



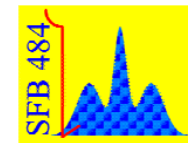
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Exact many-electron ground states on
triangle, diamond, and pentagon
Hubbard chains

Dieter Vollhardt

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"Interaction and Nanostructural Effects in Low-Dimensional Systems"
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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

"Complexity"

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

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

Simplified by flat bands

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

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

Step 2: Construct many-electron ground state

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

ground state

ground-state energy

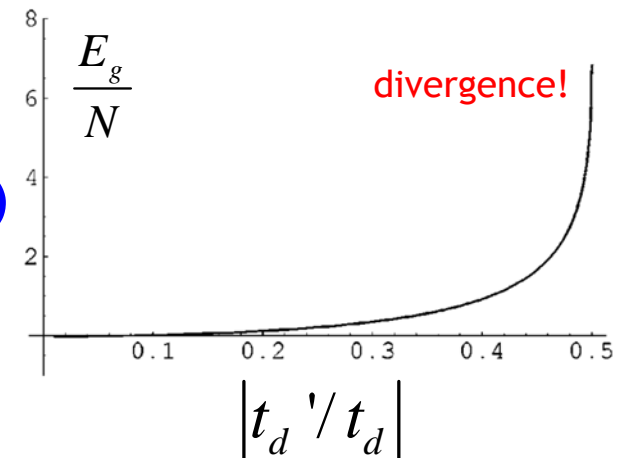
- Applicable to any model with sufficiently many microscopic parameters
- Works in any dimension
- No “integrability” required

Application to Hubbard and Periodic Anderson model

Brandt, Gieseke (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 $\frac{3}{4}$ filling

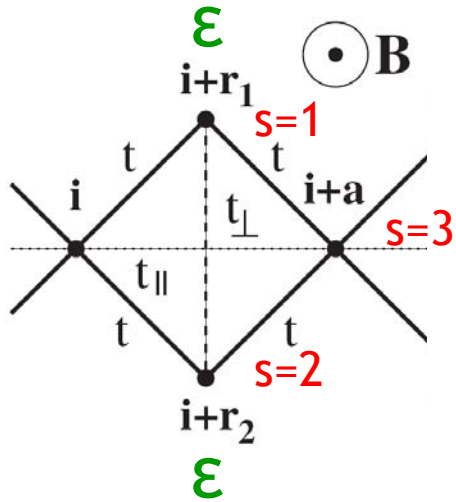


Gulacsi, Vollhardt (2003, 2005)

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 \rightarrow 3 bands

$s=1,2,3$ sublattice index

$N_c = \#$ cells

$N = \#$ electrons

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

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

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

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

Peierls phase factor

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

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

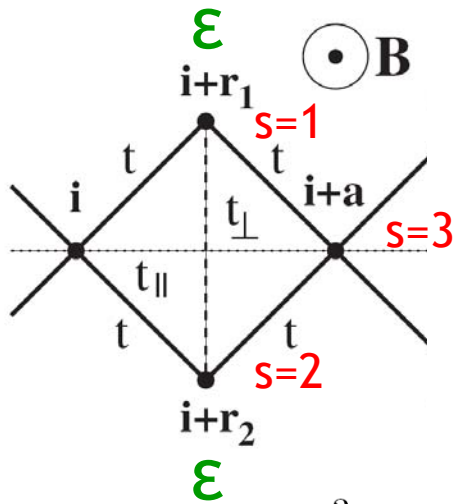
$$t_{j,j'}(\mathbf{B}) = t_{j,j'}(0) \exp[(i2\pi/\Phi_0) \int_j^{j'} \mathbf{A} \cdot d\mathbf{l}]$$

