Center for
Electronic Correlations and Magnetism
University of Augsburg

Exact many-electron ground states on triangle, diamond, and pentagon Hubbard chains

Dieter Vollhardt

Theoretical Physics III, Group Seminar; January 23, 2008

Supported by Deutsche Forschungsgemeinschaft through SFB 484

Outline:

- Construction of exact many-electron ground states

- Exact many-electron ground states on
  diamond Hubbard chains
  triangle Hubbard chains
  → application to $CeRh_3B_2$
  pentagon Hubbard chains

In collaboration with
Zsolt Gulacsi and Arno Kampf

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
- gigantic non-linear optical effects

with

Technological applications:

- sensors, switches
- magnets/magnetic storage
- spintronics, e.g., spin valves

Exact solutions of correlation models particularly important (and difficult)

Construction of exact many-electron ground states

Strategy

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

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

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

Simplified by flat bands

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

Step 2: Construct many-electron 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

Step 3: Prove uniqueness of many-electron ground state: $\left| \Psi_g \right\rangle$ spans $\ker(\hat{H}')$

$$:= \left\{ |\phi\rangle \;\middle|\; \hat{H}' |\phi\rangle = 0 \right\}$$

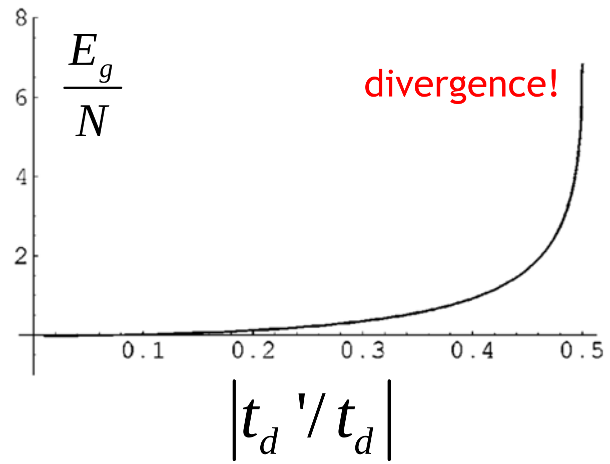
- Works in any dimension
- No "integrability" required
- Applicable to any Hamiltonian with sufficiently many microscopic parameters

Application to Hubbard and Periodic Anderson model

Brandt, Giesekus (1992)
Strack (1993)
Strack, Vollhardt (1993, 1994)
Orlik, Gulacsi (1998, 2001)
Gurin, Gulacsi (2001, 2002)
Gulacsi (2002)
Sarasua, Continentino (2002, 2004)

Periodic Anderson model in d=3

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



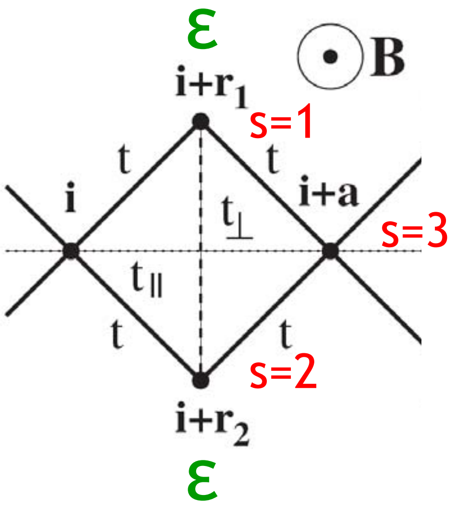
Gulacsi, Vollhardt (2003, 2005)

High sensitivity to small changes of microscopic parameters found

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

Z. Gulacsi, A. Kampf, DV

Phys. Rev. Lett. **99**, 026404 (2007)



3 sites per cell → 3 bands

s=1,2,3 sublattice index

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

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

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

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

Peierls phase factor

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

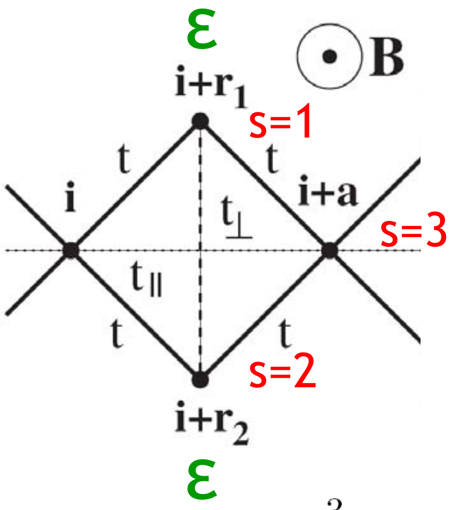
$t_{\mathbf{j},\mathbf{j}'}(\mathbf{B}) = t_{\mathbf{j},\mathbf{j}'}(0)\exp[(i2\pi/\Phi_0)\int_{\mathbf{j}}^{\mathbf{j}'}\mathbf{A}\cdot d\mathbf{l}]$

One flux quantum per unit cell (triangle): $\delta = \pi$

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

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

No Zeeman Term



3 sites per cell → 3 bands

s=1,2,3 sublattice index

N_c = # cells

N = # electrons

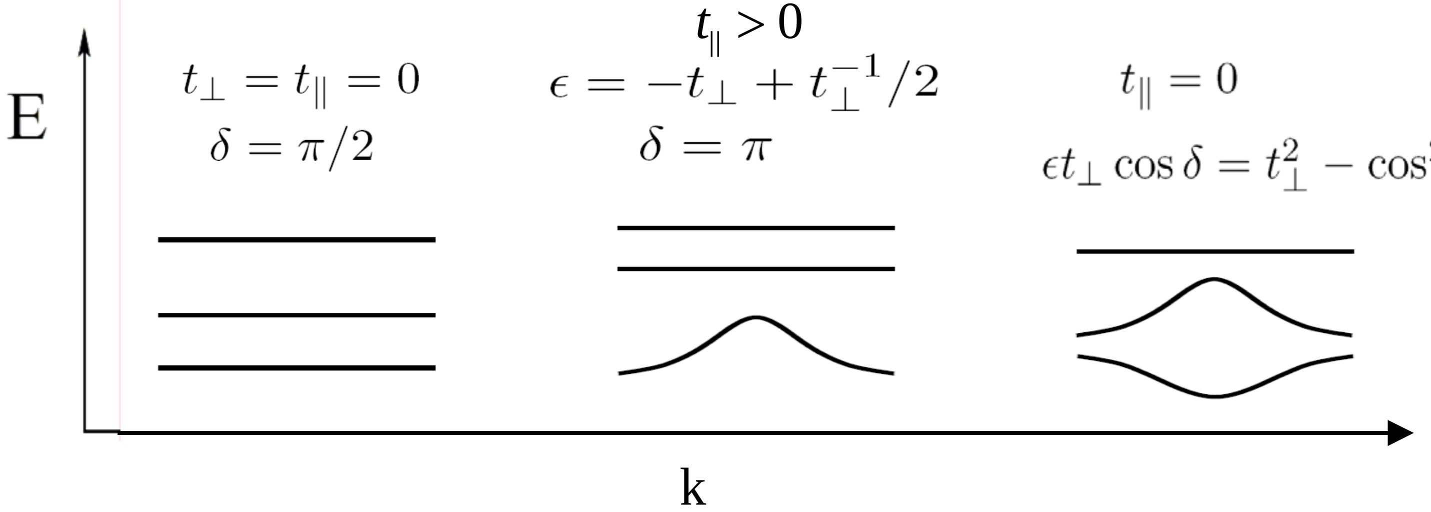
$n = \dfrac{N}{3N_c}$ electron density

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:

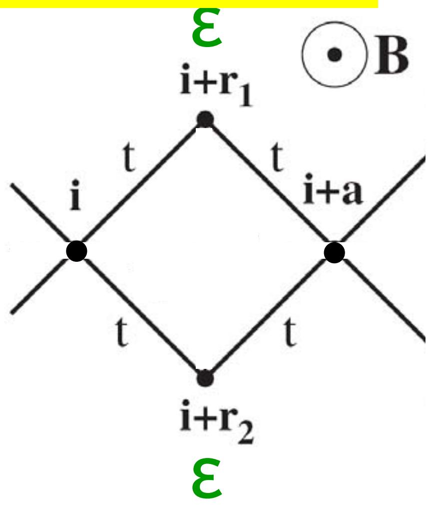
Energy unit: $2t$



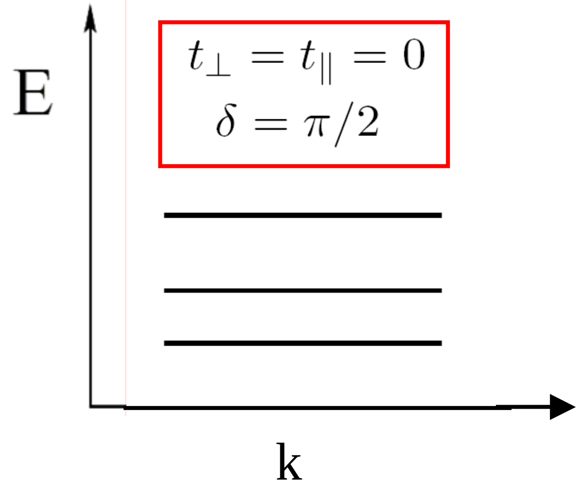
Single-electron bands

Solution I: Flat-band ferromagnetism

Solution I: Flat-band ferromagnetism



Single-electron bands



"Aharonov-Bohm cage"

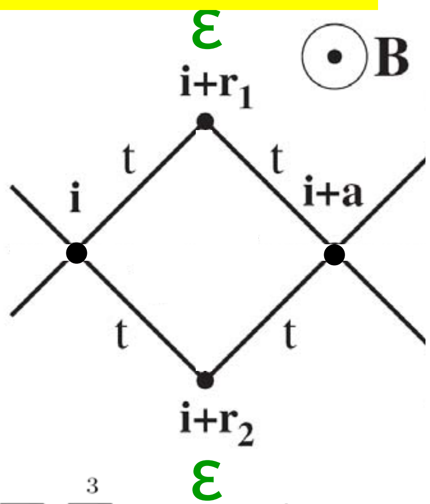
Vidal, Doucot, Mosseri, Butaud (2000)

ε=0, 2 electrons: excited singlet eigenstates

- localized if U=0
- delocalized if U>0

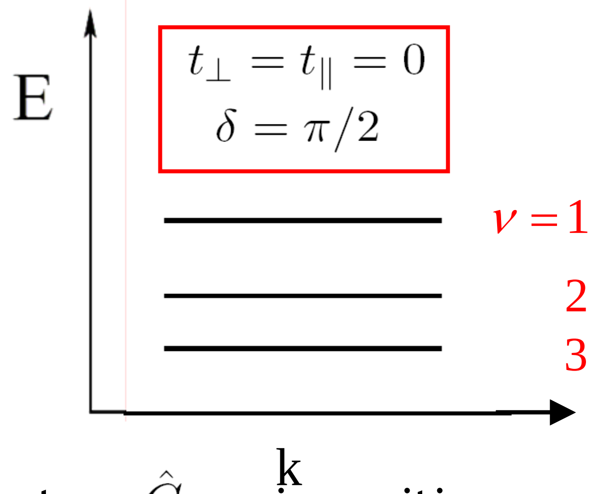
Delocalization also for finite densities ?

Solution I: Flat-band ferromagnetism



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

Single-electron bands

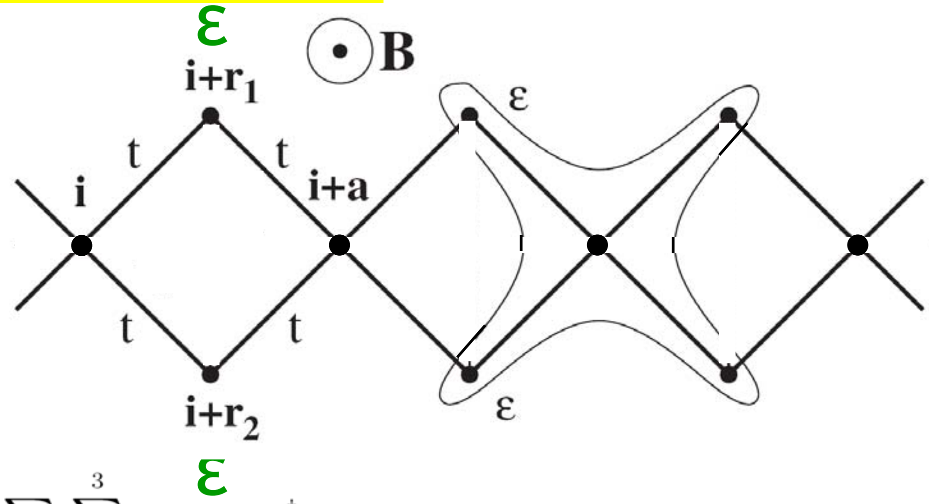


Diagonalization: → New canonical fermionic operators $\hat{C}_{\nu,\mathbf{i},\sigma}$ in position space

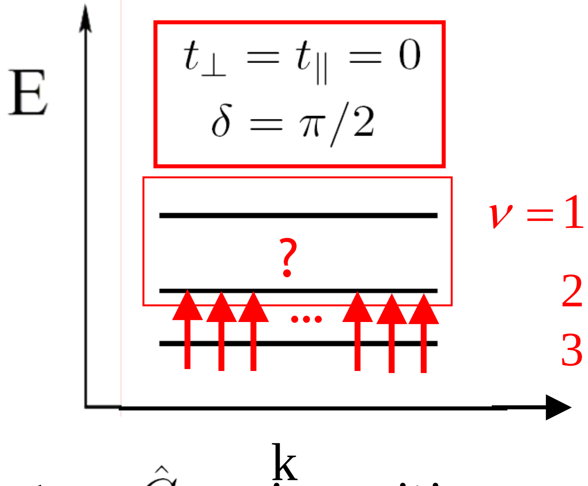
$$\hat{H}_0 = \sum_{\mathbf{i},\sigma} \sum_{\nu=1}^{3} E_\nu \underbrace{\hat{C}^\dagger_{\nu,\mathbf{i},\sigma} \hat{C}_{\nu,\mathbf{i},\sigma}}_{\hat{n}_{\nu,\mathbf{i},\sigma}} \qquad E_2 = \epsilon,\ E_{2\pm1} = (\epsilon \mp \sqrt{\epsilon^2 + 4})/2$$

$\hat{n}_{\nu,\mathbf{i},\sigma}$ and $\hat{H}_U$ positive semidefinite operators

Solution I: Flat-band ferromagnetism



Example 1:



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

Diagonalization: → New canonical fermionic operators $\hat{C}_{\nu,\mathbf{i},\sigma}$ in position space (localized Wannier eigenstate)

$$\hat{H}_0 = \sum_{\mathbf{i},\sigma} \sum_{\nu=1}^{3} E_\nu \hat{C}^\dagger_{\nu,\mathbf{i},\sigma} \hat{C}_{\nu,\mathbf{i},\sigma} \qquad E_2 = \epsilon,\ E_{2\pm1} = (\epsilon \mp \sqrt{\epsilon^2 + 4})/2$$

