Construction of exact ground states for non-integrable lattice fermion models

Workshop on “Resonating Valence Bond Physics: Spin Liquids and Beyond“

Dedicated to the memory of Patrik Fazekas

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VARIATIONAL GROUND STATE FOR
THE PERIODIC ANDERSON MODEL.

Hungarian Academy of Sciences
CENTRAL RESEARCH INSTITUTE FOR PHYSICS
BUDAPEST
First International Workshop on Ordering Phenomena in Transition Metal Oxides
7.-10. October 2001, Kloster Irsee;
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First International Workshop on Ordering Phenomena in Transition Metal Oxides
7.-10. October 2001, Kloster Irsee;
Second International Workshop on Ordering Phenomena in Transition Metal Oxides
26.-29. September 2004, Wildbad Kreuth
Outline:

- Transformation of a Hamiltonian into positive semidefinite form
- Construction of exact many-electron ground states
- Triangle Hubbard chains → application to CeRh$_3$B$_2$
- Pentagon Hubbard chains → application to organic polymers

In collaboration with
Zsolt Gulacsi (Univ. Debrecen, Hungary)
Arno Kampf (Augsburg)
Highly desirable:
Exact solutions of correlation models
Construction of exact many-electron ground states from positive semidefinite Hamiltonians

Strategy

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

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

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

e.g., \( \hat{P}_n = \Omega^\dagger \Omega, \quad \Omega \Omega^\dagger \)

\[ \rightarrow \text{well-defined lower bound of spectrum} \]

Transformation feasible
- usually in several different ways
- on a subspace of the full parameter space
Construction of exact many-electron ground states from positive semidefinite Hamiltonians

**Strategy**

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

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

**Step 2: Construct 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
Strategy

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

Step 3: Prove uniqueness of many-electron ground state:

\[ |\Psi_g \rangle \text{ spans } \ker(\hat{H}') := \{ |\phi \rangle \mid \hat{H}'|\phi \rangle = 0 \} \]

- Works in any dimension
- No integrability required
- Applicable to any Hamiltonian with sufficiently many microscopic parameters (so far not possible for Hamiltonians with too simple structure)
In particular: Exact ground states with flat bands

Condensed matter systems with macroscopic degeneracies

→ very sensitive reaction to perturbations
→ emergent behavior

Examples:

• Electrons in a magnetic field in 2D               Landau (1930)
• Spins on lattices with geometric frustration    Moessner, Ramirez (2006)
• Dispersionless (“flat“) bands in solids          Mielke (1991)
                                                Mielke, Tasaki (1993)
                                                Arita, Suwa Kuroki, Aoki (2002)

→ Find exact solutions of correlation models with flat bands
High sensitivity to small changes of microscopic parameters found

PAM in $d=3$

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

Gulacsi, DV (2003, 2005)
1. Exact many-electron ground states on triangle Hubbard chains

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

2 sites per cell → 2 bands

\[ N_c = \# \text{ cells} \]
\[ N = \# \text{ electrons} \]
\[ n = \frac{N}{2N_c} \quad \text{electron density} \]

Müller-Hartmann (1995)
Penc, Shiba, Mila, Tsukagoshi (1996)
Fazekas (1997)
Derzho, Honecker, Richter (2007)
Derzho, Honecker, Richter, Maksymenko, Moessner (2010)
2 sites per cell → 2 bands

\[ N_c = \# \text{ cells} \]
\[ N = \# \text{ electrons} \]
\[ n = \frac{N}{2N_c} \text{ electron density} \]

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

\[ \epsilon_1 - \epsilon_0 > -2t \]

**Solution I:** \[ U_0, U_1 > 0 \]

**Step 1**

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

**Step 2**

Construct operators \( \hat{B} \) with

\[ \{ \hat{A}_{i,\sigma}, \hat{B}_{i',\sigma'}^\dagger \} = 0 \]

\[ \hat{B}_{i,\sigma} = \left[ \hat{c}_{i-a+r,\sigma} + \hat{c}_{i+r,\sigma} - (t'/t)\hat{c}_{i,\sigma} \right] \]

**Ground state**

\[ |\psi_{tri}(N)\rangle = \prod_i \hat{B}_{i,\sigma_i}^\dagger |0\rangle \]
2 sites per cell $\rightarrow$ 2 bands

$N_c = \# \text{ cells}$

$N = \# \text{ electrons}$

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

Solution I: $U_0, U_1 > 0$

Physical properties

$n < 1/2 : \text{ ferromagnetic clusters}$

$n = 1/2 : \text{ fully saturated ferromagnet}$

Mielke, Tasaki (1993)

Derzho, Honecker, Richter (2007)