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

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

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

No
Zeeman
Term



3 sites per cell \rightarrow 3 bands

$s=1,2,3$ sublattice index

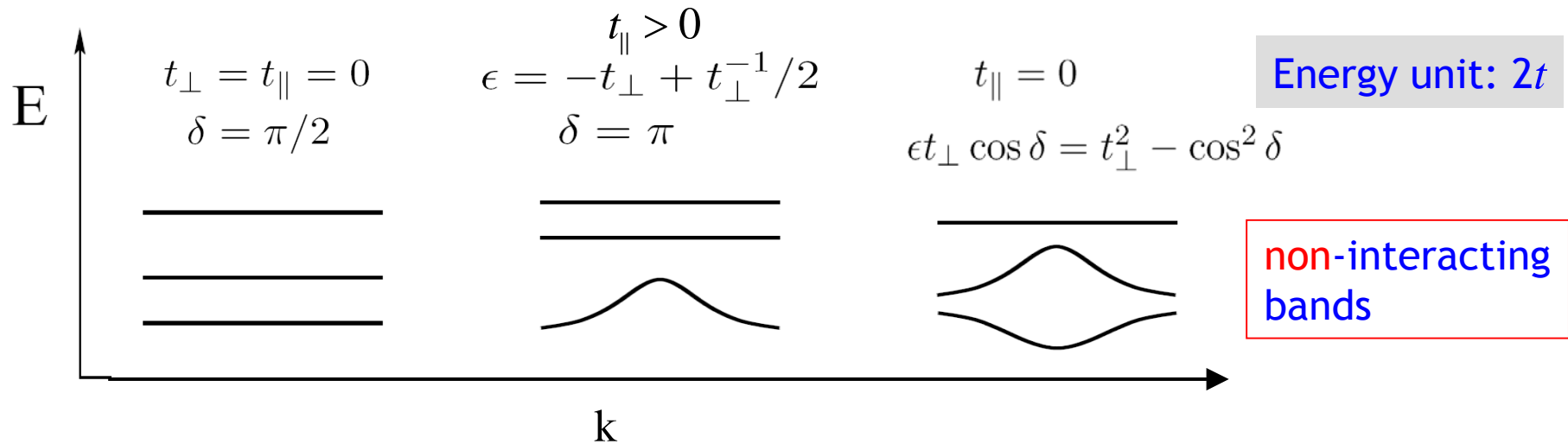
N_c = # cells

N = # electrons

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

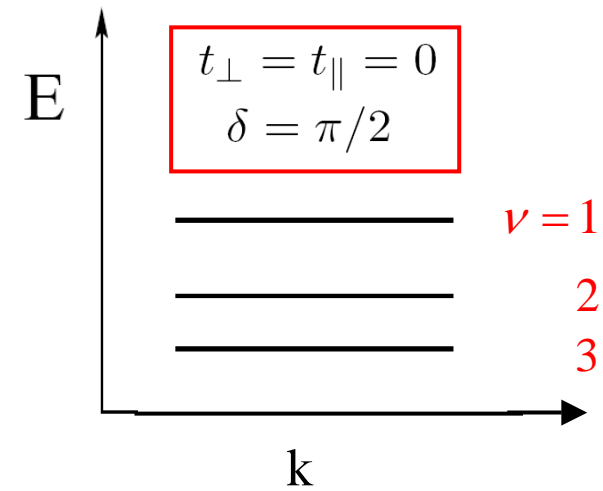
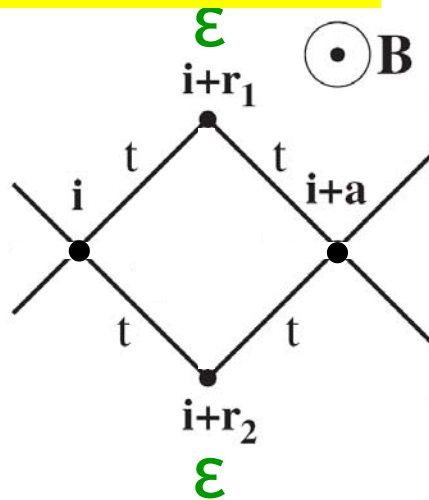
FT
$$\hat{H}_0 = \sum_{\mathbf{k}, \sigma} \sum_{s, s'=1}^3 M_{s, s'}(\mathbf{k}) \hat{C}_{s, \mathbf{k}, \sigma}^\dagger \hat{C}_{s', \mathbf{k}, \sigma}$$

Examples:



Solution I: Flat-band ferromagnetism

Solution I: Flat-band ferromagnetism



“Aharonov-Bohm cage”

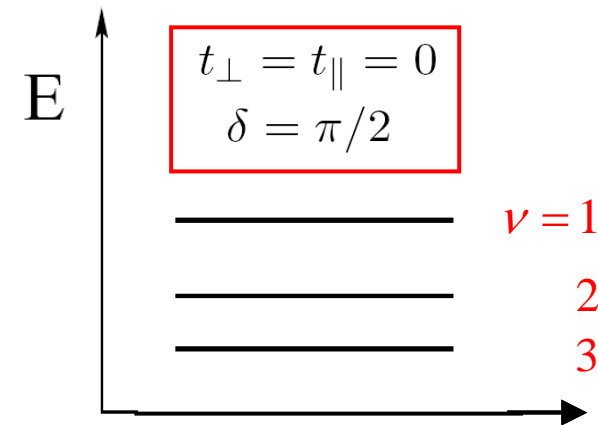
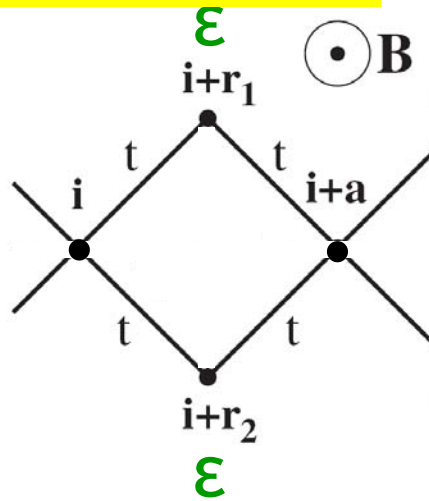
Vidal, Doucot, Mosseri, Butaud (2000)

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

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

Delocalization also for finite densities ?

Solution I: Flat-band ferromagnetism

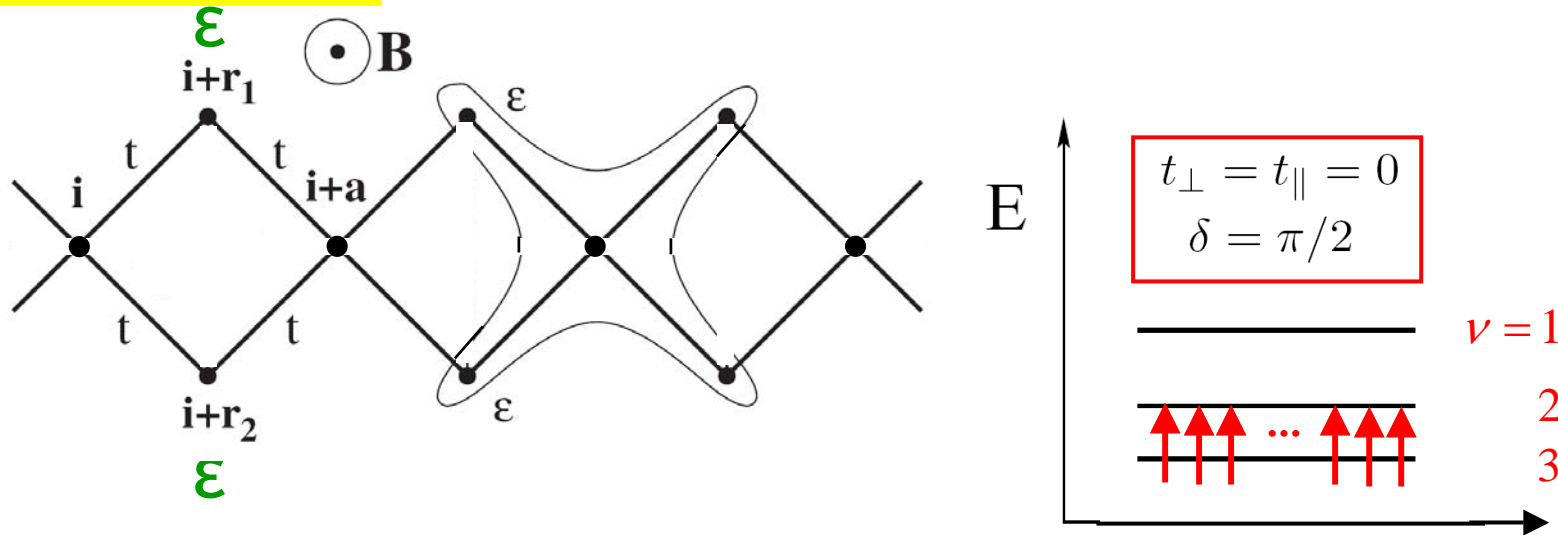


Diagonalization: \rightarrow New canonical fermionic operators $\hat{C}_{\nu, \mathbf{i}, \sigma}^{\mathbf{k}}$ in position space