Ground state of $\hat{H}$

$N \le N_c\,,\ U > 0$

$$|\Psi^I_g(N)\rangle = \prod_{\mathbf{i}=1}^{N} \hat{C}^\dagger_{3,\mathbf{i},\sigma_\mathbf{i}} |0\rangle$$

$$E^I_g = E_3 N$$

n<1/3 : ferromagnetic clusters

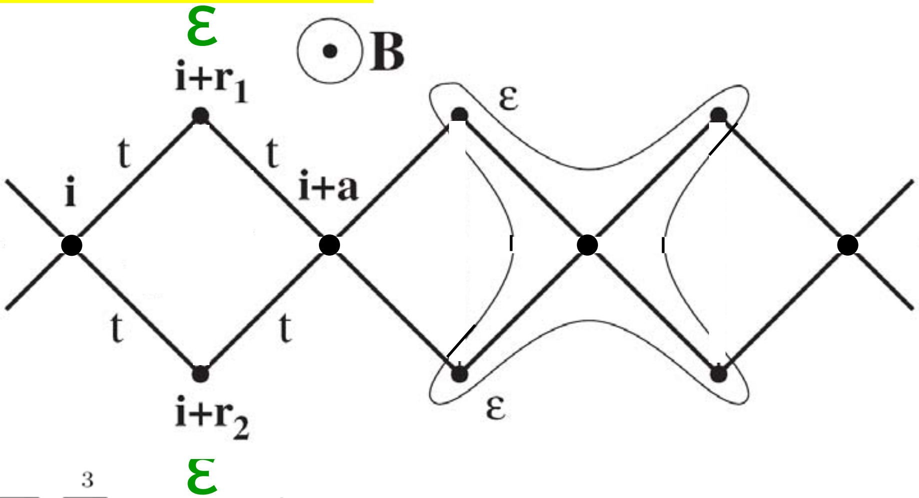
n=1/3 : fully saturated ferromagnet

- Prove uniqueness of $|\Psi^I_g(N)\rangle$

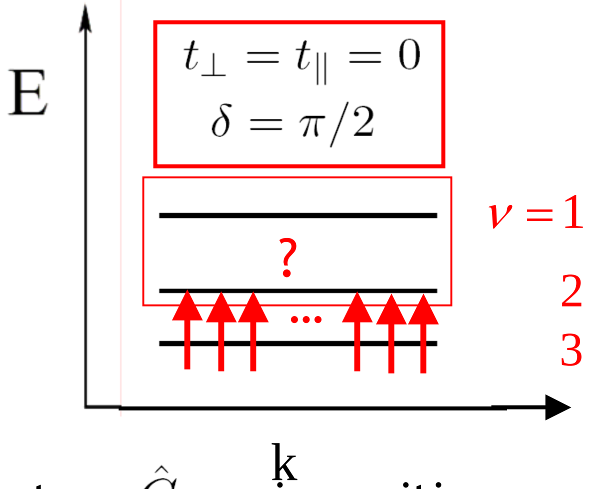
Mielke, Tasaki (1993)

→ **Flat-band ferromagnetism:** Realizes ideas of Gutzwiller and Kanamori from 1963 about the origin of itinerant ferromagnetism

Solution I: Flat-band ferromagnetism



Example 1:



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

Diagonalization: → New canonical fermionic operators $\hat{C}_{\nu,\mathbf{i},\sigma}$ in position space (localized Wannier eigenstate)

$$\hat{H}_0 = \sum_{\mathbf{i},\sigma} \sum_{\nu=1}^{3} E_\nu \hat{C}^\dagger_{\nu,\mathbf{i},\sigma} \hat{C}_{\nu,\mathbf{i},\sigma} \qquad E_2 = \epsilon,\ E_{2\pm1} = (\epsilon \mp \sqrt{\epsilon^2 + 4})/2$$

Ground state of $\hat{H}$

$$|\Psi_g^I(N)\rangle = \prod_{\mathbf{i}=1}^{N} \hat{C}^\dagger_{3,\mathbf{i},\sigma_\mathbf{i}} |0\rangle$$

$N \le N_c$, $U > 0$

$$E_g^I = E_3 N$$

n<1/3 : ferromagnetic clusters

n=1/3 : fully saturated ferromagnet

- Prove uniqueness of $|\Psi_g^I(N)\rangle$

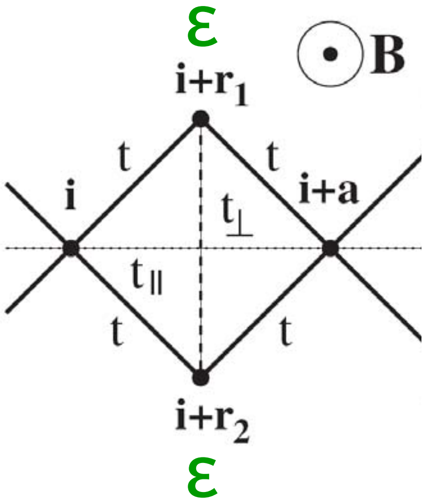
Mielke, Tasaki (1993)

U>0: lowest band flat only for $\delta = \pi/2$ (localized)
dispersive for $\delta = 0$ (conducting)

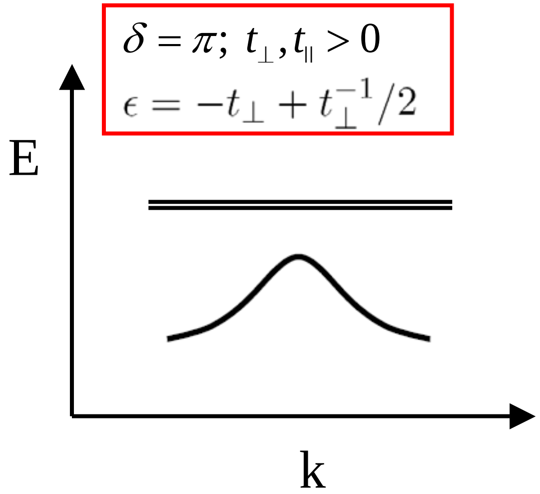
→ magnetic field induced metal-insulator transition

Solution II: Correlated half-metal

Itinerant states easier to realize at $\delta \neq \pi/2$?

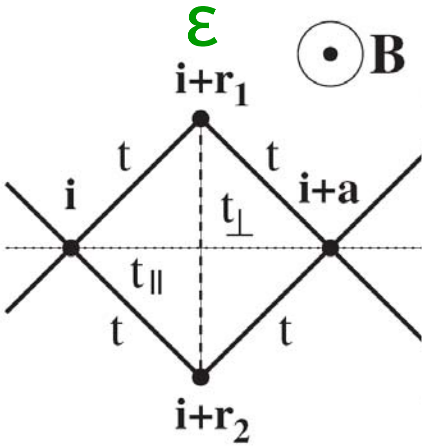


→ Investigate



Single-electron bands

Transformation of the Hamiltonian into positive semi-definite form



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

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

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

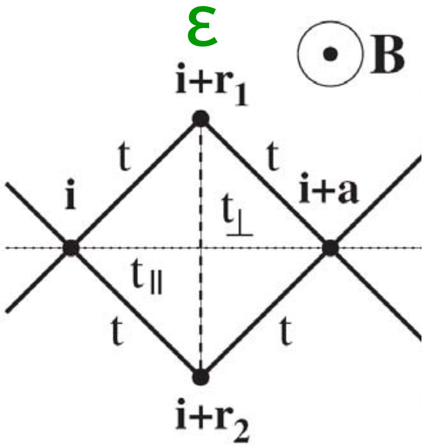
$$\{\hat{A}_{\mathbf{i},\sigma}, \hat{A}^\dagger_{\mathbf{j},\sigma}\} \neq \delta_{\mathbf{i},\mathbf{j}}$$

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

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

Solution II: Correlated half-metal

Transformation of the Hamiltonian into positive semi-definite form



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

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

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

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

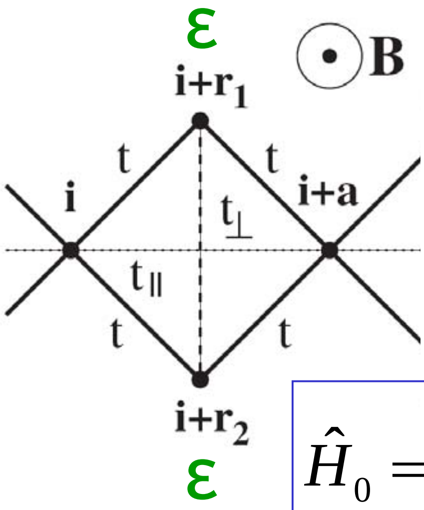
$$\Rightarrow \hat{A}^{\dagger}_{i\sigma}\hat{A}_{i\sigma} = (a_2^* a_1 \hat{c}^{\dagger}_{i+\mathbf{r}_2\sigma}\hat{c}_{i\sigma} + a_3^* a_2 \hat{c}^{\dagger}_{i+\mathbf{a}\sigma}\hat{c}_{i+\mathbf{r}_2\sigma} + a_4^* a_3 \hat{c}^{\dagger}_{i+\mathbf{r}_1\sigma}\hat{c}_{i+\mathbf{a}\sigma} + a_1^* a_4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

