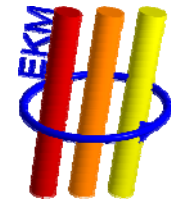




Center for Electronic Correlations and Magnetism
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Construction of exact ground states for correlated electron models

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Universität zu Köln; 20. Mai 2011

Outline:

- Electronic correlations
- Comprehensive 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

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



Correlations

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

Grammar: *either ... or*

Correlations in mathematics, natural sciences:

$$\langle AB \rangle \neq \langle A \rangle \langle B \rangle$$

e.g., densities

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

Correlations:

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

Periodic Table of the Elements

1 IA New Original	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIII	9 VIII	10 VIII	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1 H Hydrogen 1.00794	2 He Helium 4.002602	3 Li Lithium 6.941	4 Be Beryllium 9.012182	5 B Boron 10.811	6 C Carbon 12.0107	7 N Nitrogen 14.00674	8 O Oxygen 15.9994	9 F Fluorine 18.9984032	10 Ne Neon 20.1797	11 Na Sodium 22.989770	12 Mg Magnesium 24.3050	13 Al Aluminum 26.981538	14 Si Silicon 28.0855	15 P Phosphorus 30.973761	16 S Sulfur 32.066	17 Cl Chlorine 35.4527	18 Ar Argon 39.948
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955912	22 Ti Titanium 47.88	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938045	26 Fe Iron 55.845	27 Co Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.723	32 Ge Germanium 72.61	33 As Arsenic 74.92160	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.80
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 101.07	46 Pd Palladium 106.3675	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.90447	54 Xe Xenon 131.29
55 Cs Cesium 132.90545	56 Ba Barium 137.327	57 to 71 Lanthanide series	72 Hf Hafnium 178.49	73 Ta Tantalum 180.9479	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.078	79 Au Gold 196.96655	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.98038	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
87 Fr Francium (223)	88 Ra Radium (226)	89 to 103 Actinide series	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)	107 Bh Bohrium (262)	108 Hs Hassium (265)	109 Mt Meitnerium (266)	110 Uun Ununnilium (269)	111 Uuu Unununium (272)	112 Uub Unbibium (277)	113 Uuq Ununquadium (285)	114 Uuh Ununhexium (289)	115 Uuq Ununquadium (285)	116 Uuh Ununhexium (289)	117 Uue Ununseptium (289)	118 Uuo Ununoctium (293)

Partially filled d-orbitals

Atomic masses in parentheses are those of the most stable or common isotope.

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Note: The subgroup numbers 1-18 were adopted in 1984 by the International Union of Pure and Applied Chemistry. The names of elements 110-118 are the Latin equivalents of those numbers.

Partially filled f-orbitals

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 correlated
electron models

(with experimental relevance)

Construction of exact many-electron ground states

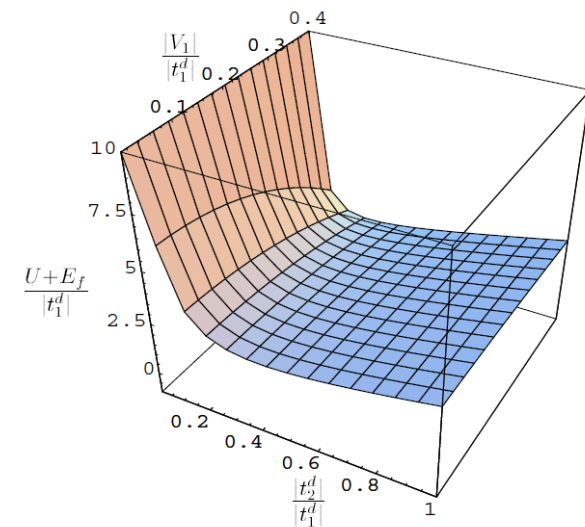
Strategy

Step 1: Transform a many-electron Hamiltonian **of your choice** on a lattice **of your choice** 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 many-electron Hamiltonian of your choice on a lattice of your choice 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)
Matrix product ground states for spin-1 chains ("Optimal ground states")	Klümper, Schadschneider, Zittartz (1993)
Exact ground states in generalized Hubbard models for arbitrary d	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)
Gossamer Hamiltonian	Laughlin (2002/2006); Bernevig <i>et al.</i> 2003, 2006)

Construction of exact many-electron ground states

Strategy

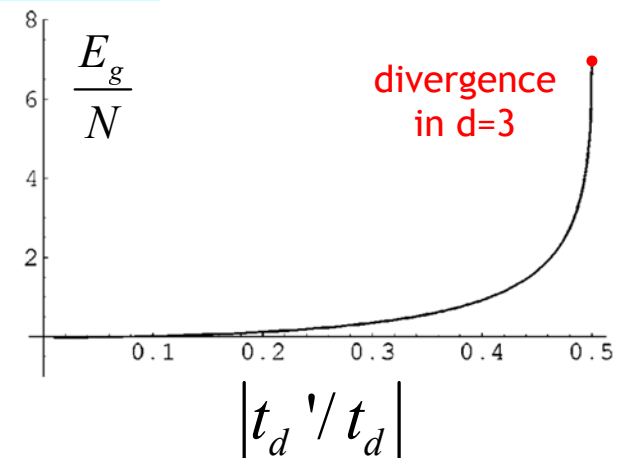
Step 1: Transform a many-electron Hamiltonian of your choice on a lattice of your choice into positive semidefinite form

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

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

(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)
- Flat band ferromagnetism Mielke (1991)
Mielke, Tasaki (1993)
Arita, Suwa Kuroki, Aoki (2002)