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

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

Solution I: Flat-band ferromagnetism



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

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

Ground state of \hat{H}

$$N \leq N_c, \quad U > 0$$

$$|\Psi_g^I(N)\rangle = \prod_{i=1}^N \hat{C}_{3,i,\sigma_i}^{\dagger} |0\rangle$$

$$E_g^I = E_3 N$$

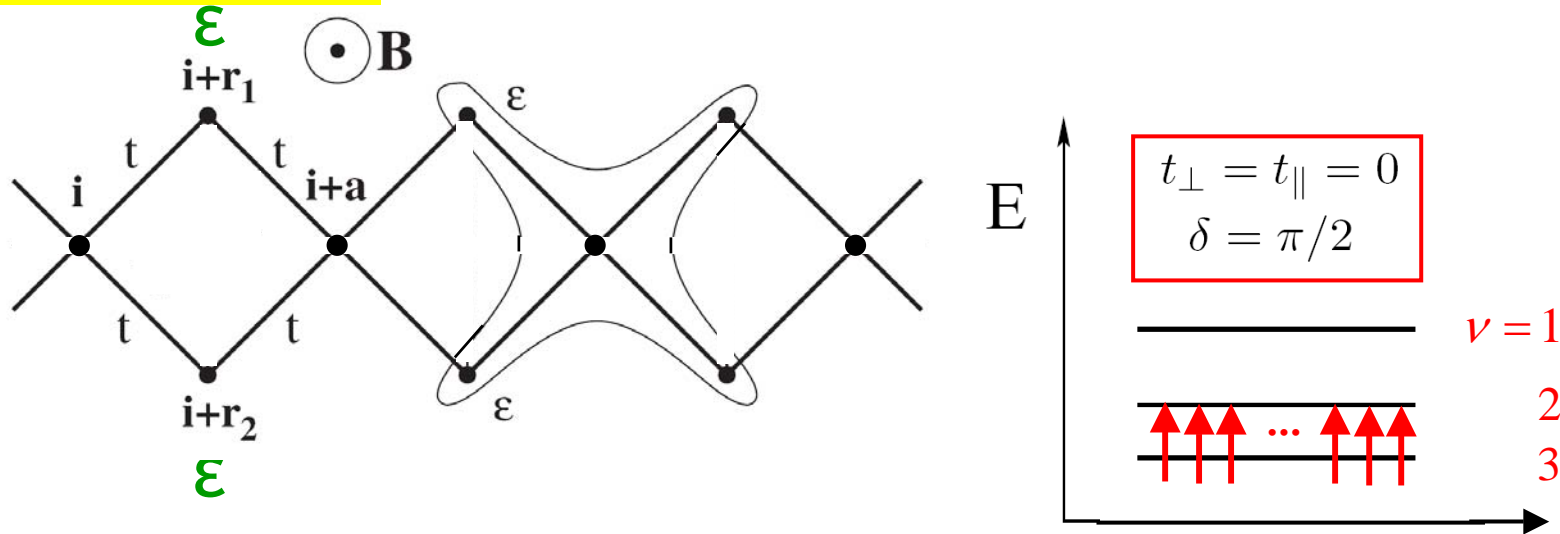
$n < 1/3$: ferromagnetic clusters

$n = 1/3$: fully saturated ferromagnet

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



Diagonalization: → New canonical fermionic operators $\hat{C}_{\nu,i,\sigma}^k$

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

Ground state of \hat{H}

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Mielke, Tasaki (1993)

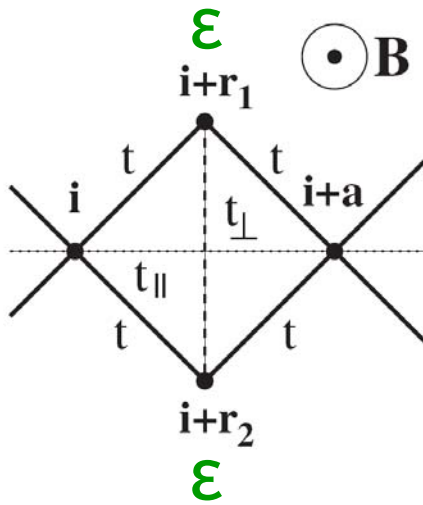
$U > 0$: **lowest** band flat only for $\delta = \pi/2$ (localized)
dispersive for $\delta = 0$ (conducting)



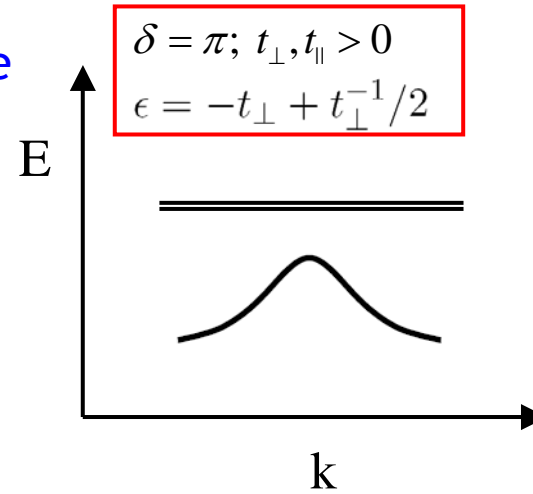
magnetic field induced
metal-insulator transition

