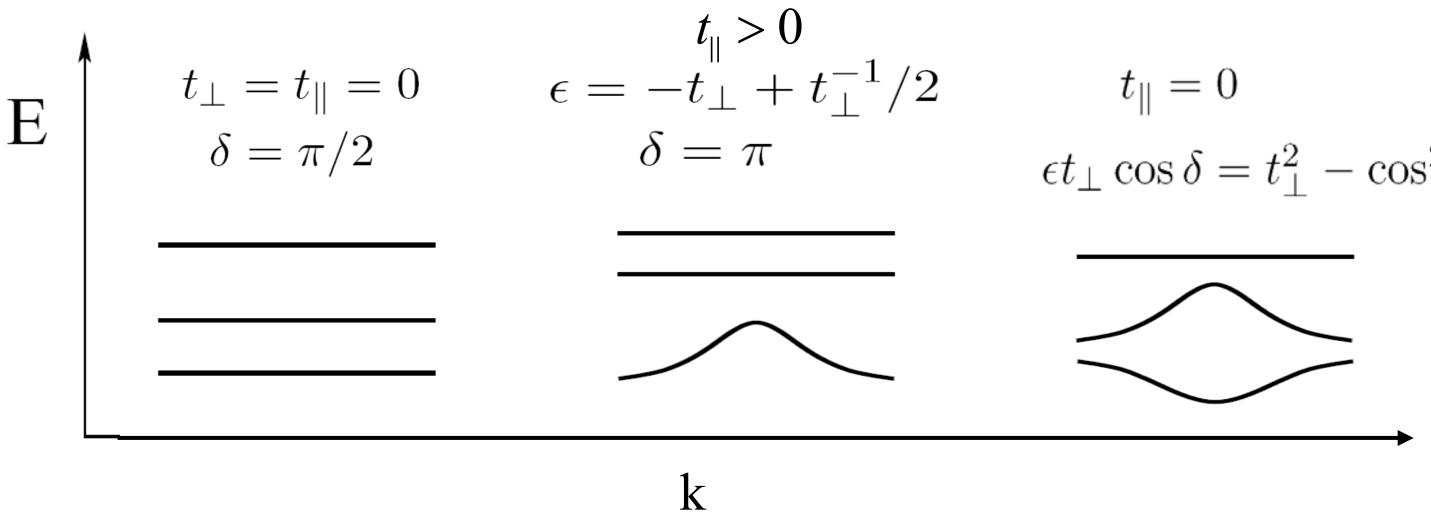
s=1,2,3 sublattice index

N_c = # cells
N = # electrons
$n = \dfrac{N}{3N_c}$ electron density

FT

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

Examples:



Energy unit: $2t$

Single-electron bands

Solution I: Correlated half-metal

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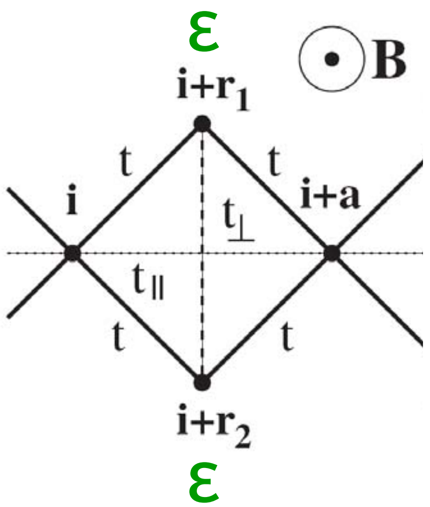
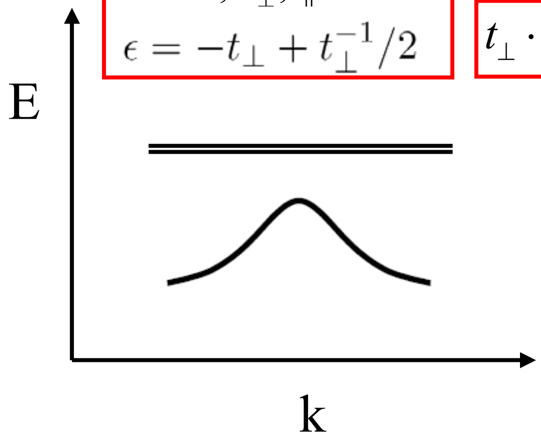


→ Investigate

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

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

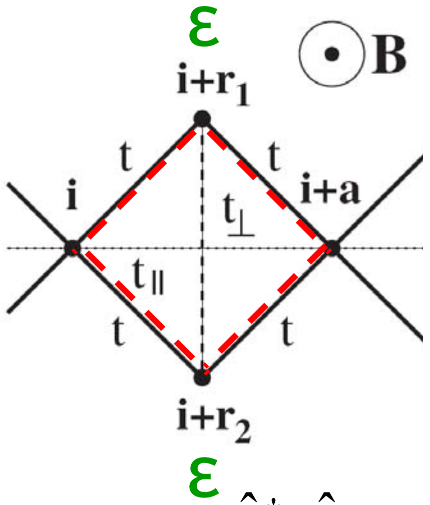
$t_\perp \cdot t_\parallel = 1/4$



Single-electron bands

Solution I: Correlated half-metal

1. Transformation of the Hamiltonian into positive semidefinite form



$\hat{H}_0$ Define non-canonical fermionic operators:

One composite operator on each plaquette

$$\hat{A}_{i,\sigma} = a_1 \hat{c}_{i\sigma} + a_2 \hat{c}_{i+\mathbf{r}_2\sigma} + a_3 \hat{c}_{i+\mathbf{a}\sigma} + a_4 \hat{c}_{i+\mathbf{r}_1\sigma}$$