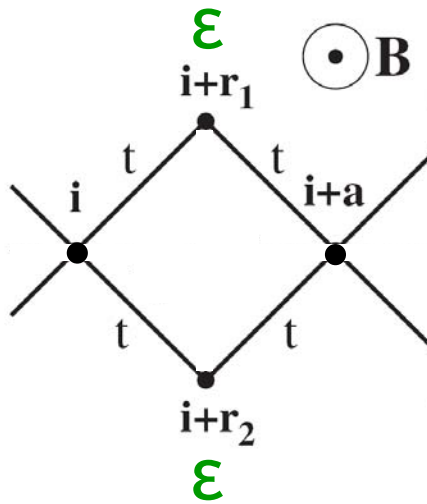
→ **First goal:**

Find exact solutions of correlation models with **flat bands**

Diamond Hubbard chains:
Correlation induced half-metallic behavior

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

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



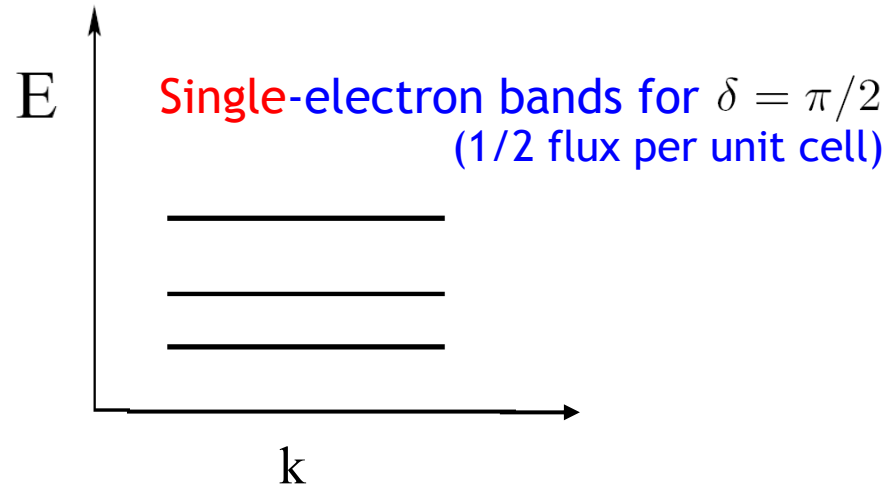
“Aharonov-Bohm cage”

Peierls phase factor

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

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

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



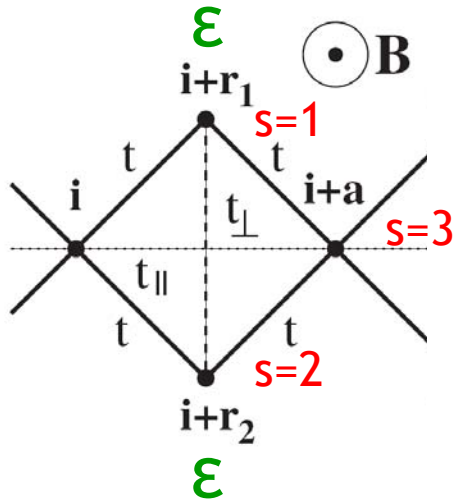
Vidal, Doucot, Mosseri, Butaud (2000):

$\epsilon=0$, $\delta = \pi/2$, 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? ✓