Solution II: Correlated half-metal

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

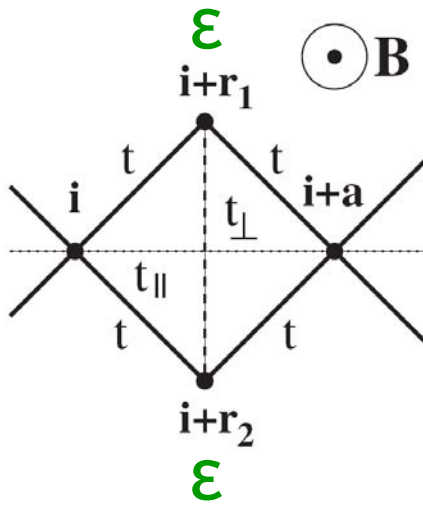


→ Investigate

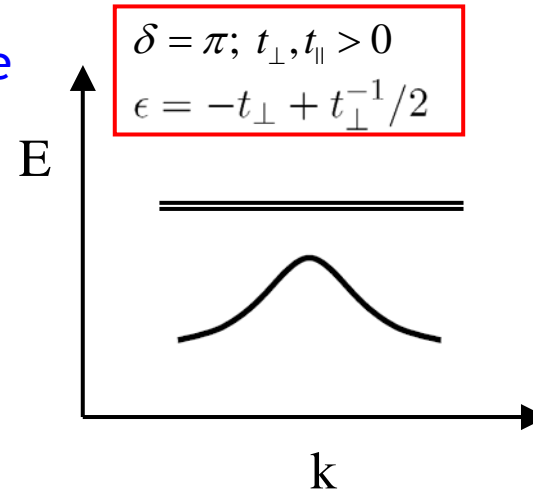


Single-electron bands

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

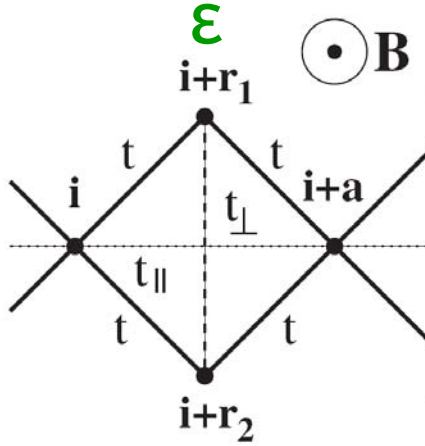


→ Investigate



Single-electron bands

Transformation of the Hamiltonian into positive semi-definite form



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

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

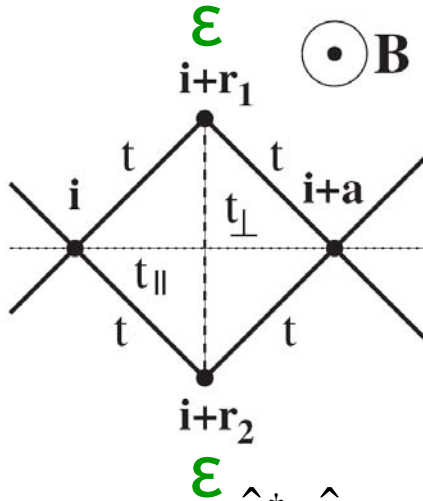
$$(\hat{A}_{i,\sigma})^2 = 0$$

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

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

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

Transformation of the Hamiltonian into positive semi-definite form



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

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

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

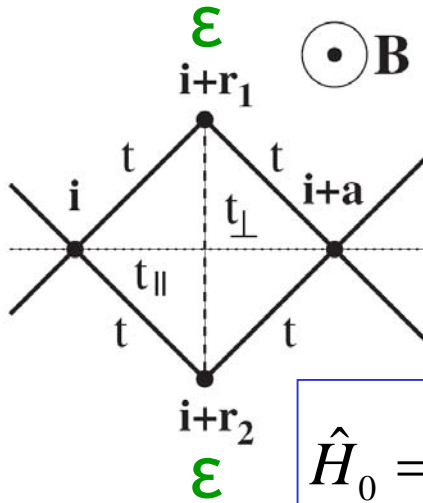
$$\{\hat{A}_{i,\sigma}, \hat{A}_{j,\sigma}^\dagger\} \neq \delta_{i,j}$$

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

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

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

Solution II: Correlated half-metal



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

$$\hat{H}_U$$

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

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

$$\Rightarrow \hat{H} = \sum_{i,\sigma} \hat{A}_{i,\sigma} \hat{A}_{i,\sigma}^\dagger + U\hat{P} + E_g^{II} \quad \text{positive semi-definite}$$

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

Construction of the ground state

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

positive semi-definite

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

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

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

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

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

Ground state

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

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

Ground state

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

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

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

One σ electron on every lattice site \rightarrow localized

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

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

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

Solution II: Correlated half-metal

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

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

Ground state

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

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

$\rightarrow \Delta N$ $-\sigma$ 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 conducting $-\sigma$ electrons
- Magnetization $M \propto (1 - \Delta N / N_c) \xrightarrow{\Delta N \rightarrow N_c} 0$
 \rightarrow Low carrier-density metallic behavior

Solution II: Correlated half-metal

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

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

Ground state

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

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

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

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

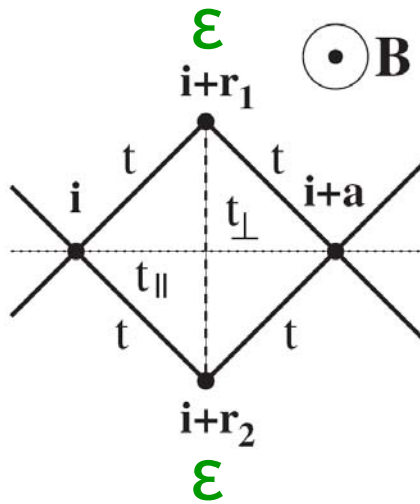
$U=0$: dispersionless, localized electrons
 $U>0$: **correlation-induced half-metal**

\rightarrow Correlation-induced localization-delocalization transition to a half-metal

$B=\text{const}$: Trigger transition by tuning local potential ε

Solution III:
Exact ground states for general magnetic flux

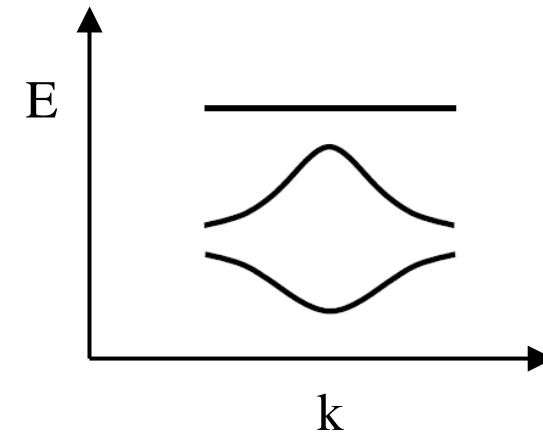
Solution III: Exact ground states for general magnetic flux



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

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

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



Single-electron bands

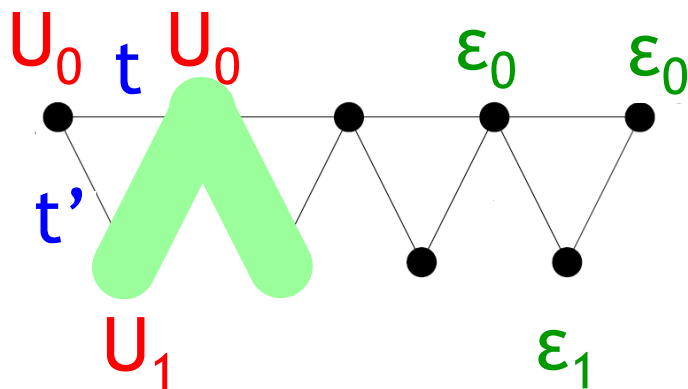
Ground states for $n \geq 5/3$

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

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



2 sites per cell \rightarrow 2 bands

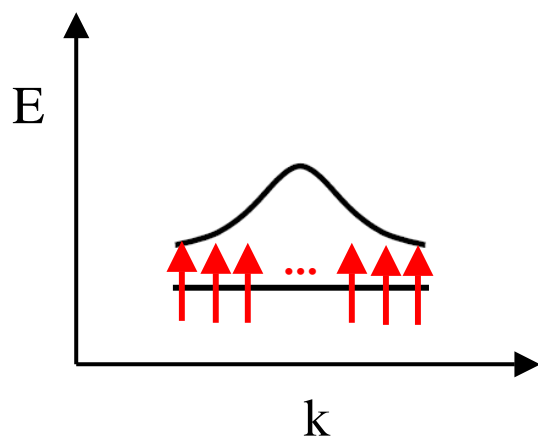
$N_c = \#$ cells

$N = \#$ electrons

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

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

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



Single-electron bands

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

Solution I:

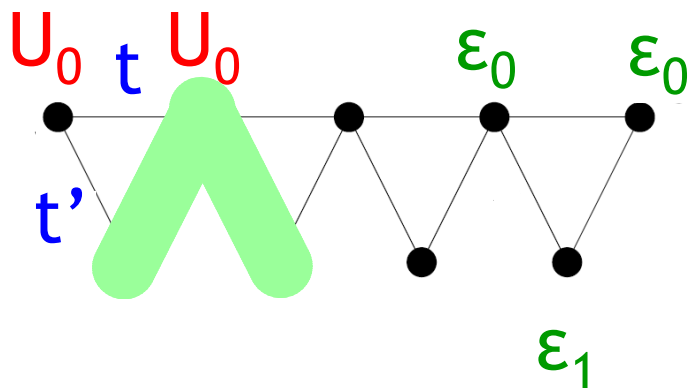
$$U_0, U_1 > 0$$

$n < 1/2$: ferromagnetic clusters

$n = 1/2$: fully saturated ferromagnet

Mielke, Tasaki (1993)