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

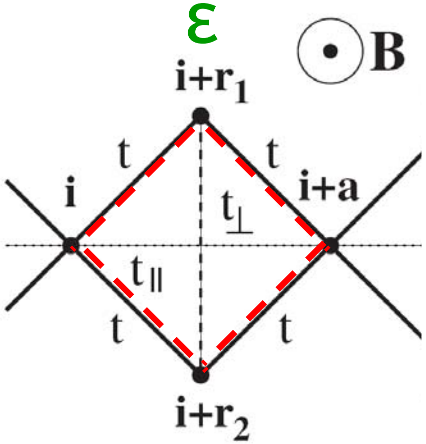
$$\{\hat{A}_{\mathbf{i},\sigma}, \hat{A}^\dagger_{\mathbf{j},\sigma}\} \neq \delta_{\mathbf{i},\mathbf{j}}$$

$$\Rightarrow \hat{A}^\dagger_{i\sigma}\hat{A}_{i\sigma} = (a_2^* a_1 \hat{c}^\dagger_{i+\mathbf{r}_2\sigma}\hat{c}_{i\sigma} + a_3^* a_2 \hat{c}^\dagger_{i+\mathbf{a}\sigma}\hat{c}_{i+\mathbf{r}_2\sigma} + a_4^* a_3 \hat{c}^\dagger_{i+\mathbf{r}_1\sigma}\hat{c}_{i+\mathbf{a}\sigma} +$$
$$a_1^* a_4 \hat{c}^\dagger_{i\sigma}\hat{c}_{i+\mathbf{r}_1\sigma} + a_2^* a_4 \hat{c}^\dagger_{i+\mathbf{r}_2\sigma}\hat{c}_{i+\mathbf{r}_1\sigma} + a_3^* a_1 \hat{c}^\dagger_{i+\mathbf{a}\sigma}\hat{c}_{i\sigma} + \text{H.c.}) +$$
$$|a_1|^2 n_{i\sigma} + |a_2|^2 n_{i+\mathbf{r}_2\sigma} + |a_3|^2 n_{i+\mathbf{a}\sigma} + |a_4|^2 n_{i+\mathbf{r}_1\sigma}$$

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

Solution I: Correlated half-metal

1. Transformation of the Hamiltonian into positive semidefinite form



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

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

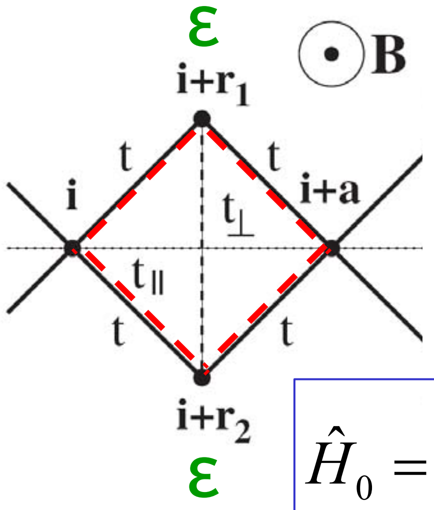
$$\Rightarrow \hat{A}^\dagger_{i\sigma} \hat{A}_{i\sigma} = (a_2^* a_1 \hat{c}^\dagger_{i+\mathbf{r}_2\sigma} \hat{c}_{i\sigma} + a_3^* a_2 \hat{c}^\dagger_{i+\mathbf{a}\sigma} \hat{c}_{i+\mathbf{r}_2\sigma} + a_4^* a_3 \hat{c}^\dagger_{i+\mathbf{r}_1\sigma} \hat{c}_{i+\mathbf{a}\sigma} +$$
$$a_1^* a_4 \hat{c}^\dagger_{i\sigma} \hat{c}_{i+\mathbf{r}_1\sigma} + a_2^* a_4 \hat{c}^\dagger_{i+\mathbf{r}_2\sigma} \hat{c}_{i+\mathbf{r}_1\sigma} + a_3^* a_1 \hat{c}^\dagger_{i+\mathbf{a}\sigma} \hat{c}_{i\sigma} + \text{H.c.}) +$$
$$|a_1|^2 n_{i\sigma} + |a_2|^2 n_{i+\mathbf{r}_2\sigma} + |a_3|^2 n_{i+\mathbf{a}\sigma} + |a_4|^2 n_{i+\mathbf{r}_1\sigma}$$

$$-\sum_{i\sigma} \hat{A}^\dagger_{i\sigma} \hat{A}_{i\sigma} \overset{!}{=} \hat{H}_0 \Rightarrow \boxed{\begin{array}{l} a_2^* a_1 = a_3^* a_2 = a_4^* a_3 = a_1^* a_4 = -t e^{i\delta/2} \\ a_2^* a_4 = -t_\perp \\ a_3^* a_1 = -t_\parallel \\ |a_1|^2 + |a_3|^2 = \varepsilon + |a_2|^2 = \varepsilon + |a_4|^2 \end{array}} \Rightarrow$$

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

Solution I: Correlated half-metal

1. Transformation of the Hamiltonian into positive semidefinite form



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

Positive semidefinite

$$\boxed{\hat{H}_U} \qquad \hat{H}_U = U \sum_{\mathbf{i}}^{3N_c} \hat{n}_{\mathbf{i}\uparrow}\hat{n}_{\mathbf{i}\downarrow} = U\hat{P} + U\hat{N} - UN_c$$

N_c: # unit cells

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

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

positive semidefinite

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

Solution I: Correlated half-metal

2. Construction of the ground state

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

positive semidefinite

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

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

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

Creates one σ and one -σ electron in each unit cell

At least one electron required at each site

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

Creates two more electrons with fixed spin σ on arbitrary sites of each unit cell

Ground state for

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

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

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

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

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

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

Prove $\boxed{\left|\Psi_g^I(4N_c)\right\rangle \text{ spans } \ker(\hat{H}') := \left\{ |\phi\rangle \;\middle|\; \hat{H}'|\phi\rangle = 0 \right\},\ \hat{H}' \equiv \hat{H} - E_g}$

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

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

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

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

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

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

Theorem 1: ker($\hat{A}_{i\sigma}\hat{A}^{\dagger}_{i\sigma}$) is spanned by vectors of the form $|\Psi\rangle = \hat{A}^{\dagger}_{i\sigma}\hat{W}|0\rangle$,

where $\hat{W}$ is an arbitrary operator, as long as $\langle\Psi|\Psi\rangle \neq 0$.