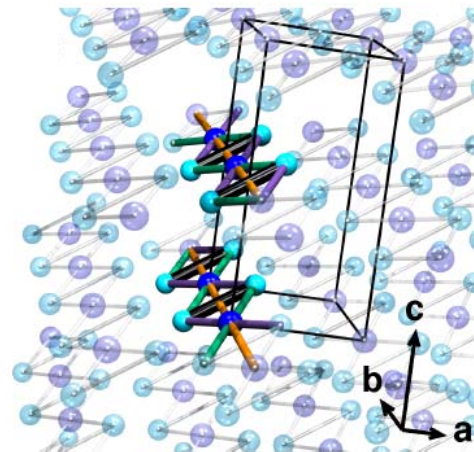
3 sites per cell → 3 bands

s=1,2,3 sublattice index

$N_c = \# \text{ cells}$

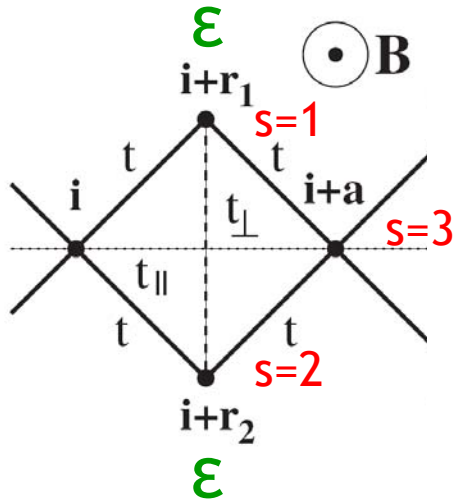
$N = \# \text{ electrons}$

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

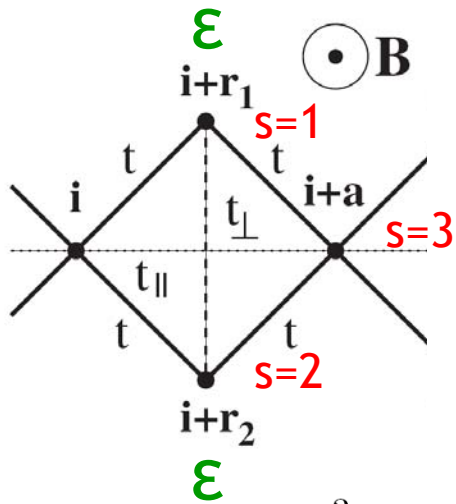
N = # electrons

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

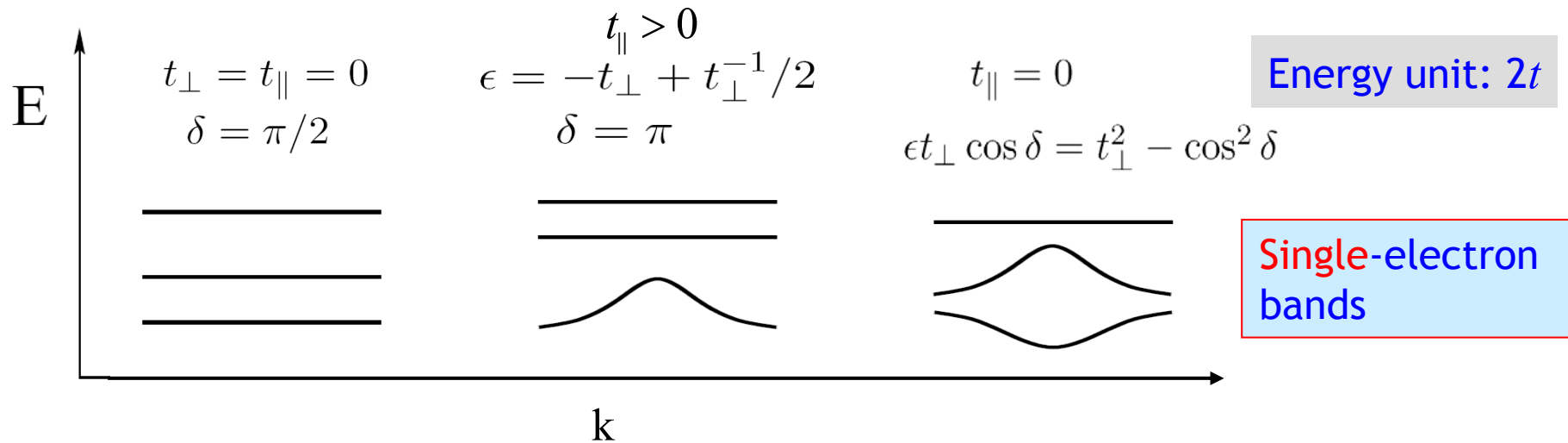
$N_c = \#$ cells

$N = \#$ electrons

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

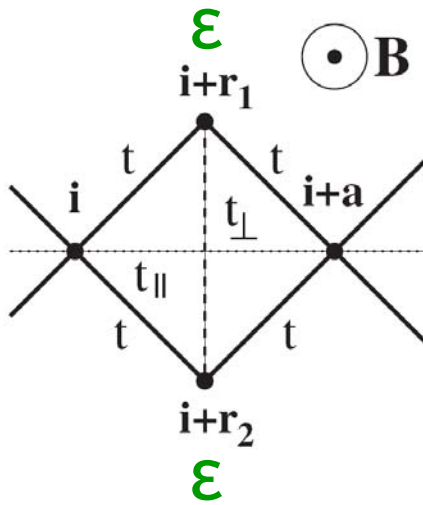
FT
$$\hat{H}_0 = \sum_{\mathbf{k}, \sigma} \sum_{s, s'=1}^3 M_{s, s'}(\mathbf{k}) \hat{C}_{s, \mathbf{k}, \sigma}^\dagger \hat{C}_{s', \mathbf{k}, \sigma}$$

Examples:

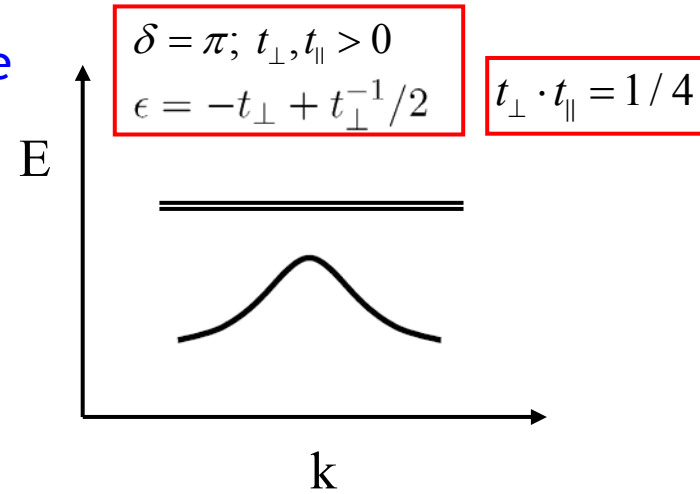


Solution I: Correlated half-metal

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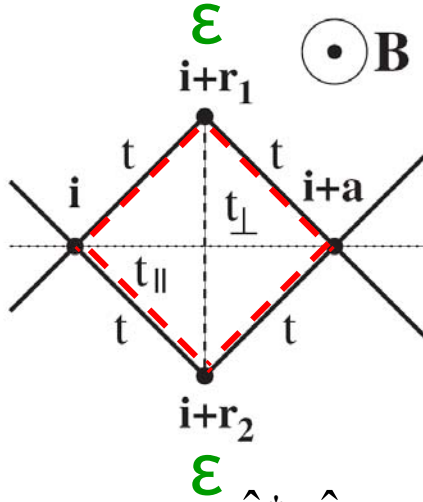


→ Investigate



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

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

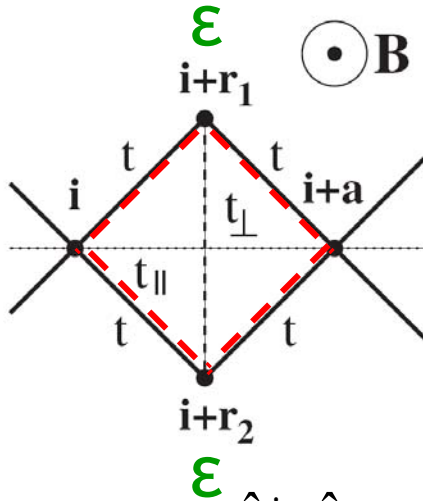
$$(\hat{A}_{i,\sigma})^2 = 0$$

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

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

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

1. Transformation of the Hamiltonian into positive semidefinite form



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

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

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

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

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

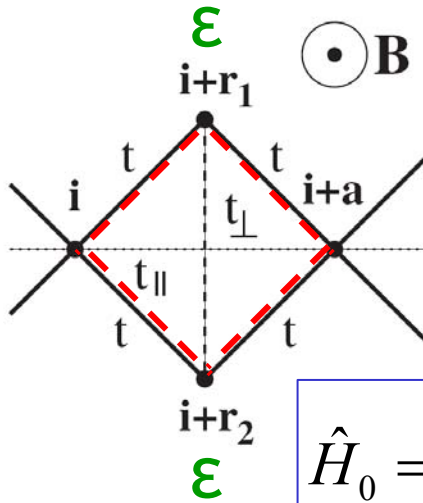
$$-\sum_{i\sigma} \hat{A}_{i\sigma}^\dagger \hat{A}_{i\sigma} \stackrel{!}{=} \hat{H}_0 \Rightarrow$$

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

\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 $\ker(\hat{H}') := \{|\phi\rangle \mid \hat{H}'|\phi\rangle = 0\}$, $\hat{H}' \equiv \hat{H} - E_g$

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

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

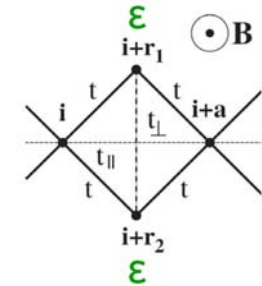
$$\epsilon = -t_{\perp} + t_{\perp}^{-1}/2$$