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

\[ \epsilon_1 - \epsilon_0 > -2t \]

\[ \rightarrow \text{ Flat-band ferromagnetism: Realizes ideas of Gutzwiller and Kanamori from 1963 about the origin of itinerant ferromagnetism} \]

Not related to Stoner theory: $\chi(\omega=0, q=0) = \infty \rightarrow \text{UN}(E_F)=1$
2 sites per cell → 2 bands

\[ N_c = \# \text{ cells} \]
\[ N = \# \text{ electrons} \]

\[ n = \frac{N}{2N_c} \]

electron density

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

\[ \epsilon_1 - \epsilon_0 > -2t \]

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 $\rightarrow$ 2 bands

$N_c = \# \text{ cells}$

$N = \# \text{ electrons}$

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

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

$n = 1/2$ : fully saturated ferromagnet
2 sites per cell $\rightarrow$ 2 bands

\[ N_c = \# \text{ cells} \]
\[ N = \# \text{ electrons} \]
\[ n = \frac{N}{2N_c} \] electron density

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

n=1/2 : fully saturated ferromagnet

Change of notation:

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

1D periodic Anderson model
CeRh$_3$B$_2$ is an interesting $4f$-system because:

- RKKY interaction cannot explain ferromagnetism
- Small $f$-moment $0.45 \, \mu_B$ (free Ce$^{3+}$ ion: $2.14 \, \mu_B$)
Application of the 1D periodic Anderson model to CeRh$_3$B$_2$
Mechanism for $f$-electron ferromagnetism in CeRh$_3$B$_2$?

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

Evaluations by variational Monte Carlo (VMC) Kono, Kuramoto (2006)
$t = 0.34 \text{ eV, } V = 0.24 \text{ eV, } E_f = -0.714 \text{ eV, } U = 7 \text{ eV, } n = 0.55$

Gulacsi, Kampf, DV (2008)

- saturated ferromagnetism, bare flat band unchanged by $U$
- almost flat band

Kono, Kuramoto (2006)

- exact ground state (Solution III)

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

$E_f > -2t$

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

Free Ce\(^{3+}\) ion

\[ m_f = 2.14 \mu_B \]

Experiment:

\[ m_f = 0.45 \mu_B \]  
Galatanu et al. (2003)

VMC

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

\[ m_f = 0.94 \mu_B \]  
Kono, Kuramoto (2006)

Exact ground state

\[ \frac{V^2}{t} = E_f + 2t, \ t > 0, \ E_f > -2t \]

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

\[ m_f = 0.68 \mu_B \]  
Gulacsi, Kampf, DV (2008)
2. Exact many-electron ground states on pentagon chain polymers

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

Conducting polymers: wide range of applications in

- Nanoelectronics
- Nanooptics
- Medicine

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

Candidate: Flat-band ferromagnetism in organic polymers

**Polymethylaminotriazole**

Spin-DFT


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

Brocks, van den Brink, Morpurgo (2004)
Polymethylaminotriazole

Gulacsi, Kampf, DV (arXiv:1007.4994)

6 sites per cell $\rightarrow$ 6 bands

$N_c = \# \text{ cells}$

$N = \# \text{ electrons}$

\[ n = \frac{N}{6N_c} \quad \text{electron density} \]

Arbitrary

- local interactions $U_n > 0$
- on-site potentials $\varepsilon_n$
- hopping amplitudes $t_{n,n'}$
Single-particle bands

Gulacsi, Kampf, DV (arXiv:1007.4994)

Band dispersion

\[ \epsilon = E_\nu(k), \ \nu \leq 6\quad k = k \cdot a \]

\[
2t_c t^2 [(\epsilon_6 - \epsilon)T_h - t_h T_f] \cos k + T_f \{t^2 t^2_h - (\epsilon_2 - \epsilon)^2 t^2_c + [(\epsilon_1 - \epsilon)(\epsilon_2 - \epsilon) - t^2]_2 - (\epsilon_1 - \epsilon)^2 t^2_h \} \\
+ 2(\epsilon_6 - \epsilon)t^2 \{(\epsilon_2 + t_h - \epsilon) - (\epsilon_1 - \epsilon)T_h \} = 0,
\]

with \( T_h = (\epsilon_2 - \epsilon)^2 - t^2_h, \ T_f = (\epsilon_6 - \epsilon)(\epsilon_5 - \epsilon) - t^2_f \)

\[
t_c \equiv t_{4,7} = 0.5, \ t_h \equiv t_{3,2} = -1.1, \ t_f \equiv t_{5,6} = 1.2 \\
\epsilon_1 = \epsilon_4 = -2.5, \ \epsilon_2 = \epsilon_3 = -2.0, \ \epsilon_5 = -2.1, \ \epsilon_6 = -2.1
\]
Define operators acting on blocks $\mathcal{B}_1$

$$\hat{G}_\alpha^\dagger = \sum_{\ell \in \mathcal{B}_{i,\alpha}} d_{\alpha, \ell} \hat{c}_{i+r_{\ell,\sigma}} \quad \alpha = 1, \ldots, 5$$