Proof:

a) $\hat{A}_{i\sigma}\hat{A}^{\dagger}_{i\sigma}|\Psi\rangle \overset{\left(\hat{A}^{\dagger}_{i\sigma}\right)^2=0}{=} 0 \Rightarrow |\Psi\rangle \in$ ker($\hat{A}_{i\sigma}\hat{A}^{\dagger}_{i\sigma}$) √

b) To show that all vectors $|\Psi\rangle \in$ ker($\hat{A}_{i\sigma}\hat{A}^{\dagger}_{i\sigma}$) can be written

in the form $|\Psi\rangle = \hat{A}^{\dagger}_{i\sigma}\hat{W}|0\rangle$ we assume $|\Phi\rangle = \hat{Y}|0\rangle \in$ ker($\hat{A}_{i\sigma}\hat{A}^{\dagger}_{i\sigma}$), i.e., $\hat{A}_{i\sigma}\hat{A}^{\dagger}_{i\sigma}\hat{Y}|0\rangle=0$.

$$\Rightarrow |\Phi\rangle = \hat{Y}|0\rangle \overset{\left\{\hat{A}_{i\sigma},\hat{A}^{\dagger}_{i\sigma}\right\}=a_{i\sigma}=const}{=} \frac{1}{a_{i\sigma}}(\cancel{\hat{A}_{i\sigma}\hat{A}^{\dagger}_{i\sigma}} + \hat{A}^{\dagger}_{i\sigma}\hat{A}_{i\sigma})\hat{Y}|0\rangle = \hat{A}^{\dagger}_{i\sigma}\underbrace{(\frac{1}{a_{i\sigma}}\hat{A}_{i\sigma}\hat{Y})}_{\hat{W}}|0\rangle = \hat{A}^{\dagger}_{i\sigma}\hat{W}|0\rangle$$

q.e.d.

Theorem 2: ker($\sum_{\sigma}\sum_{i=1}^{N_c}\hat{A}_{i\sigma}\hat{A}^{\dagger}_{i\sigma}$) is spanned by vectors of the form $|\Psi\rangle = [\prod_{\sigma}\prod_{i=1}^{N_c}\hat{A}^{\dagger}_{i\sigma}]\hat{W}|0\rangle$,

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.

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

Spanned by states which have at least one electron per site

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

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

Theorem 3: For N=4N$_c$, $\hat{W} = \hat{F}_\sigma^\dagger = \prod_{\mathbf{i}}[\hat{c}^\dagger_{\mathbf{i}+\mathbf{r}_{s_{\mathbf{i},1}},\sigma}\hat{c}^\dagger_{\mathbf{i}+\mathbf{r}_{s_{\mathbf{i},2}},\sigma}]$

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

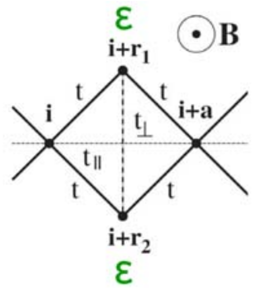
$\epsilon = -t_\perp + t_\perp^{-1}/2$

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

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

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

is the unique ground state



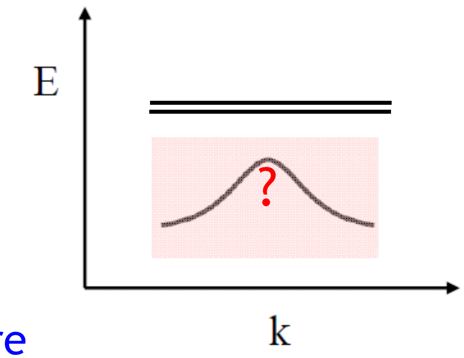
Physical properties:

Effective band structure

$$\hat{H}_{kin} = -\sum_{i\sigma} \hat{A}^\dagger_{i\sigma}\hat{A}_{i\sigma} + \text{const}$$

quadratic in the original c-operators

→ Interaction dependent band structure



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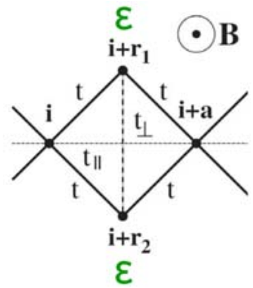
is the unique ground state



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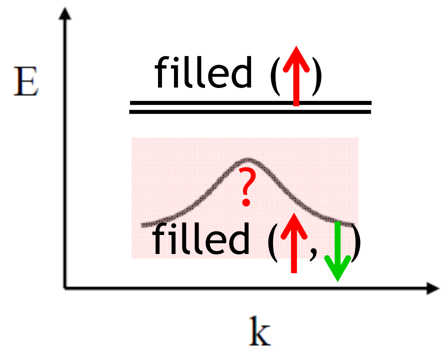


One σ electron on every lattice site → localized

-σ electrons:

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

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

→ -σ electrons: spatially extended but localized for $N_c \to \infty$

N_c: # unit cells

Solution I: Correlated half-metal

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

N_c: # unit cells

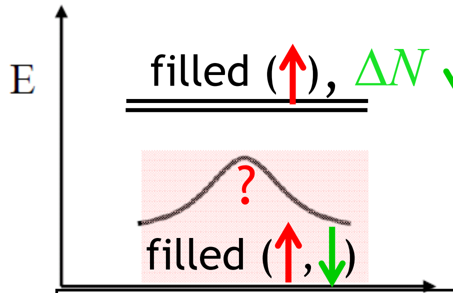
Ground state

$$\boxed{|\Psi_g^I(4N_c + \Delta N)\rangle = \prod_{\alpha=1}^{\Delta N} \hat{c}^\dagger_{n_\alpha, \mathbf{k}_\alpha, -\sigma} |\Psi_g^I(4N_c)\rangle}$$

$n_\alpha: \quad s = 1,2,3$

plane wave-type states due to $-\sigma$ electrons

Physical properties:



- charge gap $\Delta\mu = E_g(N) - 2E_g(N-1) + E_g(N-2) = 0$
- $\Gamma_{r,\ -\sigma} \propto$ plane wave results

→ ΔN many $-\sigma$ electrons itinerant

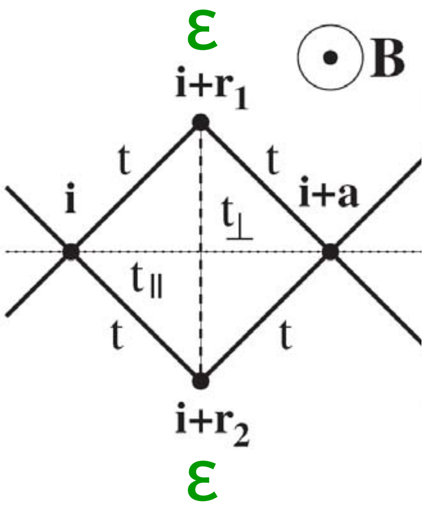
Ground state for $4/3 < n < 5/3$

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

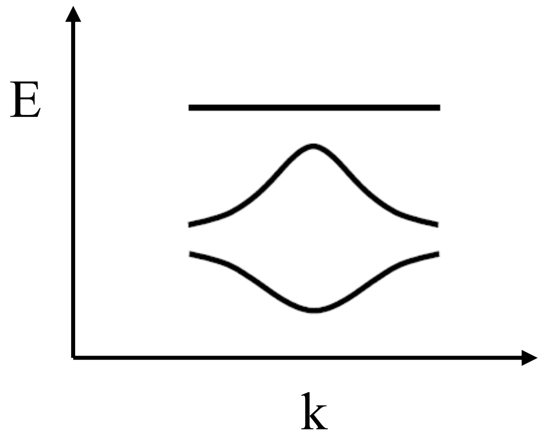
U=0: dispersionless, localized electrons
U>0: correlation induced half-metal