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

$$a_2^* a_1 = a_3^* a_2 = a_4^* a_3 = a_1^* a_4 = -t e^{i\delta/2}$$
$$a_2^* a_4 = -t_{\perp}$$
$$a_3^* a_1 = -t_{\parallel}$$
$$|a_1|^2 + |a_3|^2 = \varepsilon + |a_2|^2 = \varepsilon + |a_4|^2$$

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

Solution II: Correlated half-metal



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

$\hat{H}_U$

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

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

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

positive semi-definite

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

Solution II: Correlated half-metal

Construction of the ground state

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

positive semi-definite

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

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

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

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

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

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

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

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

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

- Prove uniqueness of $|\Psi_g^{II}(4N_c)\rangle$

Proof of the uniqueness of the ground state $|\Psi_g^{II}(4N_c)\rangle$

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

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

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

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

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

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

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

Proof of the uniqueness of the ground state

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

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., $\hat{A}_{i\sigma}\hat{A}^{\dagger}_{i\sigma}\hat{Y}|0\rangle=0$.

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

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.

Proof of the uniqueness of the ground state

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

Spanned by states which have at least one electron per site

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

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

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

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.

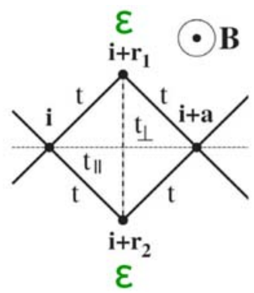
For $\delta = \pi;\ t_{\perp}, t_{\parallel} > 0$

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

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

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

is the unique ground state



Solution II: Correlated half-metal

Ground state

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

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

One σ electron on every lattice site → localized

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

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

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

Solution II: Correlated half-metal

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

ΔN -σ electrons added: $n_\sigma = 1,\ n_{-\sigma} = 1/3 + \Delta N / N_c$

Ground state

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

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

plane wave-type states due to -σ electrons

→ ΔN -σ electrons itinerant

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

- $3N_c$ immobile σ electrons
- N_c -σ electrons confined to localized Wannier function + ΔN conducting -σ electrons
- Magnetization $M \propto (1 - \Delta N/N_c) \xrightarrow{\Delta N \to N_c} 0$

→ Low carrier-density metallic behavior

Solution II: Correlated half-metal

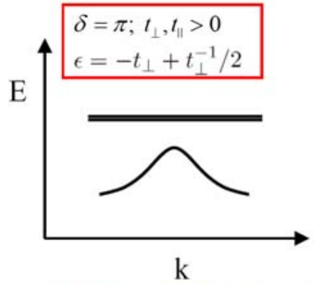
$N > 4N_c \Leftrightarrow n > 4/3$

ΔN -σ electrons added: $n_\sigma = 1,\ n_{-\sigma} = 1/3 + \Delta N / N_c$

Ground state

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

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



Single-electron bands

plane wave-type states due to -σ electrons

→ ΔN -σ electrons itinerant

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

U=0: dispersionless, localized electrons

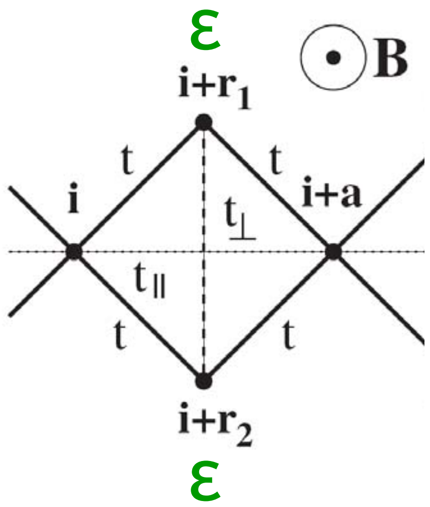
U>0: correlation-induced half-metal

→ Correlation-induced localization-delocalization transition to a half-metal

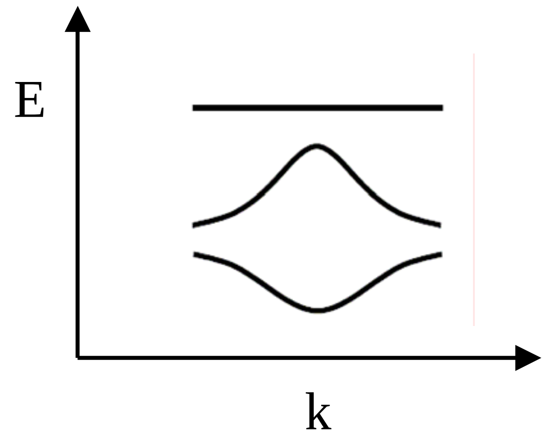
B=const: Trigger transition by tuning local potential ε

Solution III:
Exact ground states for general magnetic flux

Solution III: Exact ground states for general magnetic flux



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



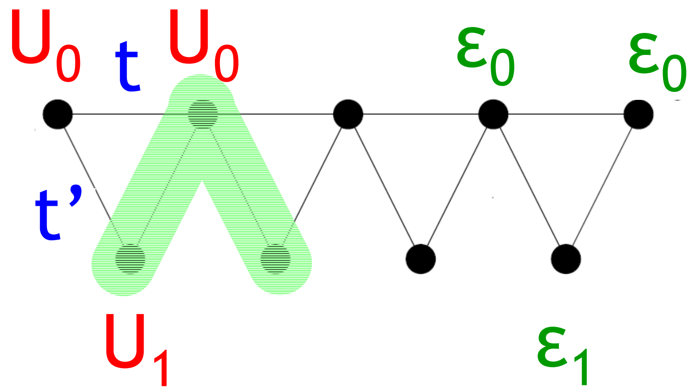
Single-electron bands

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

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

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



2 sites per cell → 2 bands

N_c = # cells

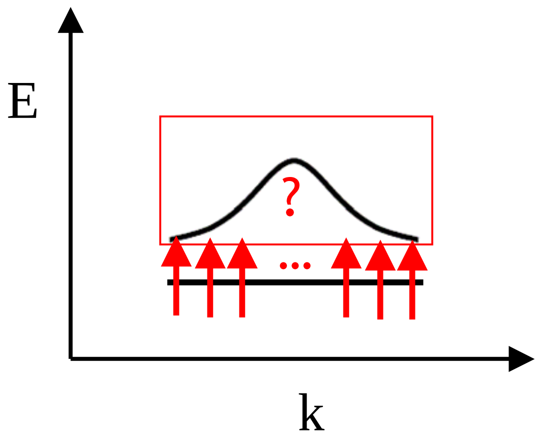
N = # electrons

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

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

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

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



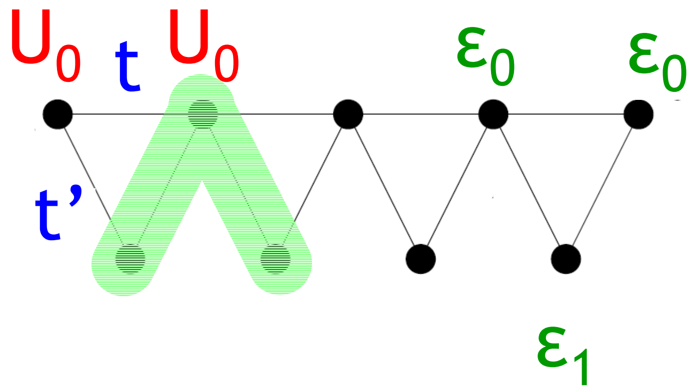
Solution I: $U_0, U_1 > 0$

n<1/2 : ferromagnetic clusters

n=1/2 : fully saturated ferromagnet

Mielke, Tasaki (1993)