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

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

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

is the **unique** ground state



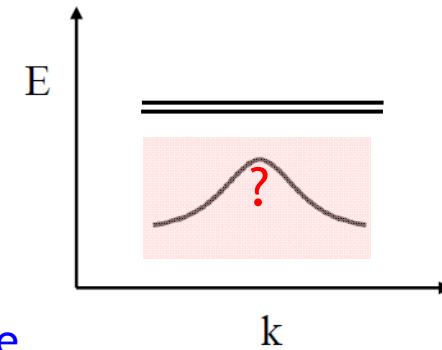
Physical properties:

Effective band structure

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

quadratic in the original c-operators

→ Interaction dependent band structure



Solution I: Correlated half-metal

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

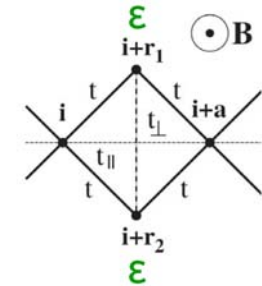
$$\epsilon = -t_{\perp} + t_{\perp}^{-1}/2$$

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

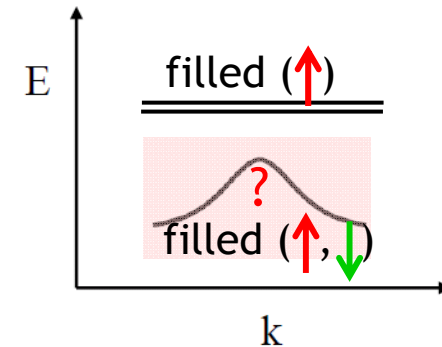
is the **unique** ground state



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 $n_\sigma = 1, n_{-\sigma} = \frac{1}{3} + \frac{\Delta N}{3N_c}$

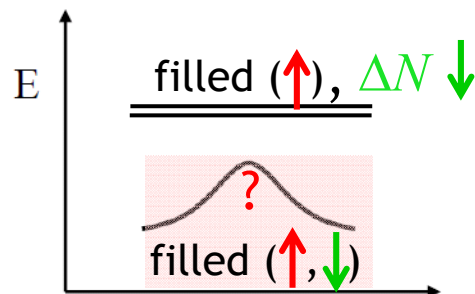
N_c : # unit cells

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

$\rightarrow \Delta N$ many $-\sigma$ electrons itinerant

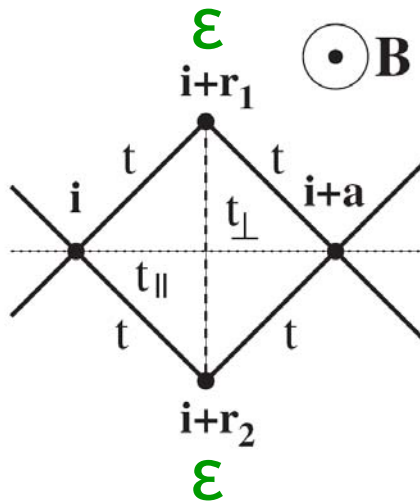
Ground state for $4/3 < n < 5/3$

- $3N_c$ 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

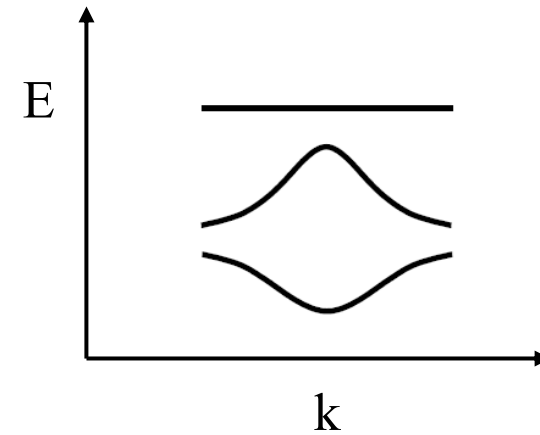
Solution II: Exact ground states for general magnetic flux



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

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

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



Single-electron bands

Ground states for $n \geq 5/3$

$B = 0$: localized non-magnetic ground state for $n \geq 5/3$	$B \neq 0$	Non-saturated ferromagnet • insulating for $n=5/3$ • metallic for $n>5/3$
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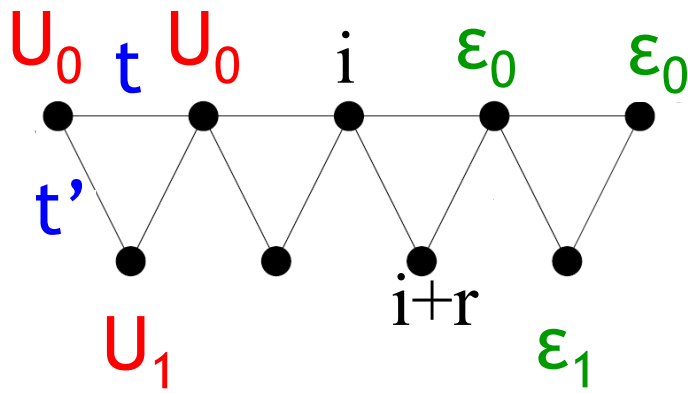
Conclusion

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

Triangle Hubbard chains:
Explanation of the strange ferromagnetism in CeRh_3B_2

Flat bands in the single-electron band structure stay flat 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

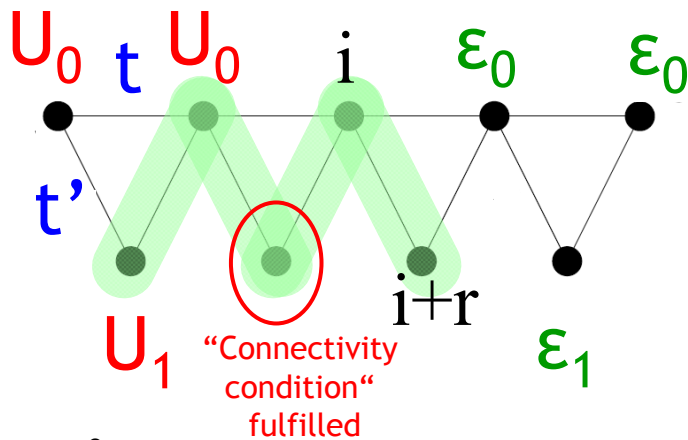
Müller-Hartmann (1995)