Solution II:
Exact ground states for general magnetic flux

Solution II: Exact ground states for general magnetic flux



$$\delta \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$$
$$t_{\|} = 0,\ t_{\perp} < 0$$
$$b \equiv -\cos\delta / t_{\perp},\quad \varepsilon = b - b^{-1}$$



Single-electron bands

Ground states for $n \geq 5/3$

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

$\xrightarrow{B \neq 0}$

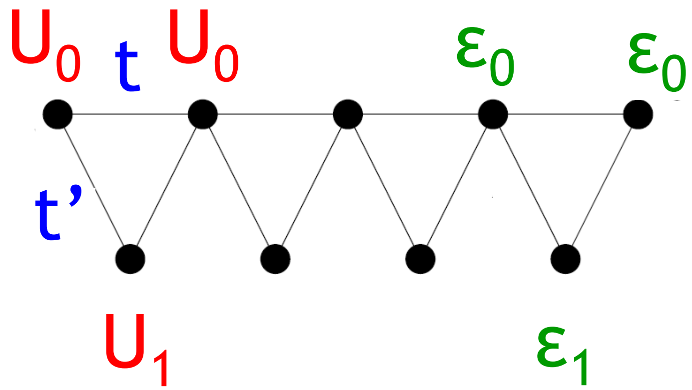
Non-saturated ferromagnet
- insulating for n=5/3
- metallic for n>5/3

Conclusion
- Diamond Hubbard chain has remarkably complex properties
- Switch between different ground states by variation of B, 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 → 2 bands

N_c = # cells

N = # electrons

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

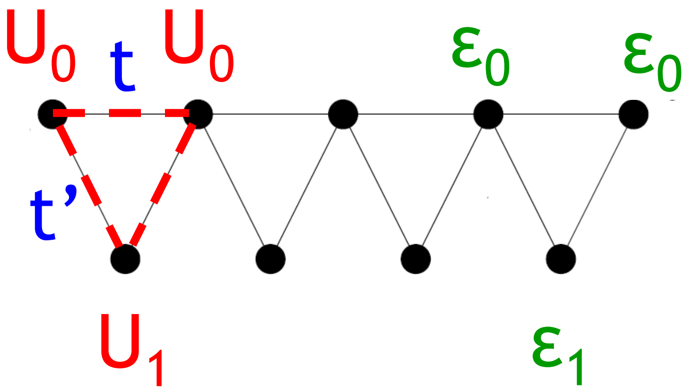
Müller-Hartmann (1995)

Penc, Shiba, Mila, Tsukagoshi (1996)

Fazekas (1997)

Derzho, Honecker, Richter (2007)

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



2 sites per cell → 2 bands

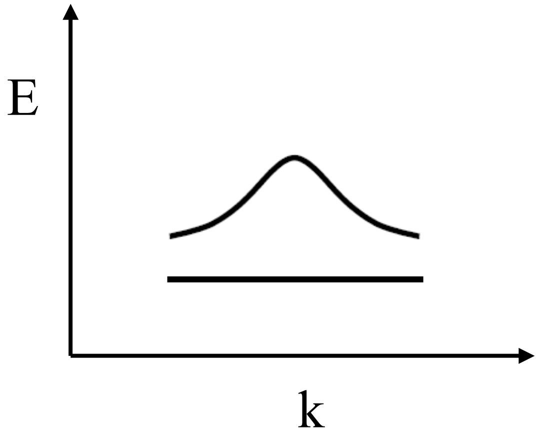
N_c = # cells

N = # electrons

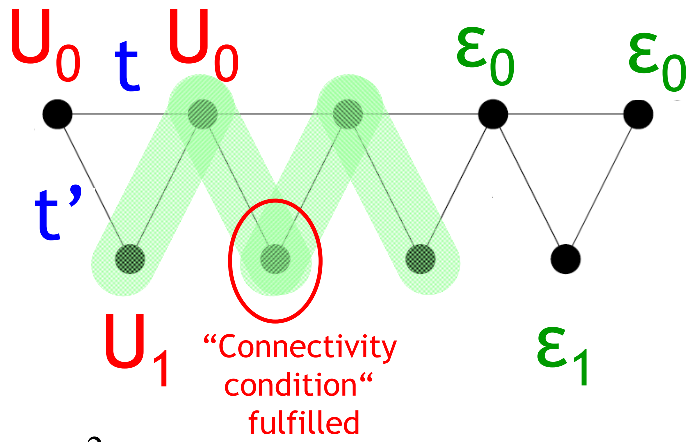
$n = \dfrac{N}{2N_c}$ electron density

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

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



Single-electron bands



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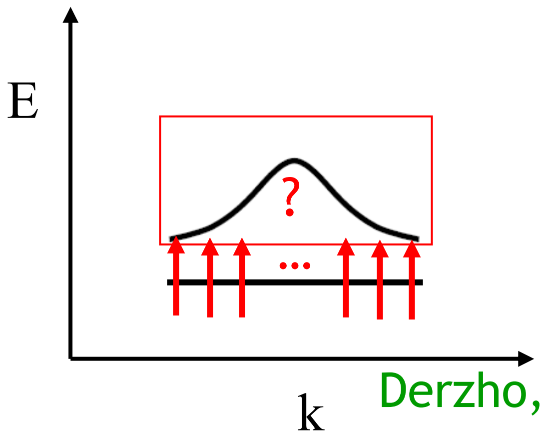