Derzho, Honecker, Richter (2007)



2 sites per cell \rightarrow 2 bands

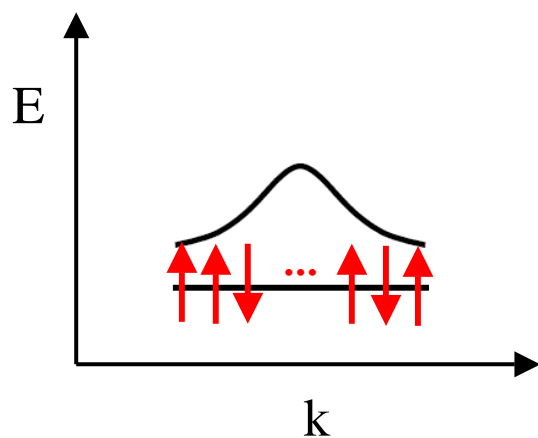
$N_c = \# \text{ cells}$

$N = \# \text{ electrons}$

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

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

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



Single-electron bands

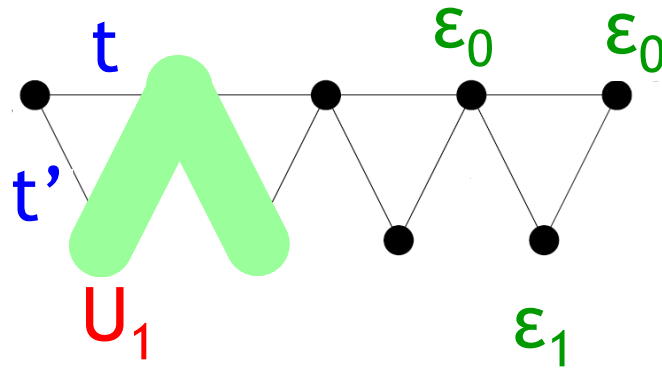
$$\hat{H} = \hat{H}_0 + \hat{H}_U$$

Solution II:

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

$n=1/2$: non-magnetic

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



2 sites per cell \rightarrow 2 bands

$N_c = \#$ cells

$N = \#$ electrons

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

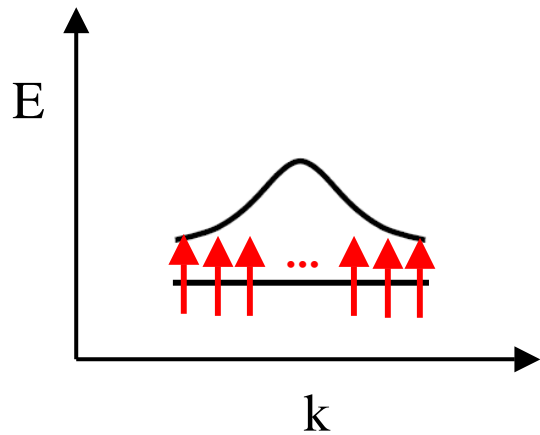
$$\frac{(t')^2}{t} = \epsilon_1 - \epsilon_0 + 2t, \quad t > 0$$

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

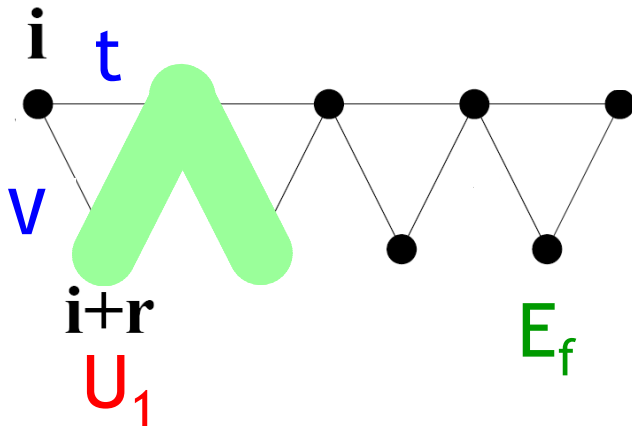
$$\hat{H} = \hat{H}_0 + \hat{H}_U$$

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

$n=1/2$: fully saturated ferromagnet



Single-electron bands



2 sites per cell \rightarrow 2 bands

$N_c = \#$ cells

$N = \#$ electrons

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

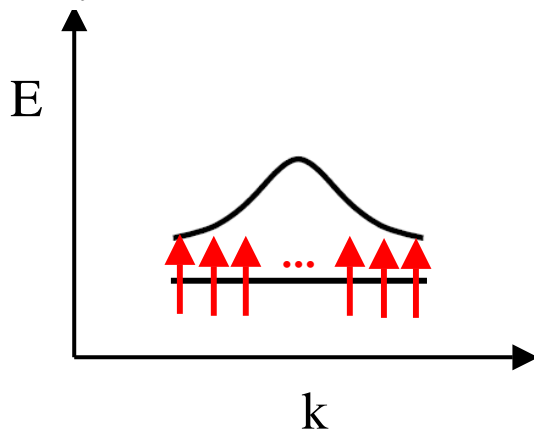
$$\frac{V^2}{t} = E_f + 2t, \quad t > 0, \quad t > 0$$

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

$$E_f > -2t$$

Solution III:

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



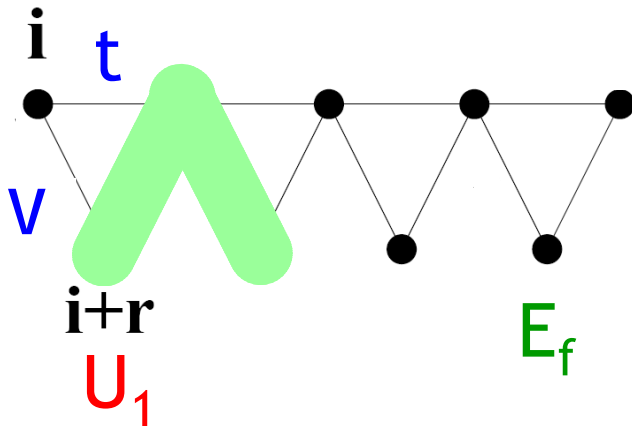
$n=1/2$: fully saturated ferromagnet

Change of notation:

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

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

1D periodic Anderson model



2 sites per cell \rightarrow 2 bands

$N_c = \#$ cells

$N = \#$ electrons

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

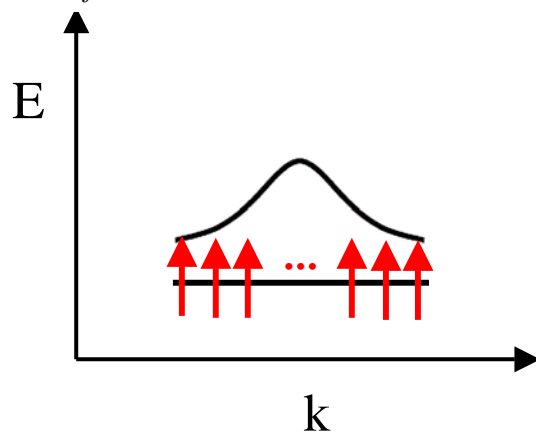
$$\frac{V^2}{t} = E_f + 2t, \quad t > 0, \quad t > 0$$