Penc, Shiba, Mila, Tsukagoshi (1996)

Fazekas (1997)

Derzho, Honecker, Richter (2007)

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



2 sites per cell \rightarrow 2 bands

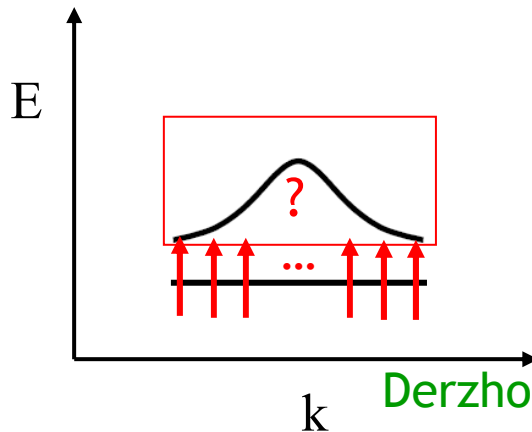
$$N_c = \# \text{ cells}$$

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

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

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

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



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

Solution I:

$$U_0, U_1 > 0$$

$n < 1/2$: ferromagnetic clusters

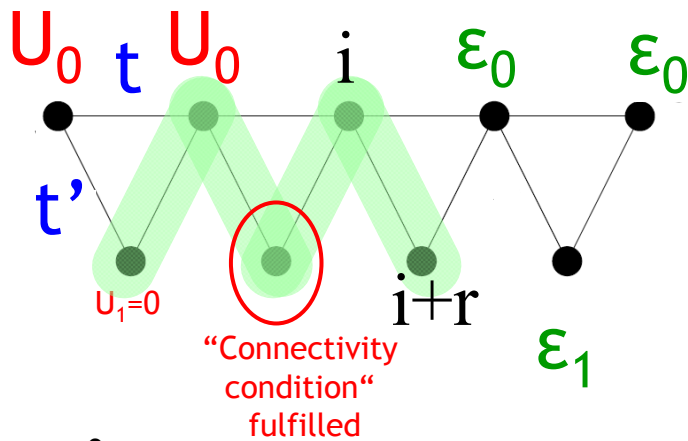
$n = 1/2$: fully saturated ferromagnet

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

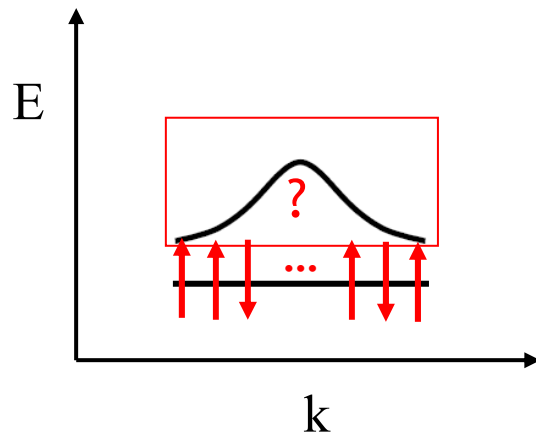
$$N_c = \# \text{ cells}$$

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

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

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

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

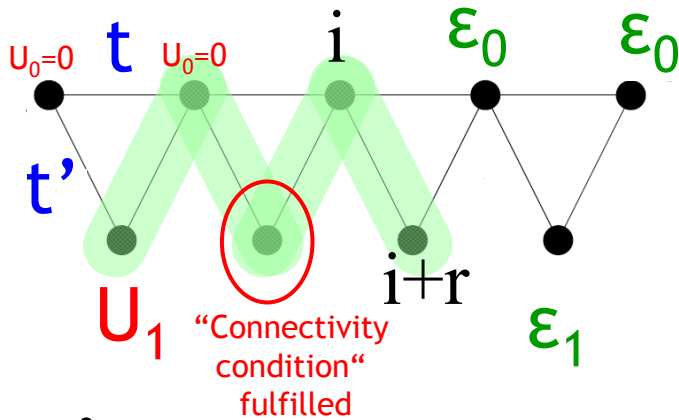


Solution II:

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

$n=1/2$: non-magnetic

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



2 sites per cell \rightarrow 2 bands

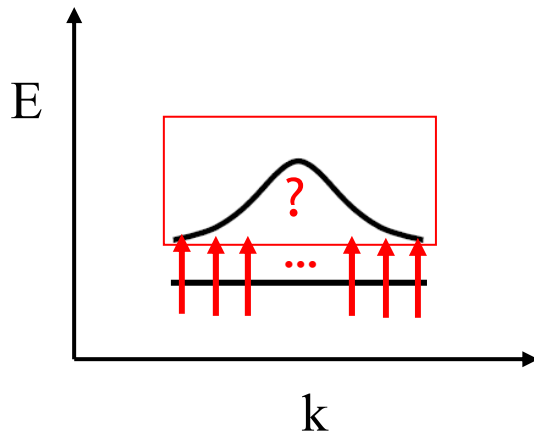
$N_c = \#$ cells

$N = \#$ electrons

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

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

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



Solution III:

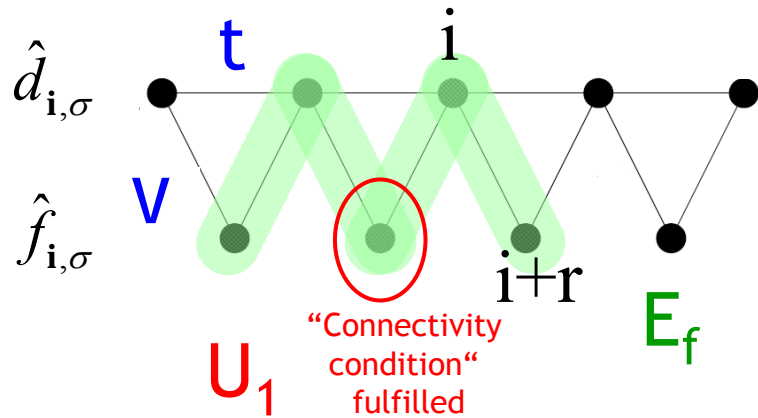
$$U_0 = 0, \quad U_1 > 0$$

$n=1/2$: fully saturated ferromagnet

Change of notation:

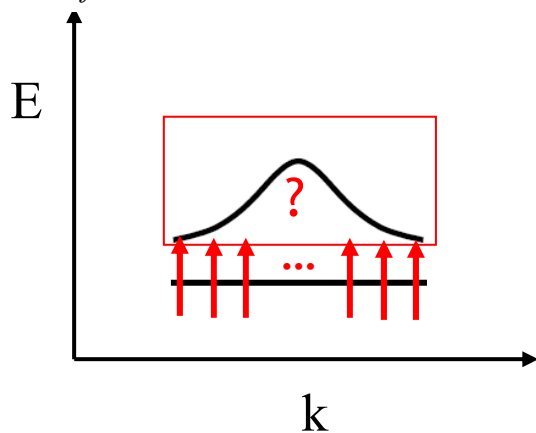
$$\hat{d}_{i,\sigma} \equiv \hat{c}_{i,\sigma},$$

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



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

$$E_f > -2t$$



2 sites per cell \rightarrow 2 bands

$N_c = \#$ cells

$N = \#$ electrons

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

Solution III:

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

$n=1/2$: fully saturated ferromagnet

Change of notation:

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

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

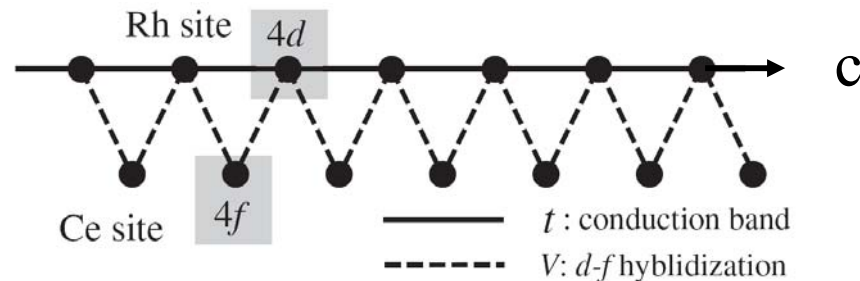
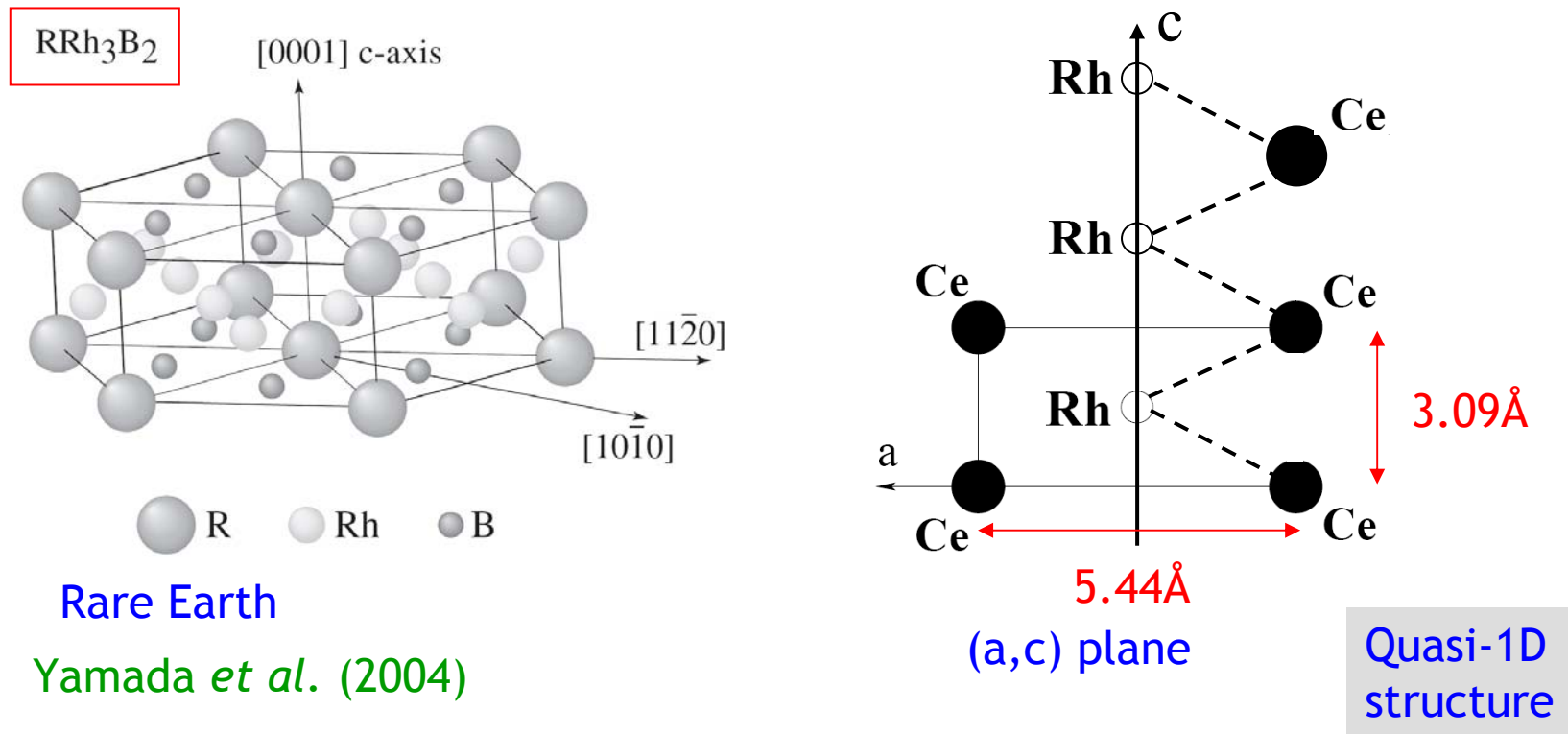
1D periodic Anderson model