Derzho, Honecker, Richter (2007)

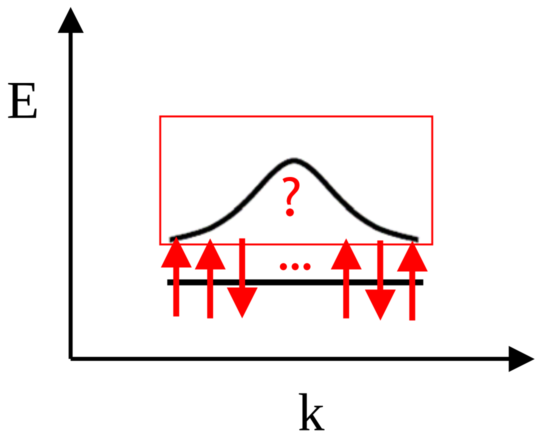


2 sites per cell → 2 bands

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

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

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

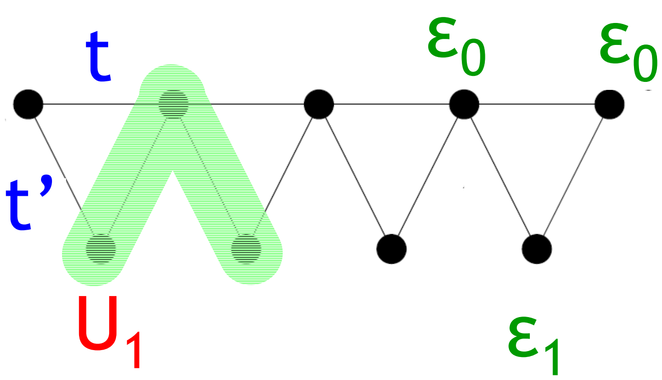


$$\hat{H} = \hat{H}_0 + \hat{H}_U$$

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

n=1/2 : non-magnetic

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



2 sites per cell → 2 bands

N_c = # cells

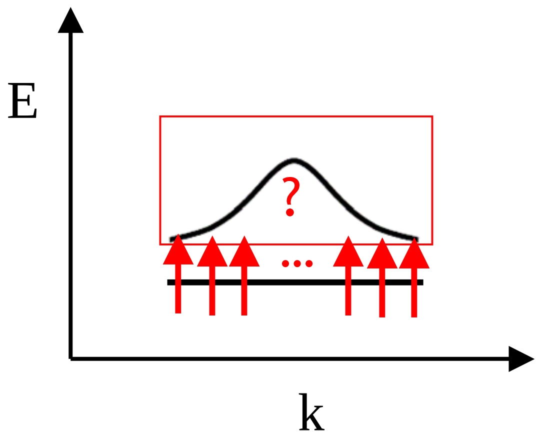
N = # electrons

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

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

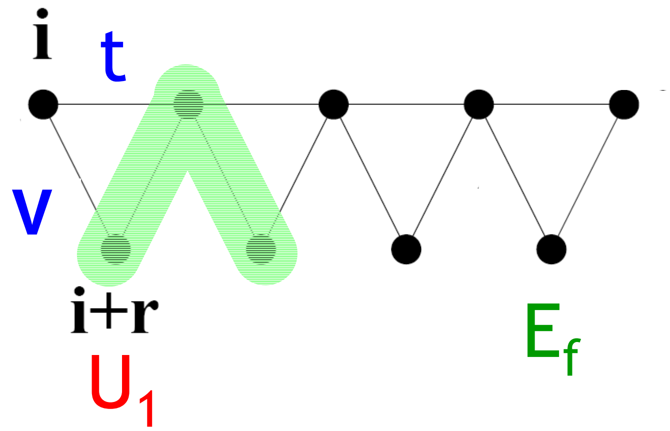
$$\epsilon_1 - \epsilon_0 > -2t$$

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



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

n=1/2 : fully saturated ferromagnet



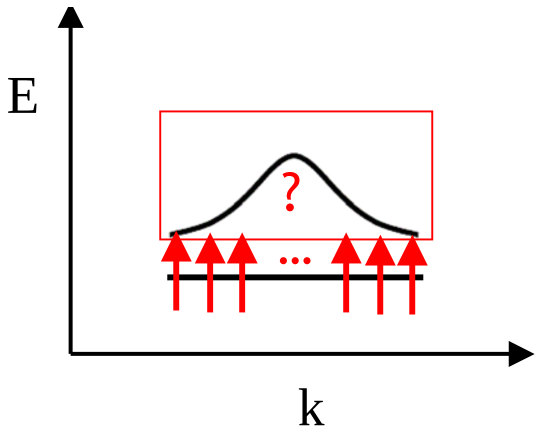
2 sites per cell → 2 bands

N_c = # cells
N = # electrons

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

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

$$E_f > -2t$$



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

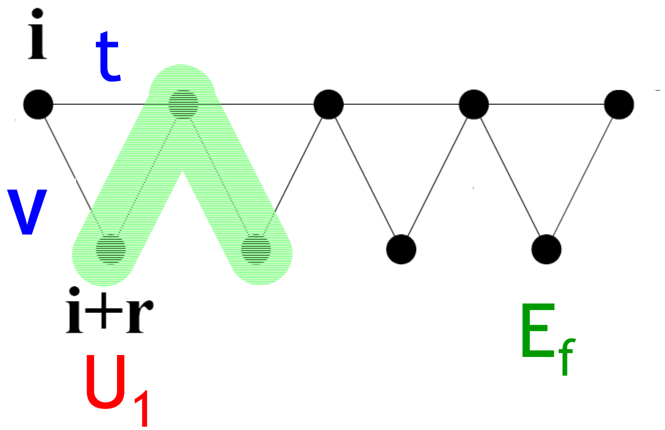
Solution III: $U_0 = 0, \; U_1 > 0$

n=1/2 : fully saturated ferromagnet

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

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

1D periodic Anderson model



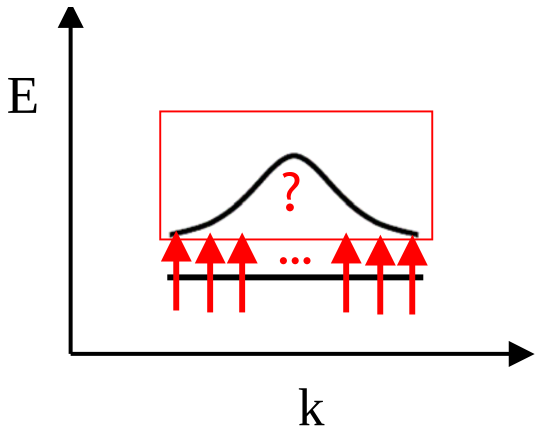
2 sites per cell → 2 bands

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

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

$$E_f > -2t$$

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



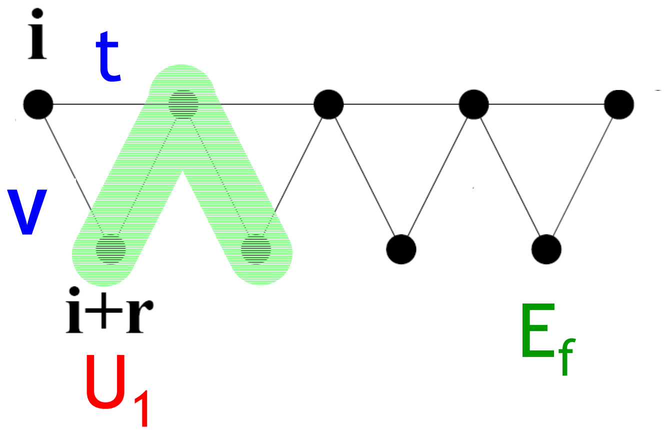
Solution III: $U_0 = 0,\ U_1 > 0$

n=1/2 : fully saturated ferromagnet

$$|\Psi_g(N = N_c)\rangle = \prod_{\mathbf{i}=1}^{N_c} [\, \hat{f}^\dagger_{\mathbf{i}-\mathbf{a}+\mathbf{r},\sigma} + \hat{f}^\dagger_{\mathbf{i}+\mathbf{r},\sigma} - \frac{V}{t}\hat{d}^\dagger_{\mathbf{i},\sigma}]|0\rangle$$