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

$$E_f > -2t$$

Solution III:

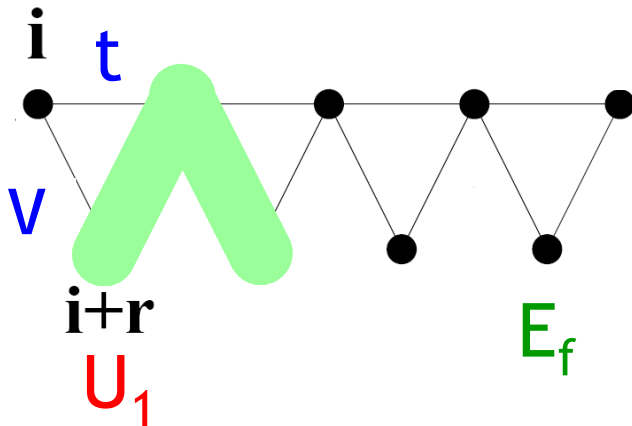
$$U_0 = 0, \quad U_1 > 0$$



$n=1/2$: fully saturated ferromagnet

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

1D periodic Anderson model



2 sites per cell \rightarrow 2 bands

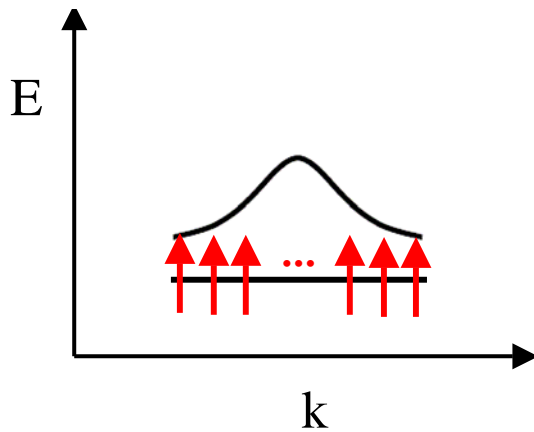
$N_c = \#$ cells

$N = \#$ electrons

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

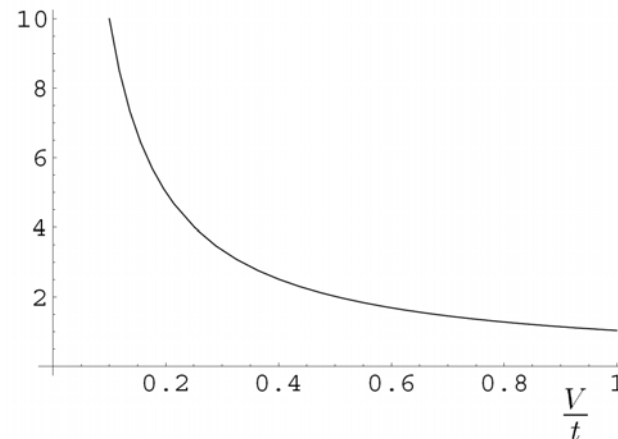
$$\frac{V^2}{t} = E_f + 2t, \quad t > 0$$

$$E_f > -2t$$



Localization length of d-electrons

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

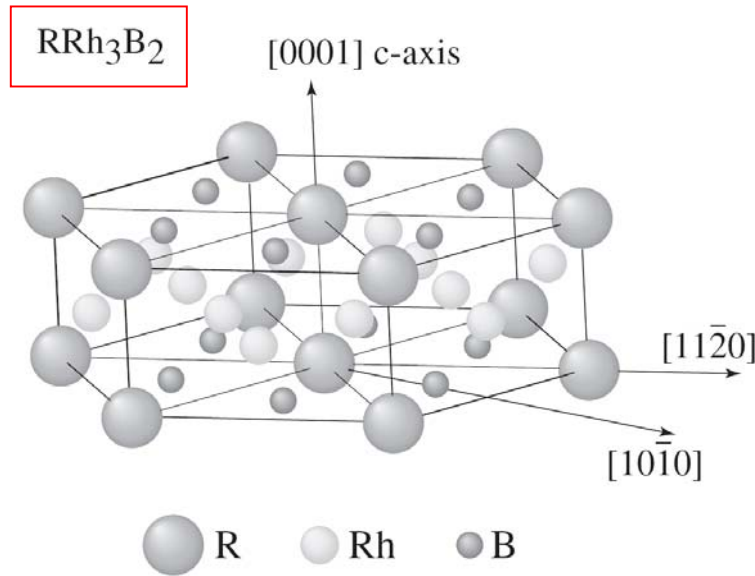


Application of the 1D periodic Anderson model to CeRh_3B_2

CeRh_3B_2 is interesting because:

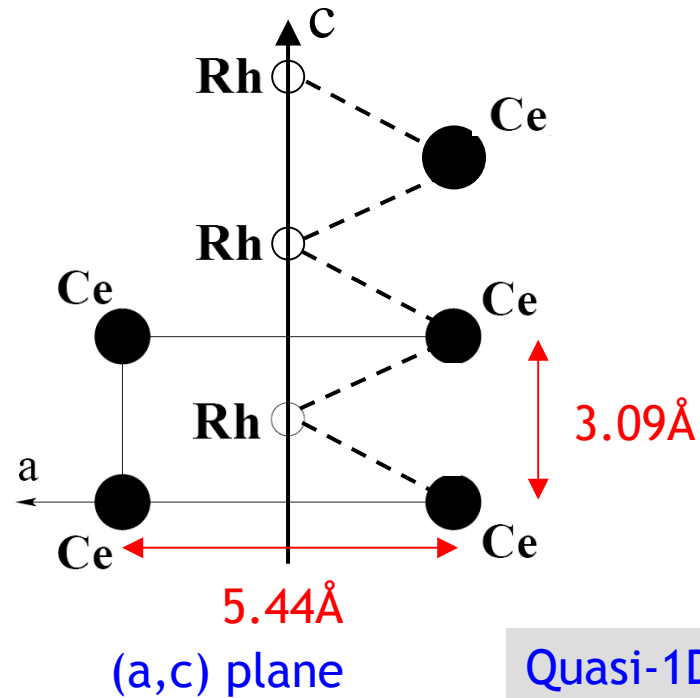
- RKKY interaction cannot explain ferromagnetism
- Small f- moment $0.45 \mu_B$ (free Ce^{3+} ion: $2.14 \mu_B$)
- Highest T_c (=120 K) among known Ce compounds with non-magnetic elements

Application of the 1D periodic Anderson model to CeRh_3B_2

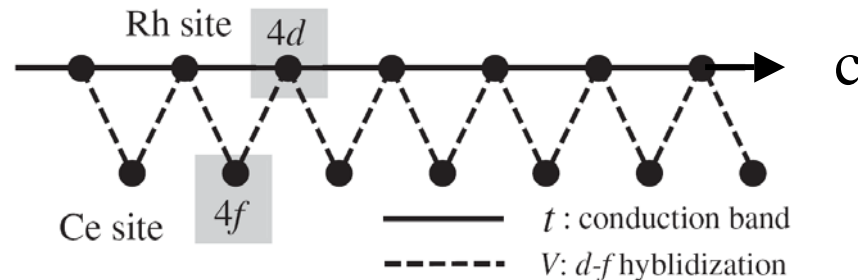


Rare Earth

Yamada *et al.* (JPSJ, 2004)



Quasi-1D
band structure



Kono, Kuramoto (JPSJ, 2006)

Mechanism for f-electron ferromagnetism in CeRh_3B_2 ?