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

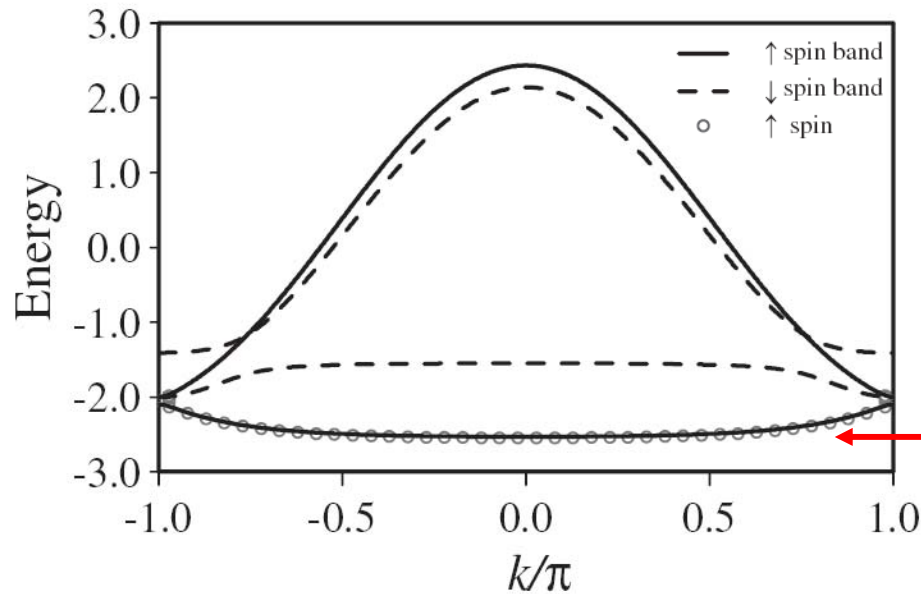
$$|\Psi\rangle = P|\Phi\rangle$$

Evaluations by variational Monte Carlo (VMC)

Kono, Kuramoto (2006)

f-electron ferromagnetism in CeRh₃B₂

VMC

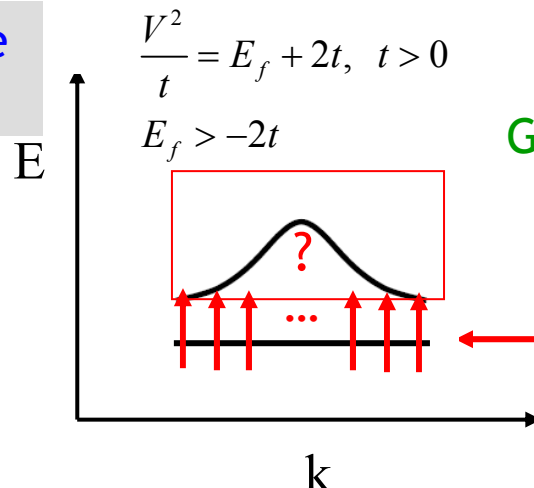


Kono, Kuramoto (2006)

almost flat band

LDA: $t = 0.34$ eV, $V = 0.24$ eV, $E_f = -0.714$ eV, $U = 7$ 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., $t = 0.34$ eV, $V = 0.23$ eV, $E_f = -0.52$ 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

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

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

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

$$m_f = 0.68 \mu_B$$

Gulacsi, Kampf, DV (2008)

Pentagon Hubbard chains:
Ferromagnetism in polymers

Exact dispersive band structure can be tuned to become flat

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

Conducting polymers: wide range of applications in

- Nanoelectronics
- Nanooptics
- Medicine

Heeger, Kivelson, Schrieffer, Su (1988)

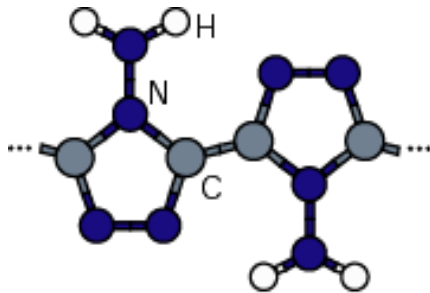
Search for **plastic** ferromagnets and ferromagnetism in systems with **non-magnetic** elements

Candidate: Flat-band ferromagnetism in organic polymers

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

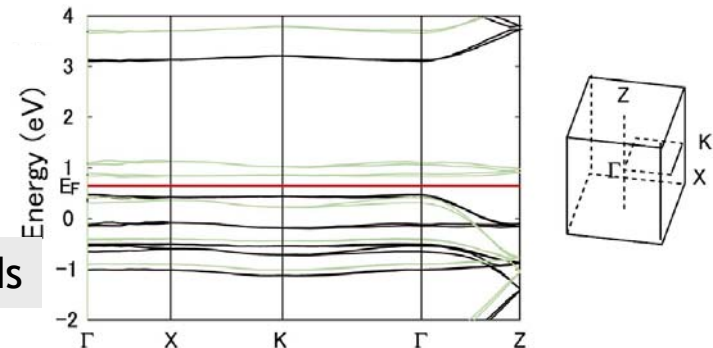
Arita, Suwa, Kuroki, Aoki (2002, 2003)

Polyaminotriazole



Spin-DFT

Single-particle bands

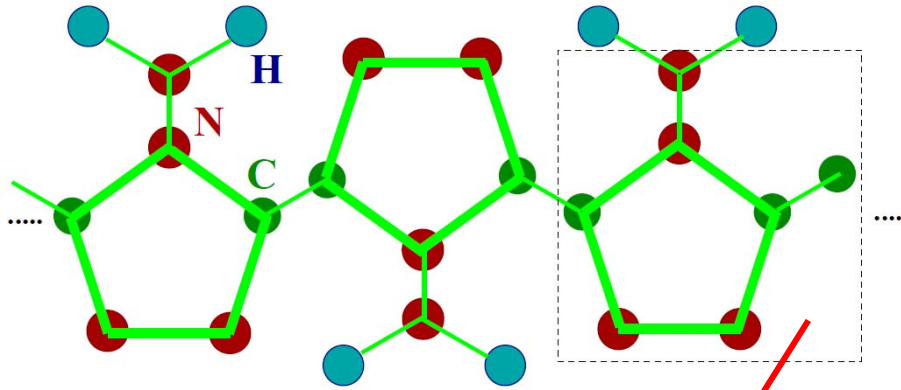


- Strong correlations in acene and thiophene organic molecular crystals
- stabilization of magnetic phases at high electron densities

Brocks, van den Brink, Morpurgo (2004)

Polyaminotriazole

Gulacsi, Kampf, DV (2010)