- Prove uniqueness of $|\Psi_g(N = N_c)\rangle$

1D periodic Anderson model



2 sites per cell → 2 bands

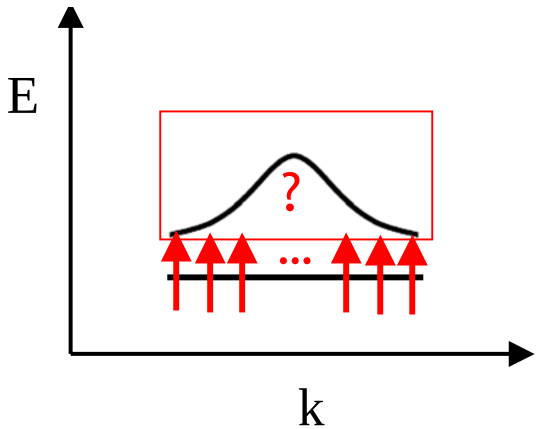
N_c = # cells

N = # electrons

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

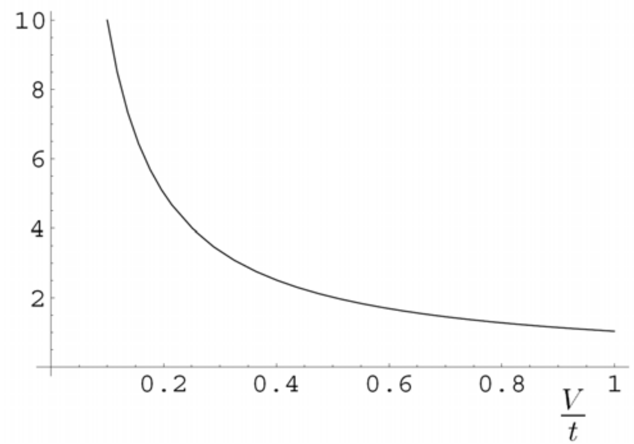
$$\frac{V^2}{t} = E_f + 2t, \quad t > 0$$

$$E_f > -2t$$



Localization length of d-electrons

$$\frac{\xi_d}{a} = \left\{ \ln\left[1 + \frac{1}{2}\bar{V}^2 \left(1 - \sqrt{1 + \frac{4}{\bar{V}^2}} \right) - \right] \right\}^{-1}, \quad \bar{V} = \frac{V}{t}$$

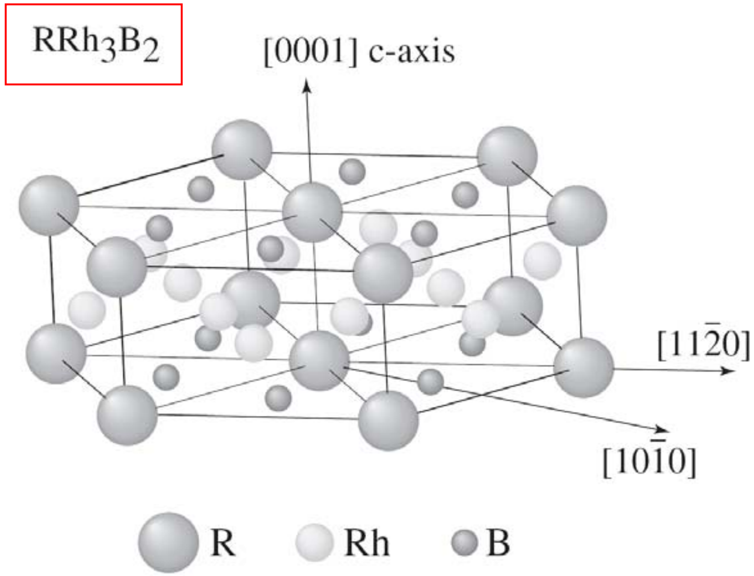


Application of the 1D periodic Anderson model to $CeRh_3B_2$

$CeRh_3B_2$ is interesting because:

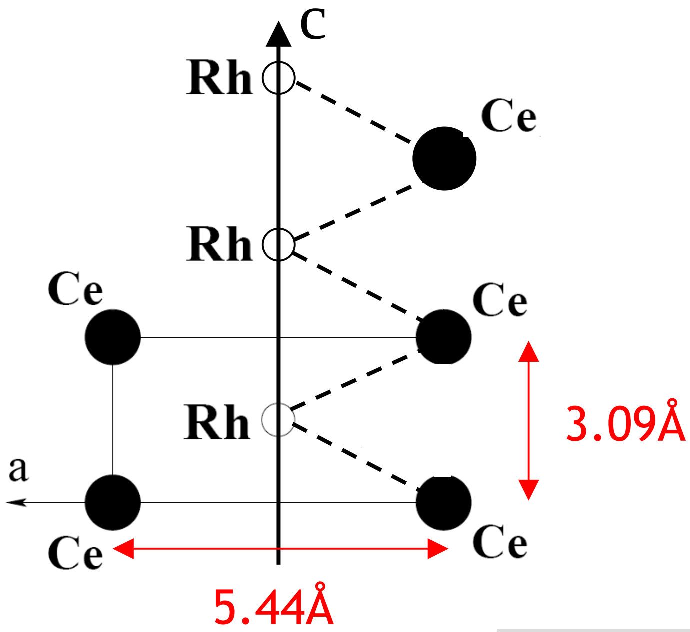
- RKKY interaction cannot explain ferromagnetism
- Small f- moment 0.45 μ_B (free Ce^{3+} ion: 2.14 μ_B)
- Highest T_c (=120 K) among known Ce compounds with non-magnetic elements

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



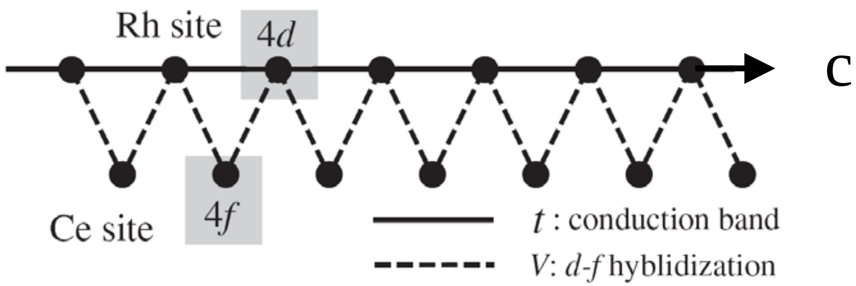
Rare Earth

Yamada *et al.* (JPSJ, 2004)



(a,c) plane

Quasi-1D
band structure



Kono, Kuramoto (JPSJ, 2006)

Mechanism for f-electron ferromagnetism in $CeRh_3B_2$?