Solution I: $U_0, U_1 > 0$

n<1/2 : ferromagnetic clusters

n=1/2 : fully saturated ferromagnet

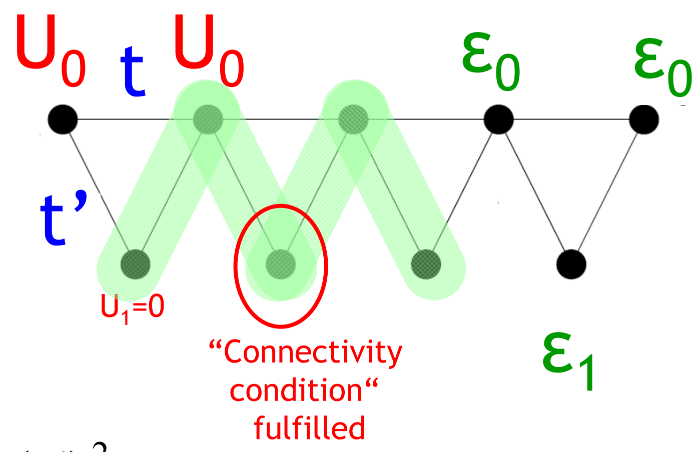
Mielke, Tasaki (1993)

Derzho, Honecker, Richter (2007)

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

→ 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 → 2 bands

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N = # electrons
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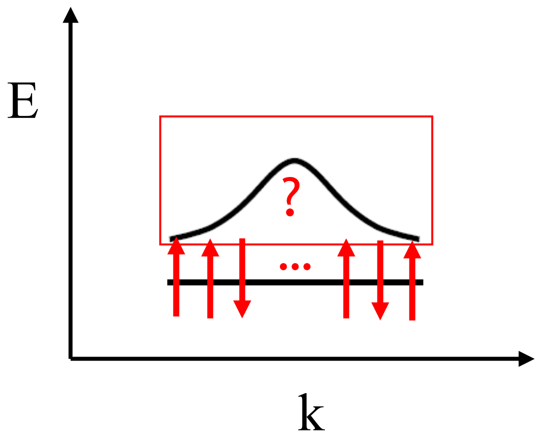
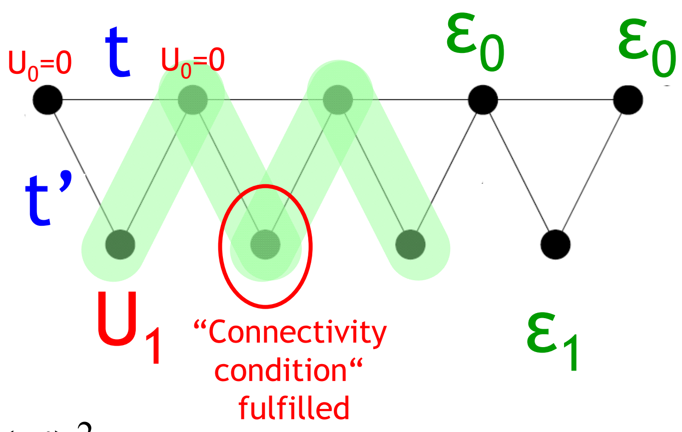
$$\epsilon_1 - \epsilon_0 > -2t$$