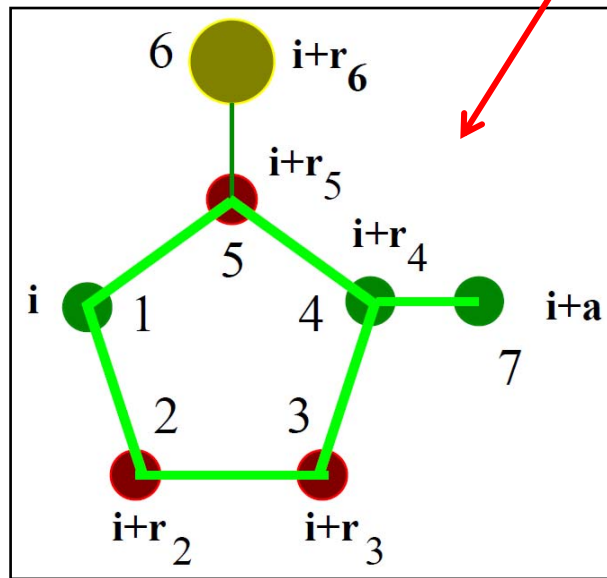


6 sites per cell \rightarrow 6 bands

$N_c = \# \text{ cells}$

$N = \# \text{ electrons}$

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



Arbitrary

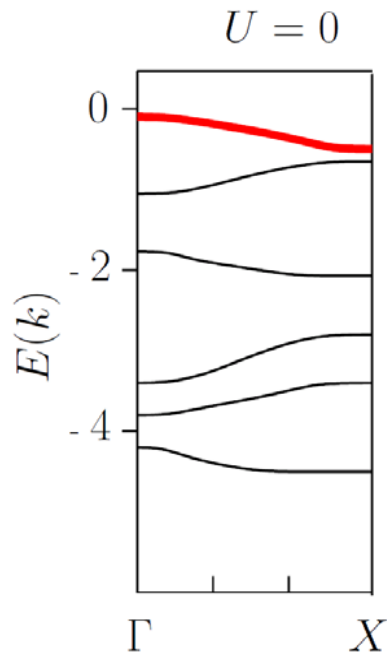
- local interactions $U_n > 0$
- on-site potentials ε_n
- hopping amplitudes $t_{n,n'}$

Single-particle bands

Gulacsi, Kampf, DV (2010)

Band dispersion

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



$$t_c \equiv t_{4,7} = 0.5, \quad t_h \equiv t_{3,2} = -1.1, \quad t_f \equiv t_{5,6} = 1.2$$
$$\epsilon_1 = \epsilon_4 = -2.5, \quad \epsilon_2 = \epsilon_3 = -2.0, \quad \epsilon_5 = -2.1, \quad \epsilon_6 = -2.1$$

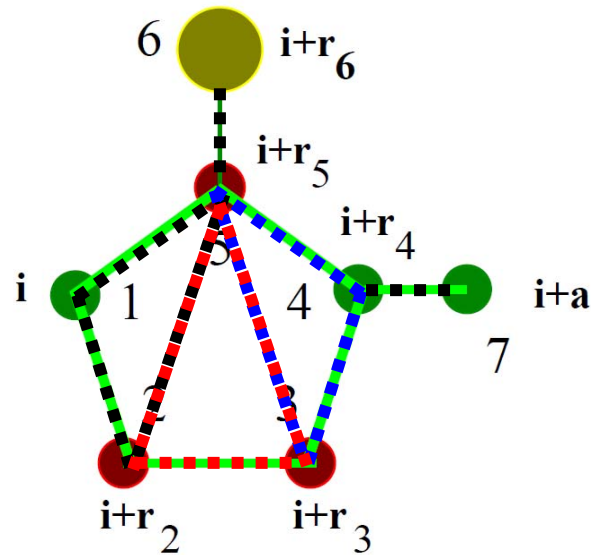
Transform Hamiltonian in positive semidefinite form

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

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

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

→ Matching conditions

No strong restrictions
on microscopic parameters

free parameters in block operators < # matching conditions

Effective band structure

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

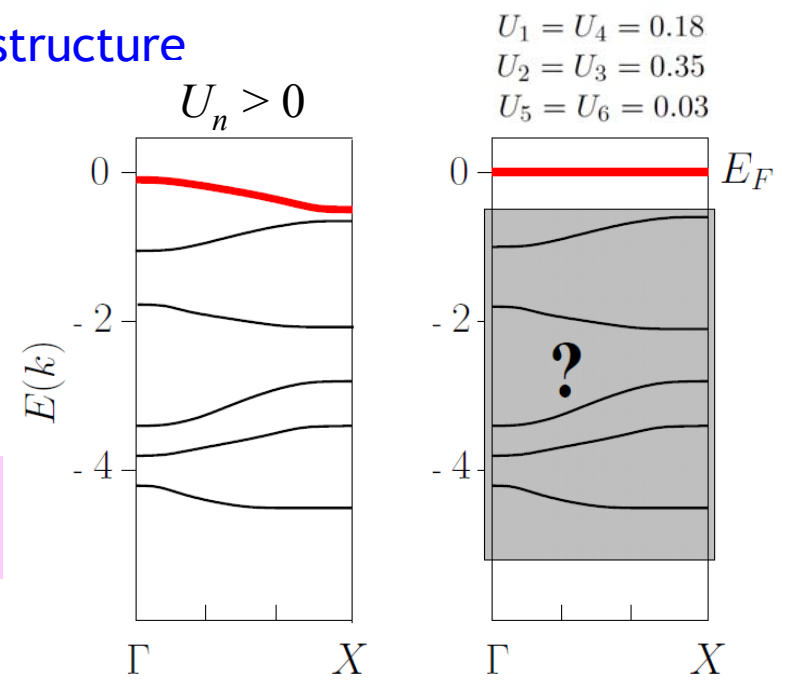
↑
quadratic in the original c-operators

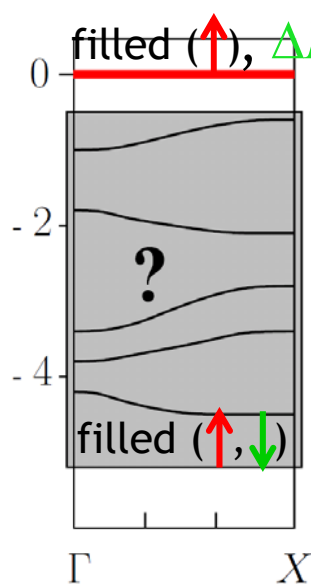
→ Effective, interaction dependent band structure
same as for H_0 but with renormalization
of local potentials

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

→ 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 $N=11N_c \rightarrow$ density $n=11/6$

Ground state for $n=11/6$:

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

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

\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 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**