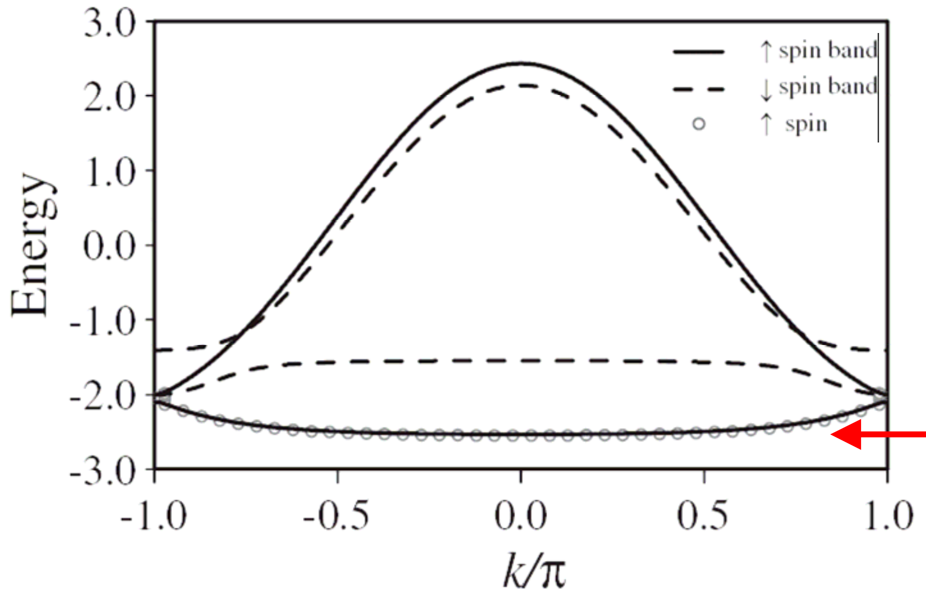
Non-interacting magnetic state $|\Phi\rangle = \prod_{\sigma} \prod_{k}^{N_\sigma - L} a^\dagger_{k\sigma} \prod_{k}^{L} b^\dagger_{k\sigma} |0\rangle$

Variational wave function $|\Psi\rangle = P|\Phi\rangle$

Gutzwiller projector $P = \prod_i (1 - \tilde{\eta} n^f_{i\uparrow} n^f_{i\downarrow})$

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

VMC



Kono, Kuramoto (JPSJ, 2006)

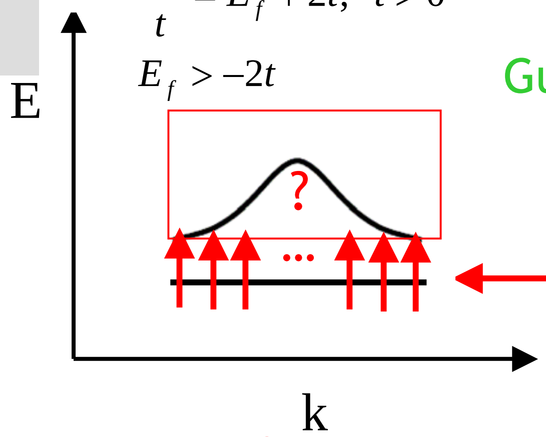
almost flat band created by U

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

Exact ground state (Solution III)

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

$$E_f > -2t$$



Gulacsi, Kampf, Vollhardt (unpublished)

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, $n = 0.5$

Both: Ferromagnetism related to a lowest flat-band

Magnetic moments

Experiment: $m_f = 0.45$ Galatanu *et al.* (2003)

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

$m_f = 0.94$ Kono, Kuramoto (JPSJ, 2006)

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

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

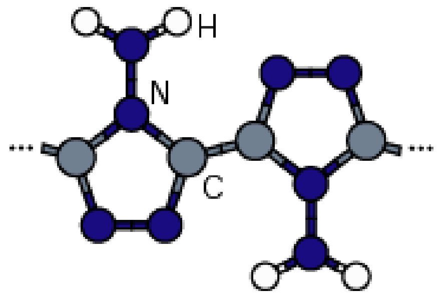
$m_f = 0.68$ Gulacsi, Kampf, Vollhardt (unpublished)

III. Exact many-electron ground states on pentagon Hubbard chains

Search for ferromagnetism in systems with non-magnetic elements

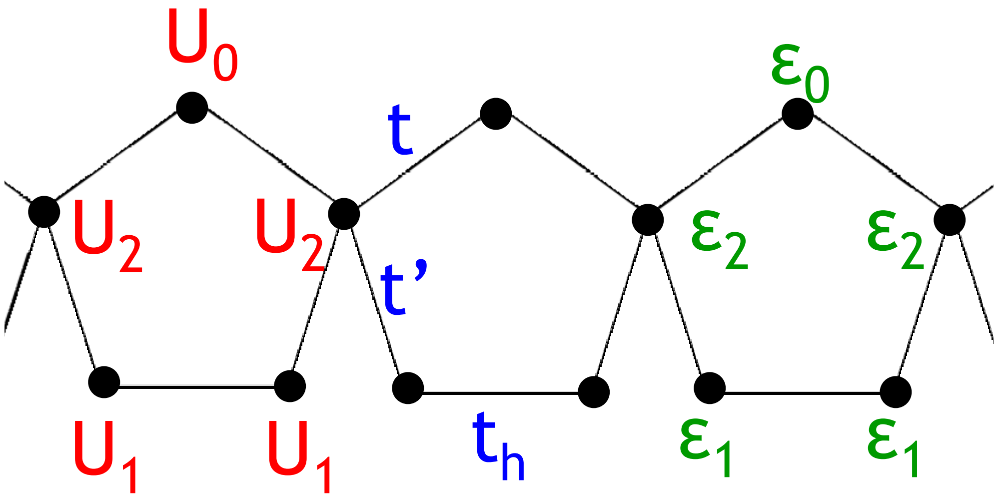
Candidate: Flat-band ferromagnetism in organic polymers

Polymethylaminotriazole



Suwa, Arita, Kuroki, Aoki (2003)

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



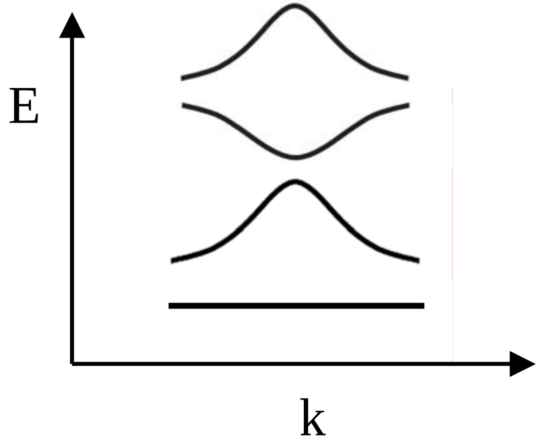
4 sites per cell → 4 bands

N_c = # cells
N = # electrons
$n = \frac{N}{4N_c}$ electron density

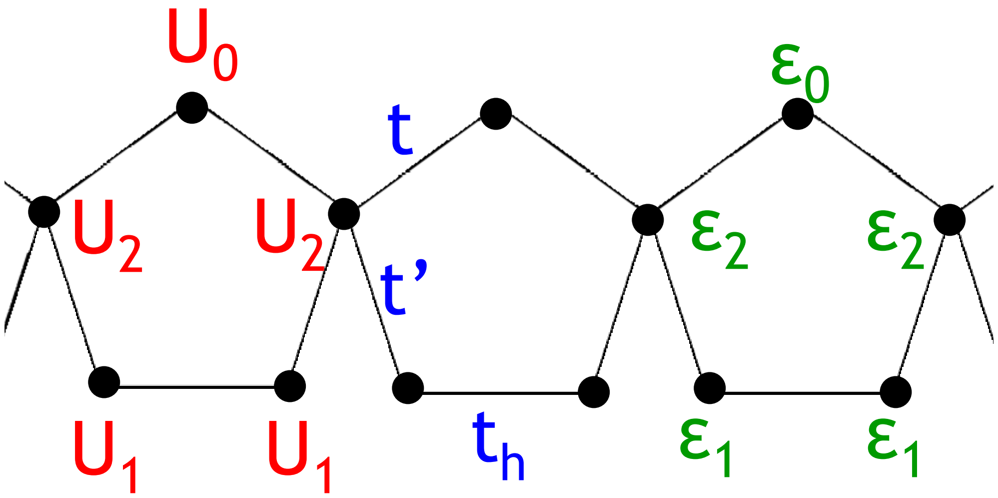
Gulacsi, Kampf, Vollhardt (unpublished)

$$\varepsilon_1 > t_h > 0, \ \varepsilon_0 = \left(\frac{t}{t'}\right)^2 \frac{\varepsilon_1^2 - t_h^2}{t_h}$$