Solution II: $U_0 > 0,\ U_1 = 0$

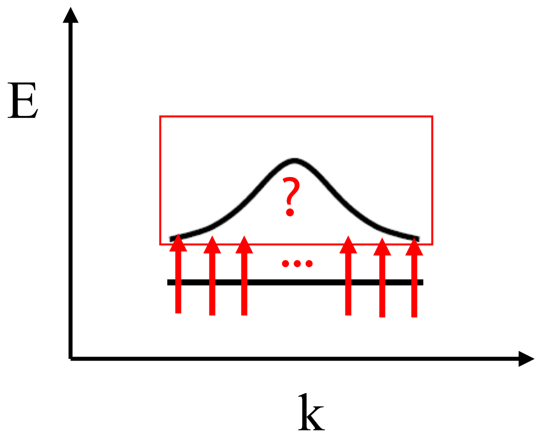
n=1/2 : non-magnetic

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



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

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



2 sites per cell → 2 bands

N_c = # cells

N = # electrons

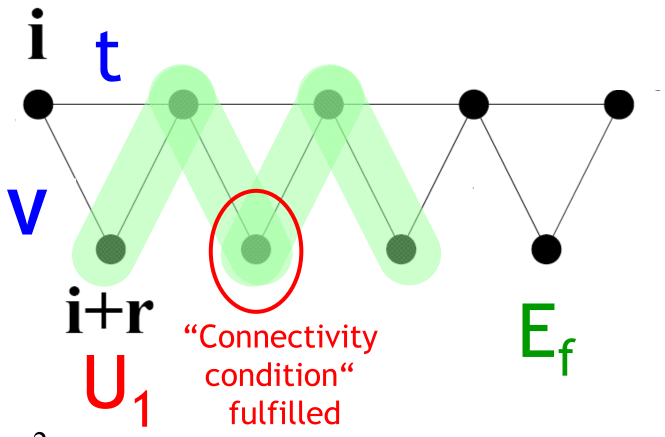
$n = \dfrac{N}{2N_c}$ electron density

Solution III: $U_0 = 0,\ U_1 > 0$

n=1/2 : fully saturated ferromagnet

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

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



2 sites per cell → 2 bands

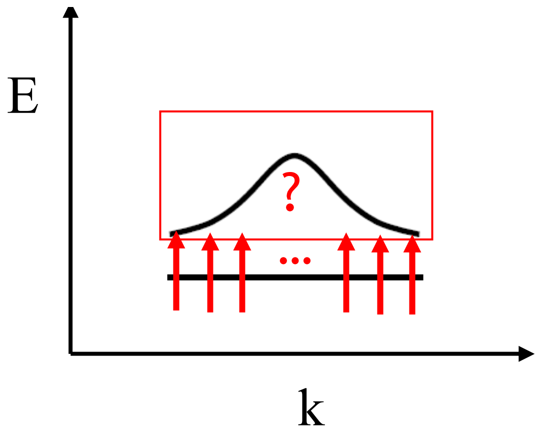
N_c = # cells

N = # electrons

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

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

$$E_f > -2t$$



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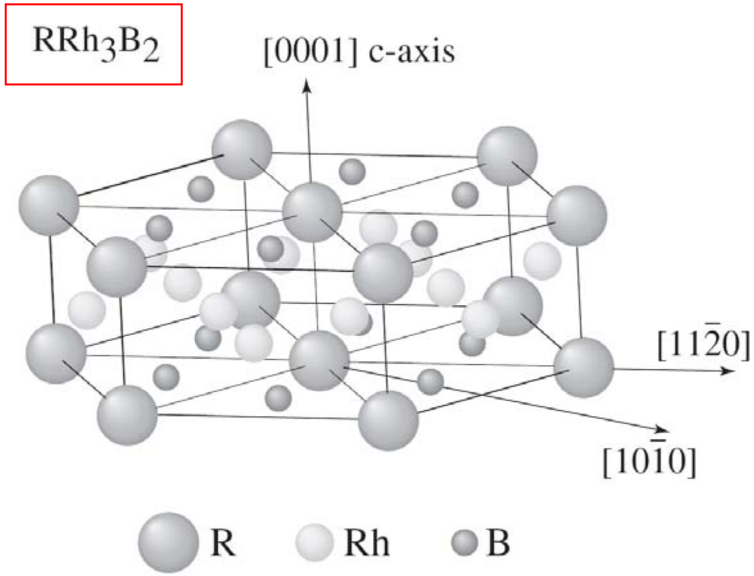
1D periodic Anderson model

Application of the 1D periodic Anderson model to $CeRh_3B_2$

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

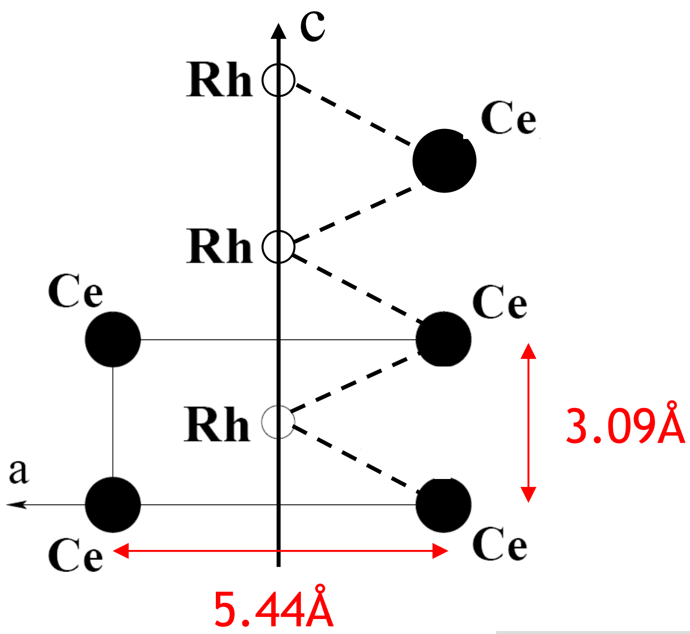
- RKKY interaction cannot explain ferromagnetism
- Small *f*-moment 0.45 μ_B (free Ce^{3+} ion: 2.14 μ_B)

Application of the 1D periodic Anderson model to $CeRh_3B_2$



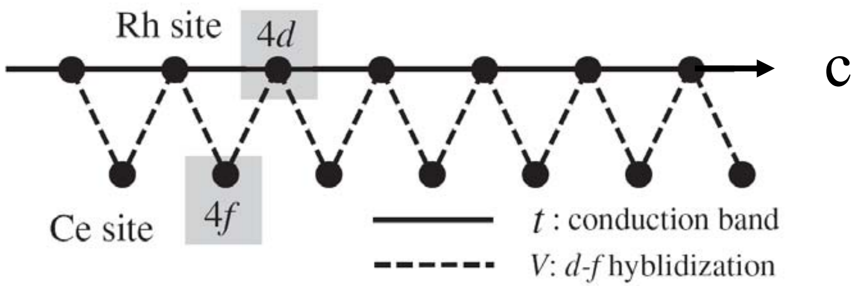
Rare Earth

Yamada *et al.* (2004)



(a,c) plane

Quasi-1D structure



Kono, Kuramoto (2006)

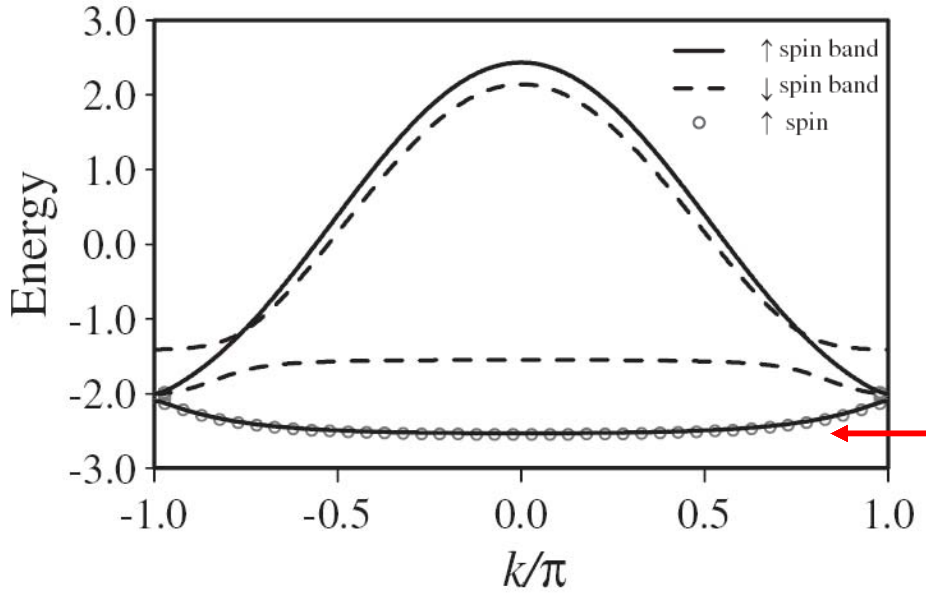
Mechanism for f-electron ferromagnetism in $CeRh_3B_2$?

