Ground-state degeneracy and low-temperature thermodynamics of correlated electrons on highly frustrated lattices

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Motivation & Summary

- Hubbard model on highly frustrated lattices: completely flat lowest single-electron band
- localized-electron states: *exact* many-body ground states (key ingredient of flat-band ferromagnetism [1])
- analogy with localized-magnon states of Heisenberg antiferromagnet in high magnetic fields [2]
- ⇒ macroscopic ground-state degeneracy for a certain value of the chemical potential
- ⇒ thermodynamic signatures: low-temperature peak in the specific heat
- ⇒ exact and numerical results for certain models (e.g., sawtooth chain) [3–7]

Models of correlated electrons

Hubbard model:

$$H = + \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle i,j \rangle} t_{i,j} \left(c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \mu \sum_{i=1}^{N} n_i$$

N: #sites $\langle i,j \rangle$: pairs of nearest neighbor lattice sites i,j
$c^{(\dagger)}_{i,\sigma}$: Fermi operators $n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$ $n_i = n_{i,\uparrow} + n_{i,\downarrow}$
$U \geq 0$: Coulomb repulsion $t_{i,j}$: hopping integrals μ: chemical potential

$t-J$ model:

$$H = + \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle i,j \rangle} t_{i,j} P \left(c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma} \right) P + \sum_{\langle i,j \rangle} J_{i,j} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right) + \mu \sum_{i=1}^{N} n_i$$

P: projector eliminating doubly occupied sites
$\vec{S}_i$: spin-1/2 operators $J_{i,j} = J$: exchange integrals

References

[1] H. Tasaki, Prog. Theor. Phys. **99** (1998) 489

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[4] O. Derzhko, A. Honecker, J. Richter, Phys. Rev. B **76** (2007) 220402(R)

[5] J. Richter, O. Derzhko, A. Honecker, arXiv:0806.0922

[6] O. Derzhko, A. Honecker, J. Richter, arXiv:0807.2991

[7] A. Honecker, O. Derzhko, J. Richter, submitted to proceedings

From flat bands to localized electrons

- flat band $\varepsilon_0(\vec{k})$ ⇒ localized states, created by

$$l^\dagger_{\text{cell},\sigma} = \sum_{i \in \text{cell}} \alpha_i c^\dagger_{i,\sigma}$$

sum runs over trapping cells (**bold red lines** at the right)

- localized many-electron states

$$l^\dagger_{\text{cell}_r,\sigma_r} \cdots l^\dagger_{\text{cell}_1,\sigma_1} |0\rangle \qquad (1)$$

with fermionic vacuum $|0\rangle$
the states (1) are **ground states for $U=0$** by construction

Lower bounds for the ground-state degeneracy

- subset of (1): also eigenstates for $U > 0$, e.g.
  1. spin-polarized states $\sigma_i = \sigma$
  2. no spatial overlap of cell$_i$ with cell$_j$ for $\sigma_i \neq \sigma_j$
- positivity of the Coulomb (U) term of the Hubbard model ⇒ such states are exact many-electron **ground states**
- also exact eigenstates of the $t-J$ model, but not necessarily ground states for $J > 0$
- $\mu = \mu_0$ ⇒ $\varepsilon_0(\vec{k}) = 0$
- **lower bounds for the ground-state entropy**:
  1. one out of b bands flat [3]:
  $$\frac{S}{N} \geq \frac{\ln 2}{b}$$
  2. disjoint unit cells (yellow regions at the right), size l [7]:
  $$\frac{S}{N} \geq \frac{\ln 3}{l}$$
  exact if all trapping cells are non-overlapping [6]

Exact results in one dimension

assumption: trapping cells overlap with both neighbors

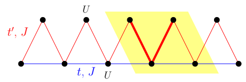
- spin-polarized clusters of consecutive occupied trapping cells
- independent $SU(2)$-rotations of the clusters: eigenstates
- flat band separated from the dispersive bands (e.g., sawtooth chain): complete basis of ground states
- choice of representative for linear combinations of (1): $\sigma_i = \downarrow$ at the right of cluster, $\sigma_i = \uparrow$ at the left
- ⇒ **dimer** model, solution by transfer matrix [4] ⇒ contribution to thermodynamic quantities, e.g., specific heat

$$\frac{C(\beta,\mu,N)}{N} = \frac{(\beta\,\varepsilon_0)^2\, \mathrm{e}^{-\beta\,\varepsilon_0}}{8\left(\frac{1}{4} + \mathrm{e}^{-\beta\,\varepsilon_0}\right)^{\frac{3}{2}}}$$