$$\varepsilon_2 = 2\frac{t'^2}{\varepsilon_1 - t_h}$$



Single-electron bands



4 sites per cell → 4 bands

N_c = # cells

N = # electrons

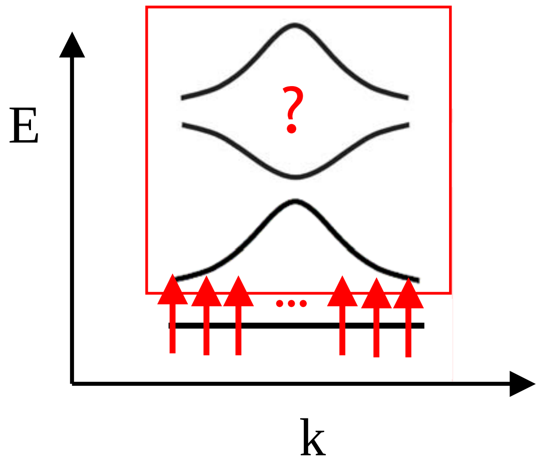
$n = \frac{N}{4N_c}$ electron density

$$\varepsilon_1 > t_h > 0,\ \varepsilon_0 = \left(\frac{t}{t'}\right)^2 \frac{\varepsilon_1^2 - t_h^2}{t_h}$$

$$\varepsilon_2 = 2\frac{t'^2}{\varepsilon_1 - t_h}$$

Gulacsi, Kampf, Vollhardt (unpublished)

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

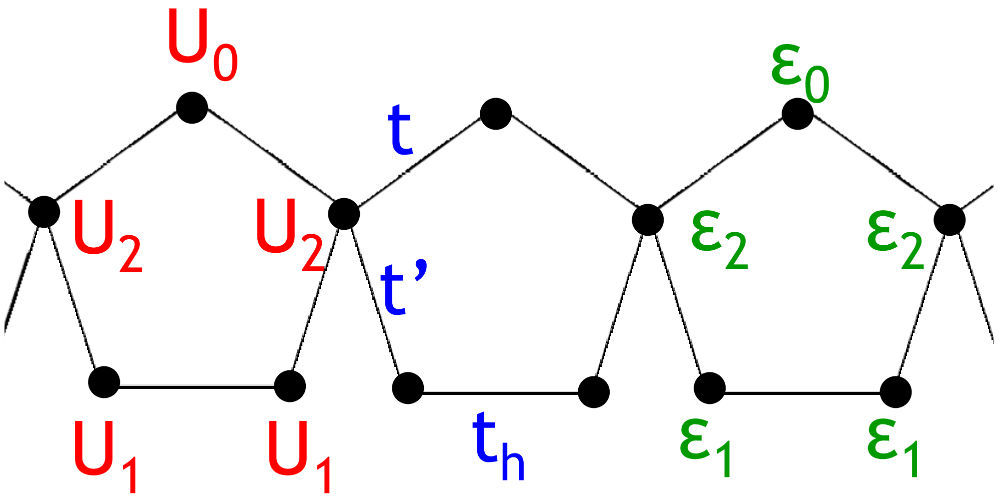


Ground state I: $U_0, U_1, U_2 > 0$

n<1/4 : ferromagnetic clusters

n=1/4 : saturated ferromagnet

Construction of lowest flat band by tuning of "gate potentials ε" only



4 sites per cell → 4 bands

N_c = # cells

N = # electrons

$n = \frac{N}{4N_c}$ electron density

Gulacsi, Kampf, Vollhardt (unpublished)

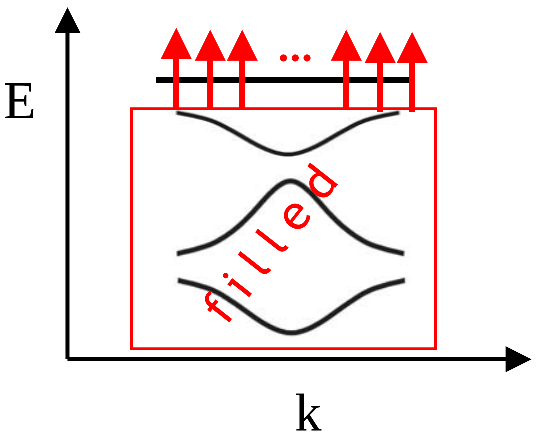
$t_h < 0$; arbitrary $t, t', \varepsilon_1, \varepsilon_2$

$U_1, U_2 > 0$

$U_0 = U_0(t, t', t_h, \varepsilon_0, \varepsilon_1, \varepsilon_2, U_1, U_2)$

$\rightarrow$ upper bound for ε_0

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



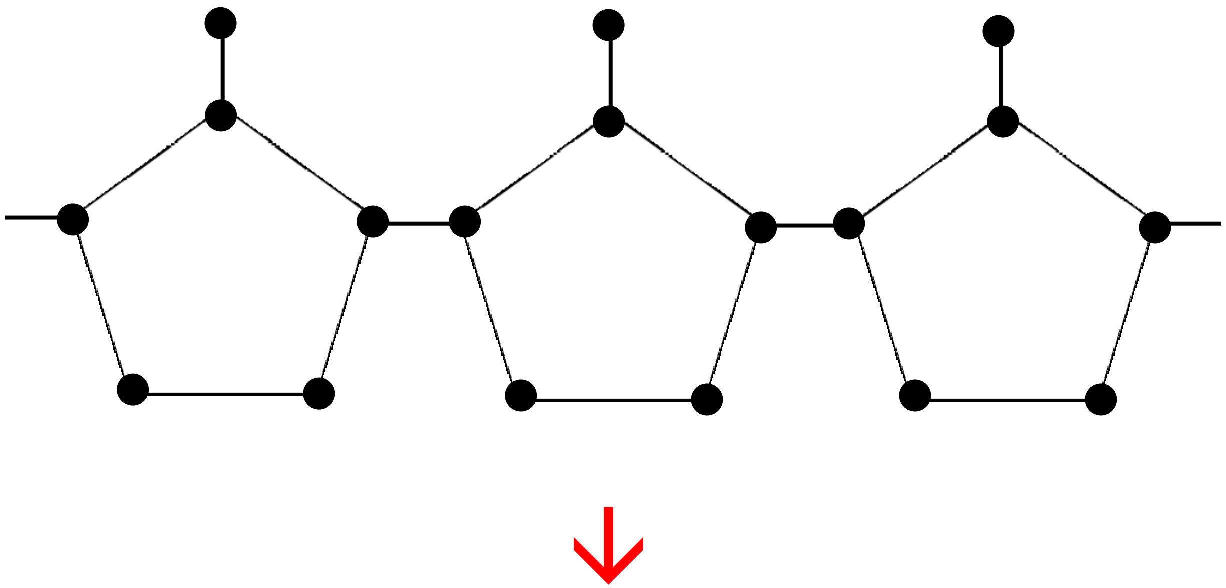
Ground state II:

n<7/4 : ferromagnetic clusters

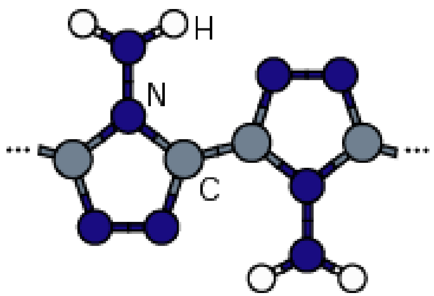
n=7/4 : non-saturated ferromagnet

Construction of a flat band by tuning the interaction U_0

Extension to more complicated structures possible



Polymethylaminotriazole



Conclusion 1:
Strategy for the construction of exact many-electron ground states

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

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

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

Simplified by flat bands

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

Step 2: Construct many-electron ground state

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

ground state | ground-state energy

Step 3: Prove uniqueness of many-electron ground state: $|\Psi_g\rangle$ spans $\ker(\hat{H}')$

$$:= \left\{ |\phi\rangle \;\middle|\; \hat{H}' |\phi\rangle = 0 \right\}$$

- 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

  → Design of new switches