Gutzwiller projected variational wave function $\boxed{|\Psi\rangle = P|\Phi\rangle}$

Evaluations by variational Monte Carlo (VMC)   Kono, Kuramoto (2006)

f-electron ferromagnetism in $CeRh_3B_2$

VMC



Kono, Kuramoto (2006)

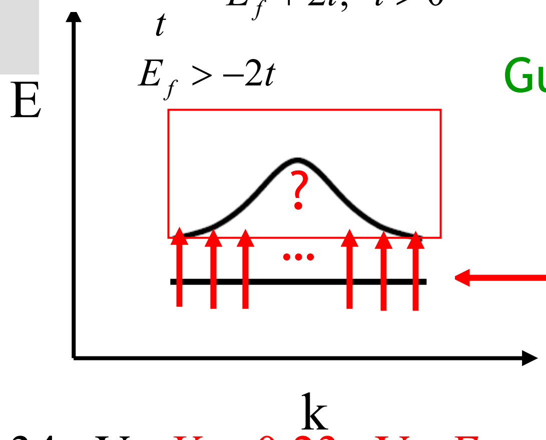
almost flat band

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

Exact ground state
(Solution III)

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

$$E_f > -2t$$



Gulacsi, Kampf, DV (2008)

saturated ferromagnetism,
bare flat band unchanged by U

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

f-electron ferromagnetism in $CeRh_3B_2$: Magnetic moments

Free Ce^{3+} 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 $\frac{V^2}{t} = E_f + 2t,\ \ t > 0,\ E_f > -2t$

$$\boxed{m_f = g\mu_B \frac{1}{2N_c} \sum_i < (\hat{n}^f_{i,\uparrow} - \hat{n}^f_{i,\downarrow}) >}$$

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

$m_f = 0.68\ \mu_B$ 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

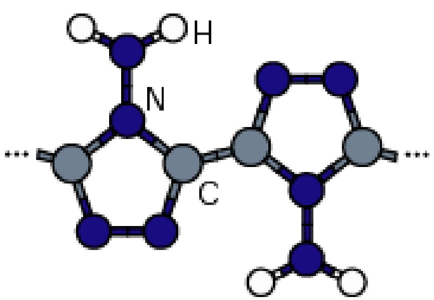
Search for plastic ferromagnets and
ferromagnetism in systems with non-magnetic elements

Candidate: Flat-band ferromagnetism in organic polymers

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

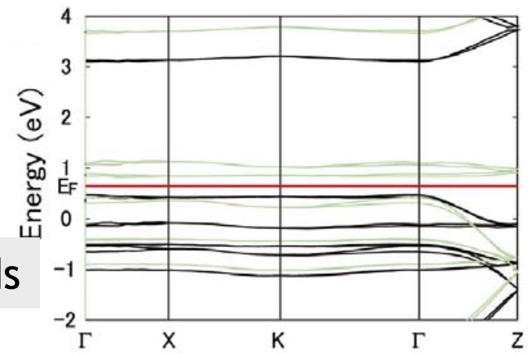
Arita, Suwa, Kuroki, Aoki (2002, 2003)

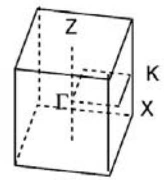
Polyaminotriazole



Spin-DFT

Single-particle bands



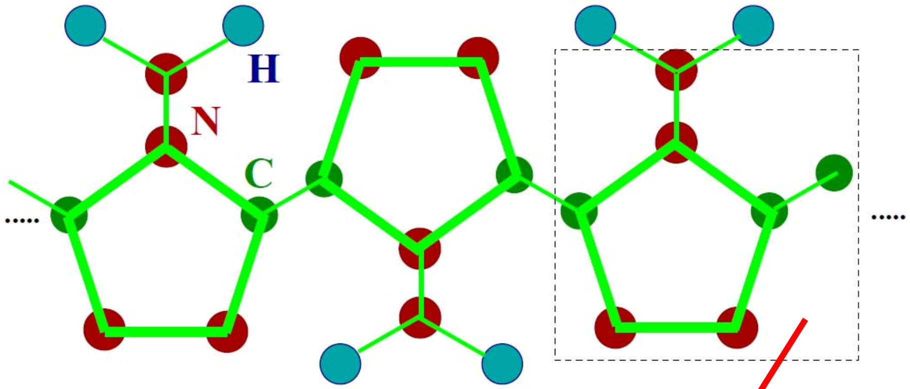


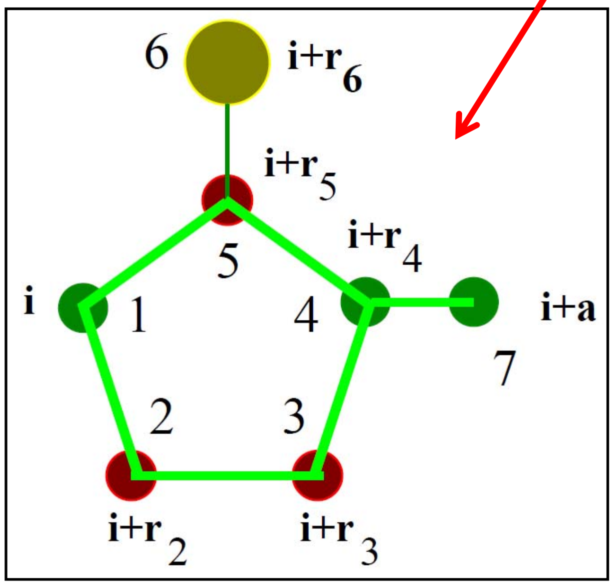
- Strong correlations in acene and thiophene organic molecular crystals
- stabilization of magnetic phases at high electron densities

Brocks, van den Brink, Morpurgo (2004)

Polyaminotriazole

Gulacsi, Kampf, DV (2010)





6 sites per cell → 6 bands

N_c = # cells
N = # electrons
$n = \dfrac{N}{6N_c}$ electron density

Arbitrary

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

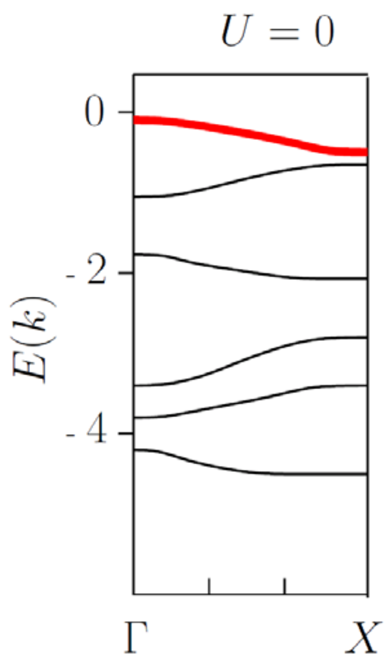
Single-particle bands

Gulacsi, Kampf, DV (2010)