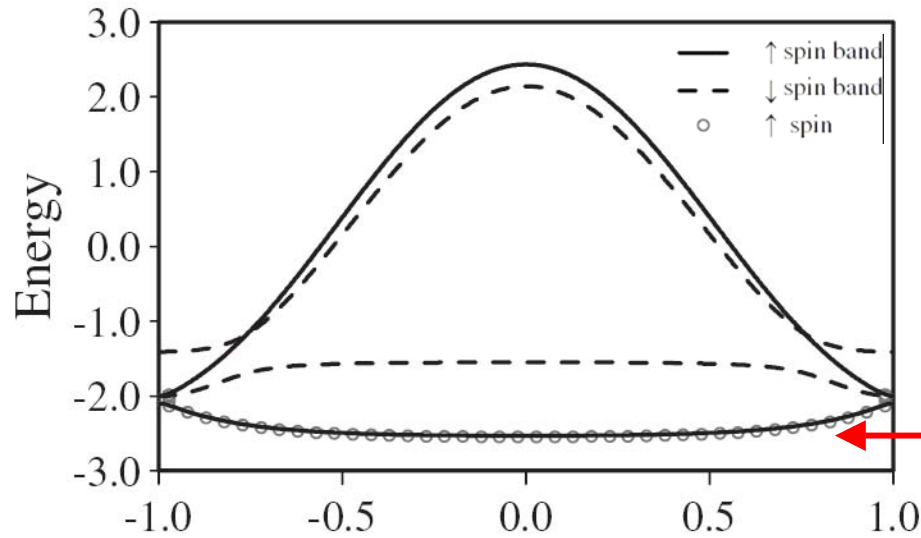
Non-interacting magnetic state $|\Phi\rangle = \prod_{\sigma} \prod_k^{N_{\sigma}-L} a_{k\sigma}^{\dagger} \prod_k^L b_{k\sigma}^{\dagger} |0\rangle$

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

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

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

VMC



Kono, Kuramoto (JPSJ, 2006)

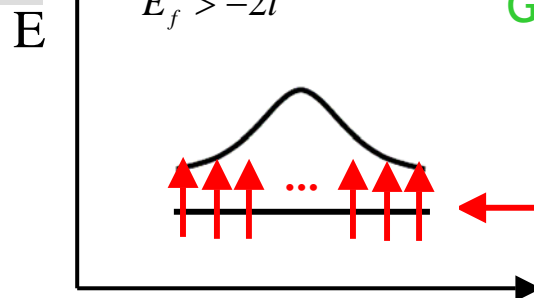
$$t = 0.34 \text{ eV}, V = 0.24 \text{ eV}, E_f = -0.714 \text{ eV}, U = 7 \text{ eV}, n = 0.55$$

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

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

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

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

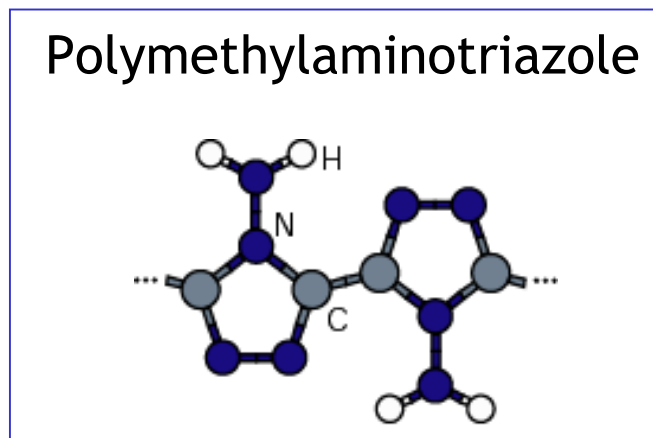
$$m_f = 0.68$$

Gulacsi, Kampf, Vollhardt (unpublished)

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

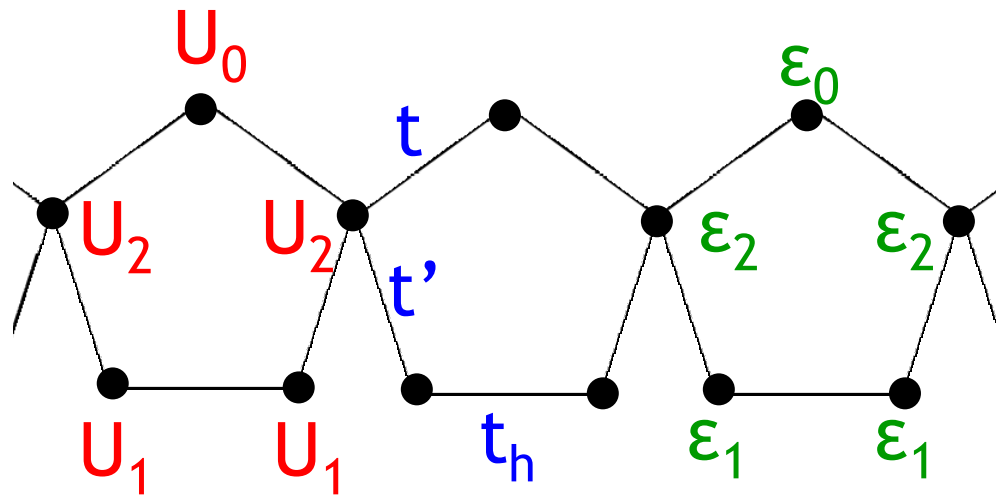
Search for ferromagnetism in systems with non-magnetic elements

Candidate: Flat-band ferromagnetism in organic polymers



Suwa, Arita, Kuroki, Aoki (2003)