3 three-site blocks
2 two-site blocks
Original form

\[ \hat{H}_0 = \sum_{\sigma, i} \sum_{n, n' (n>n')} (t_{n, n'} \hat{c}_{i + r_n, \sigma}^\dagger \hat{c}_{i + r_{n'}, \sigma} + H.c.) + \]
\[ + \sum_{\sigma, i} \sum_{n=1}^m \epsilon_n \hat{n}_{i + r_n, \sigma}, \]
\[ \hat{H}_U = \sum_{i} \sum_{n=1}^m U_n \hat{n}_{i + r_n, \uparrow} \hat{n}_{i + r_n, \downarrow}. \]

Positive semidefinite form

\[ \hat{H} - C_g = \hat{H}_G + \hat{H}_P \]

with

\[ \hat{H}_G = \sum_{i, \sigma} \sum_{\alpha=1}^{m-1} \hat{G}_{\alpha, i, \sigma} \hat{G}_{\alpha, i, \sigma}^\dagger, \quad \hat{H}_P = \sum_{n=1}^m U_n \sum_i \hat{P}_{i + r_n}, \]
\[ \hat{P}_j = \hat{n}_{j, \uparrow} \hat{n}_{j, \downarrow} - (\hat{n}_{j, \uparrow} + \hat{n}_{j, \downarrow}) + 1 \]
\[ C_g = q_U N - N_c [\sum_{n=1}^m U_n + 2 \sum_{\alpha=1}^{m-1} z_{\alpha}], \quad z_{\alpha} = \sum_{\ell} |a_{\alpha, \ell}|^2 \]
\[ q_U = (1/2) [(U_1 + \epsilon_1 + |t_c|) + (U_2 + \epsilon_2 + |t_h|) + \{(U_2 + \epsilon_2 + |t_h|) - (U_1 + \epsilon_1 + |t_c|)^2 + 4t^2\}]^{1/2} \]
Original form

\[
\hat{H}_0 = \sum_{\sigma,i} \sum_{n,n'(n>n')} (t_{n,n'} \hat{c}_{i+r_n,\sigma} \hat{c}_{i+r_{n'},\sigma} + H.c.) + \\
+ \sum_{\sigma,i} \sum_{n=1}^{m} \epsilon_n \hat{n}_{i+r_n,\sigma},
\]

\[
\hat{H}_U = \sum_{i} \sum_{n=1}^{m} U_n \hat{n}_{i+r_n,\uparrow} \hat{n}_{i+r_n,\downarrow}.
\]

Positive semidefinite form

\[
\hat{H} - C_g = \hat{H}_G + \hat{H}_P
\]

with

\[
\hat{H}_G = \sum_{i,\sigma} \sum_{\alpha=1}^{m-1} \hat{G}_{\alpha,i,\sigma} \hat{G}_{\alpha,i,\sigma}^{\dagger}, \quad \hat{H}_P = \sum_{n=1}^{m} U_n \sum_{i} \hat{P}_{i+r_n}
\]

Matching conditions:

\[
\sum_{\alpha} z_\alpha = 4Q_1 + Q_1^2/|t_h| + 2t_f^2/Q_1 + 2(|t_h| + |t_\epsilon|) + Q_3^2 + t_f^2/Q_3^2
\]

\[
Q_1 = q_U - U_2 - \epsilon_2 - |t_h|, \quad Q_2 = q_U - U_1 - \epsilon_1 - |t_\epsilon|,
\]

\[
Q_3 = |t_f| \sqrt{|t_h|/|t_h|(q_U - U_5 - \epsilon_5) - (q_U - U_2 - \epsilon_2)^2 + t_h^2}^{1/2}
\]

# free parameters in block operators < # matching conditions
Parameter space for which the transformation holds

\[ t_h < 0, \quad Z = (q_U - Q_3^2) > \epsilon_6, \]
\[ W = q_U - [(q_U - U_2 - \epsilon_2)^2 - t_h^2]/|t_h| > \epsilon_5, \]
\[ W - \epsilon_5 > U_5 > 0, \quad U_6 = Z - \epsilon_6. \]

No strong restrictions!