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

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

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



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

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

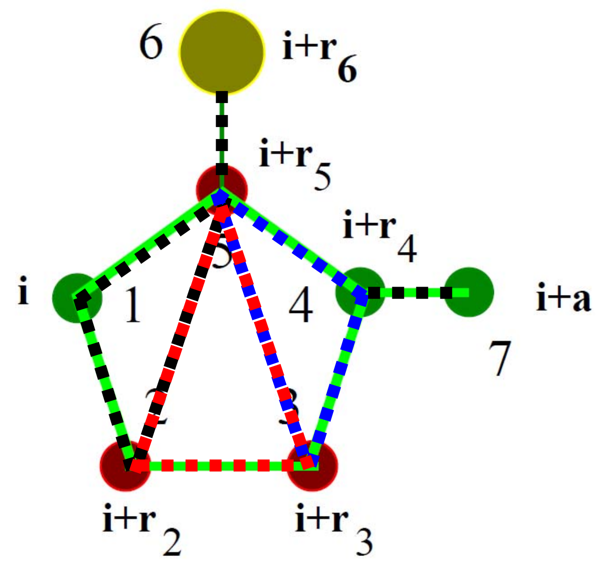
Transform Hamiltonian in positive semidefinite form

Define operators acting on blocks $\mathcal{B}_{\mathbf{i}}$

$$\boxed{\hat{G}^{\dagger}_{\alpha,\mathbf{i},\sigma} = \sum_{\ell\in\mathcal{B}_{\mathbf{i},\alpha}} a_{\alpha,\ell}\hat{c}^{\dagger}_{\mathbf{i}+\mathbf{r}_{\ell},\sigma}}$$ α=1,...,5

3 three-site blocks

2 two-site blocks



Original form

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

$$\hat{H}_0 = \sum_{\sigma,\mathbf{i}} \sum_{n,n'(n>n')} (t_{n,n'} \hat{c}^{\dagger}_{\mathbf{i}+\mathbf{r}_n,\sigma} \hat{c}_{\mathbf{i}+\mathbf{r}_{n'},\sigma} + H.c.) + \\ + \sum_{\sigma,\mathbf{i}} \sum_{n=1}^{6} \epsilon_n \hat{n}_{\mathbf{i}+\mathbf{r}_n,\sigma},$$

$$\hat{H}_U = \sum_{\mathbf{i}} \sum_{n=1}^{6} U_n \hat{n}_{\mathbf{i}+\mathbf{r}_n,\uparrow} \hat{n}_{\mathbf{i}+\mathbf{r}_n,\downarrow}.$$

Positive semidefinite form

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

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

→ 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 on parameters

Effective band structure

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

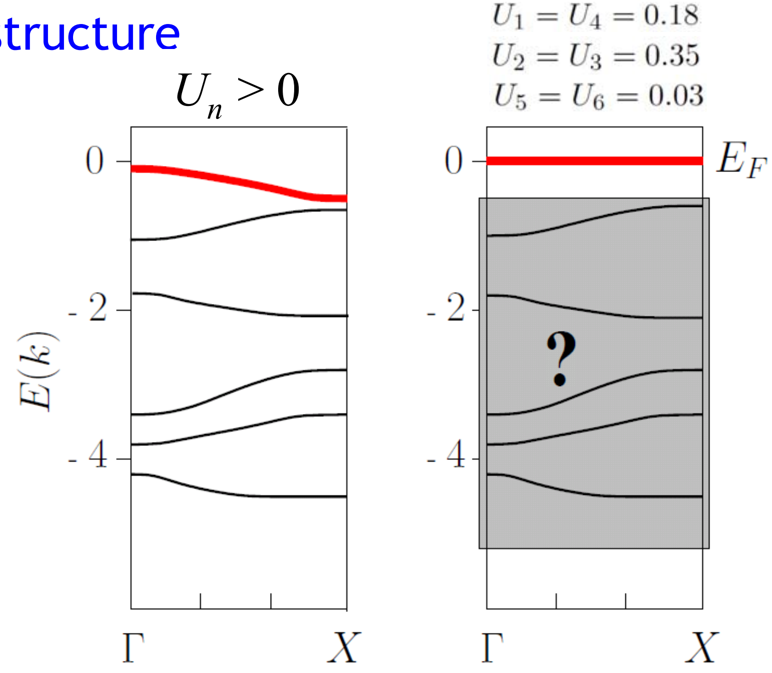
quadratic in the original c-operators

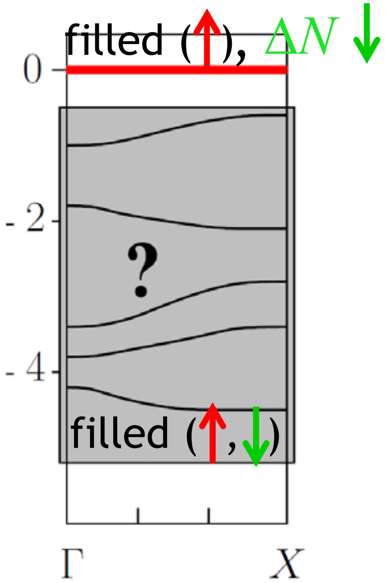
→ Effective, interaction dependent band structure
same as for H_0 but with renormalization of local potentials

$$\boxed{\epsilon_n \rightarrow \epsilon_n^R = \epsilon_n + U_n - q_U}$$

→ 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 $N=11N_c$ → density $n=11/6$

Ground state for n=11/6:

$$\left|\Psi_g(11N_c)\right\rangle = \prod_{\mathbf{i}} [(\prod_{n=1}^{6} \hat{c}^{\dagger}_{\mathbf{i}+\mathbf{r}_n,\sigma})(\prod_{\alpha=1}^{5} \hat{G}^{\dagger}_{\alpha,\mathbf{i},-\sigma})]|0\rangle$$

creates $6N_c$ σ electrons → localized

creates $5N_c$ -σ electrons

Physical properties of -σ electrons

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

→ Ground state for n = 11/6: localized ferromagnet

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

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

→ itinerant ferromagnet (half-metal)

Matching conditions are valid for

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

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 a many-electron Hamiltonian of your choice
for a given lattice of your choice into positive semidefinite form

Step 2: Construct many-electron ground state

Step 3: Prove uniqueness of 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