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



4 sites per cell \rightarrow 4 bands

N_c = # cells

N = # electrons

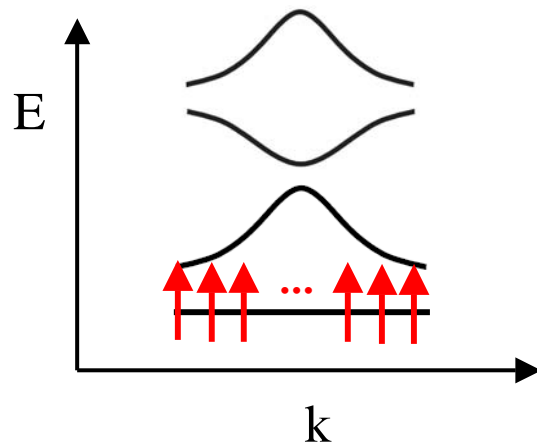
$n = \frac{N}{4N_c}$ electron density

Gulacsi, Kampf, Vollhardt (unpublished)

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

$$\epsilon_2 = 2 \frac{t'^2}{\epsilon_1 - t_h}$$

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

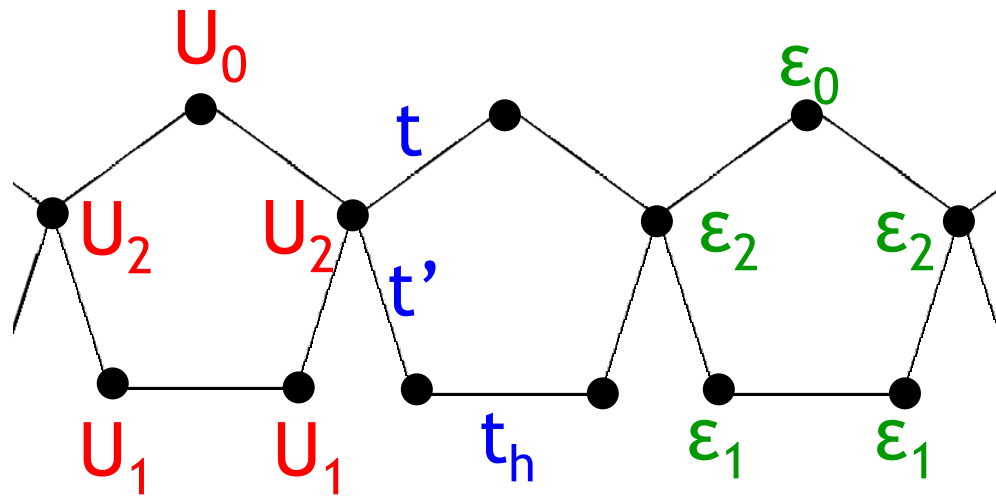


Ground state I: $U_0, U_1, U_2 > 0$

$n < 1/4$: ferromagnetic clusters

$n = 1/4$: saturated ferromagnet

Construction of lowest flat band by tuning of “gate potentials ϵ ” only



4 sites per cell \rightarrow 4 bands

$N_c = \#$ cells

$N = \#$ electrons

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

Gulacsi, Kampf, Vollhardt (unpublished)

$t_h < 0$; arbitrary $t, t', \epsilon_1, \epsilon_2$

$U_1, U_2 > 0$

$U_0 = U_0(t, t', t_h, \epsilon_0, \epsilon_1, \epsilon_2, U_1, U_2)$

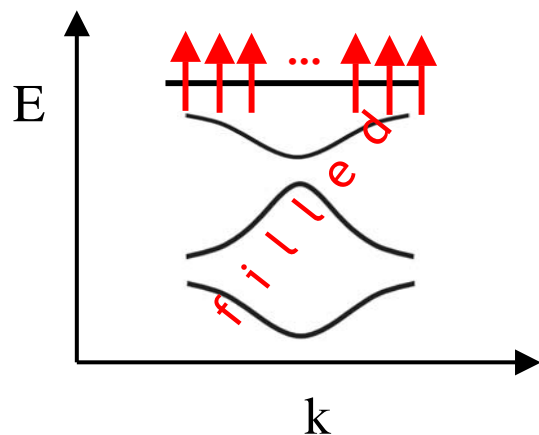
\rightarrow upper bound for ϵ_0

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

Ground state II:

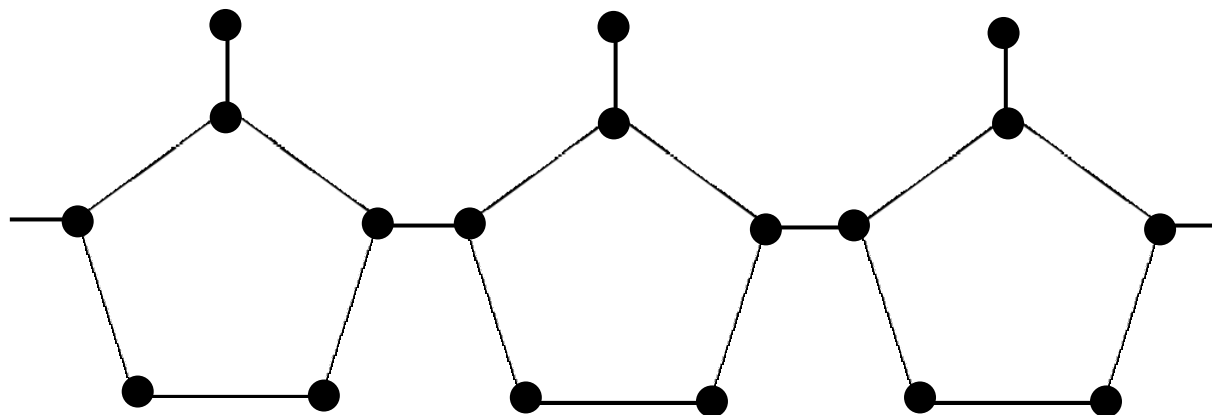
$n < 7/4$: ferromagnetic clusters

$n = 7/4$: non-saturated ferromagnet

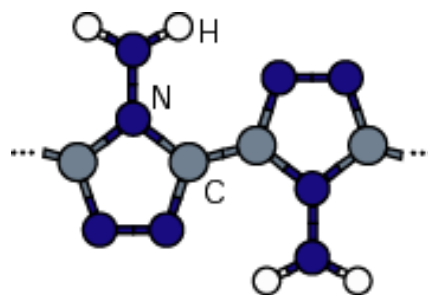


Construction of a flat band
by tuning the interaction U_0

Extension to more complicated structures possible



Polymethylaminotriazole

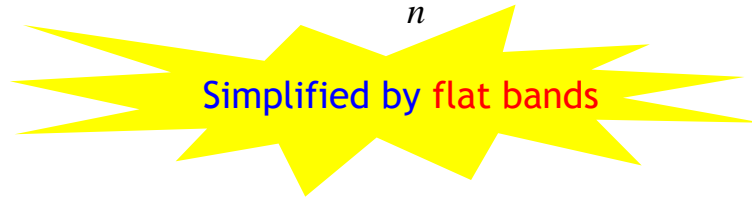


Conclusion 1:

Strategy for the construction of exact many-electron ground states

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

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



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

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

Step 2: Construct many-electron ground state

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

ground state

ground-state energy

- Applicable to any model with sufficiently many microscopic parameters
- Works in any dimension
- No “integrability” required

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