Explicit form of block operators:

\[ \hat{G}_{1,i,\sigma} = q_S \hat{b}_{i,5,2} - t/q_S \hat{c}_{i+r_1,\sigma}, \]
\[ \hat{G}_{2,i,\sigma} = -t_S \hat{b}_{i,2,3} + Q_1 \hat{c}_{i+r_5,\sigma}/t_S, \]
\[ \hat{G}_{3,i,\sigma} = q_S \hat{b}_{i,5,3} - t/q_S \hat{c}_{i+r_4,\sigma}, \]
\[ \hat{G}_{4,i,\sigma} = Q_3 \hat{c}_{i+r_6,\sigma} - t_f/Q_3 \hat{c}_{i+r_5,\sigma}, \]
\[ \hat{G}_{5,i,\sigma} = |t_c|^{1/2} [\hat{c}_{i+r_4,\sigma} - t_c \hat{c}_{i+a,\sigma}/|t_c|], \]

with \[ q_S = Q_1^{1/2}, \quad t_S = |t_h|^{1/2}, \quad \hat{b}_{i,n,m} = \sum_{p=n,m} \hat{c}_{i+r_p,\sigma} \]
Effective band structure

$$\hat{H}_G = \hat{H}_{kin} + \text{const}$$

$$\hat{H}_{kin} = -\sum_{i,\sigma} \sum_{\alpha=1}^{m-1} \hat{G}^\dagger_{\alpha,i,\sigma} \hat{G}_{\alpha,i,\sigma}$$

quadratic in the original $c$-operators

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

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

# free parameters in block operators < # matching conditions

→ exact effective band structure is in general dispersive

Upper band can be tuned to become flat due to interactions
Upper flat band half filled for $N=N^*=11N_c \rightarrow$ density $n=11/6$

Ground state for $n=11/6$:

$$|\Psi_g(N^*)\rangle = \prod_{\sigma} \hat{G}^\dagger_{\sigma} \hat{F}^\dagger |0\rangle$$

$$\hat{G}^\dagger_{\sigma} = \prod_i \prod_{\alpha=1}^{m-1} \hat{G}^\dagger_{m,i,\sigma}$$ creates $(m-1)N_c$ $\sigma$-electrons

$$\hat{F}^\dagger = \prod_i \hat{c}^\dagger_{i+r_{n_1},\sigma}$$ creates one $\sigma$-electrons in each unit cell

one $\sigma$-electron per site $\rightarrow$ localized

$-\sigma$-electron are mobile ($=\text{Slater determinant}$)
Upper flat band half filled for \( N = N^* = 11N_c \) \( \rightarrow \) density \( n = 11/6 \)

Ground state for \( n = 11/6 \):

\[
|\Psi_g(N^*)\rangle = \prod_{\sigma} \hat{G}^\dagger_{\sigma} \hat{F}^\dagger |0\rangle
\]

\[
\hat{G}^\dagger_{\sigma} = \prod_i \prod_{\alpha=1}^{m-1} \hat{G}^\dagger_{m,i,\sigma}
\]

creates \((m-1)N_c\) \( \sigma \)-electrons

\[
\hat{F}^\dagger = \prod_i \hat{c}^\dagger_{i+r_n,\sigma}
\]

creates one \( \sigma \)-electrons in each unit cell

one \( \sigma \)-electron per site \( \rightarrow \) localized

\( -\sigma \)-electron are mobile (= Slater determinant)

Physical properties

\[
\Gamma_i(r) = \langle \Psi_g(N^*) | (\hat{c}^\dagger_{i+r_n,-\sigma} \hat{c}^\dagger_{i+r_n+r,-\sigma} + H.c.) | \Psi_g(N^*) \rangle \rightarrow \frac{N_c}{\infty} e^{-r/\xi}
\]

Ground state for \( n = 11/6 \): localized ferromagnet

Ground state for \( n > 11/6 \) (\( S_{z,\text{max}} \) sector)

charge gap \( \Delta \mu = E_g(N)-2E_g(N-1)+E_g(N-2) = 0 \), \( \xi = \infty \) \( \rightarrow \) itinerant ferromagnet
Matching conditions allow for parameters

\[ n \geq \frac{11}{6}, \quad \frac{W}{t} = 0.15, \quad \text{with} \quad 0.2 \leq \frac{U_n}{W} \leq 2.3 \]

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)

Dispersive band may be tuned by interactions to become flat

→ new route for the design of ferromagnetic pentagon-chain polymers
Strategy for the construction of exact many-electron ground states:

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

**Step 2:** Construct many-electron ground state

**Step 3:** Prove uniqueness of many-electron ground state:

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

**E.g.:** Pentagon chain polymers

Tune dispersive band structure by the interaction → design flat band structure with ferromagnetic or half metallic ground state