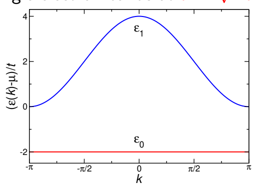
for $N \to \infty$, $\beta = \frac{1}{k_B T}$ ($\varepsilon_0 = -2\,t + \mu$ for sawtooth chain)

Examples

Sawtooth chain:



- single-electron bands at $t' = \sqrt{2}\,t$:

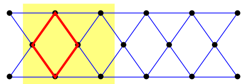


- $T=0$ entropy at $\mu = 2\,t$:

$\frac{S}{N} \geq \frac{\ln 3}{4} = 0.274\ldots$ ($l=4$) $\quad \frac{S}{N} \geq \frac{\ln 2}{2} = 0.346\ldots$ ($b=2$)

$\frac{S}{N} = \ln\left(\frac{1+\sqrt{5}}{2}\right) =: \ln\phi = 0.481\ldots$ (dimer) [4]

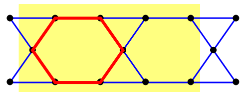
Kagome chain I:



- $T=0$ entropy at $\mu = 2\,t$:

$\frac{S}{N} \geq \frac{\ln 3}{6} = 0.183\ldots$ ($l=6$)
$\frac{S}{N} \geq \frac{\ln 2}{3} = 0.231\ldots$ ($b=3$)
$\frac{S}{N} \geq \frac{2}{3}\ln\phi = 0.320\ldots$ (dimer)

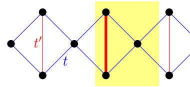
Kagome chain II:



- $T=0$ entropy at $\mu = 2\,t$:

$\frac{S}{N} \geq \frac{\ln 3}{10} = 0.109\ldots$ ($l=10$)
$\frac{S}{N} \geq \frac{\ln 2}{5} = 0.138\ldots$ ($b=5$)
$\frac{S}{N} \geq \frac{2}{5}\ln\phi = 0.192\ldots$ (dimer)

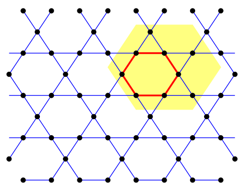
Diamond chain:



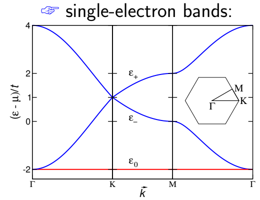
- $T=0$ entropy at $\mu = t'$ for $t' > 2\,t$:

$\frac{S}{N} = \frac{\ln 3}{3} = 0.366\ldots$ ($l=3$) [6]
$\frac{S}{N} \geq \frac{\ln 2}{3} = 0.231\ldots$ ($b=3$)

Kagome lattice:



- single-electron bands:



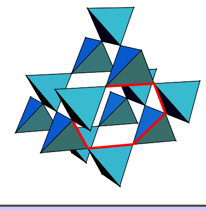
- $T=0$ entropy at $\mu = 2\,t$:

$\frac{S}{N} \geq \frac{\ln 3}{9} = 0.122\ldots$ ($l=9$) $\quad \frac{S}{N} \geq \frac{\ln 2}{3} = 0.231\ldots$ ($b=3$)

Pyrochlore lattice:

- $T=0$ entropy at $\mu = 2\,t$:

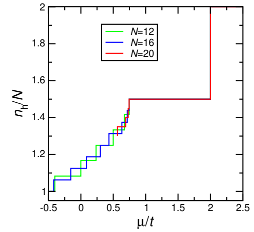
$\frac{S}{N} \geq \frac{\ln 3}{12} = 0.091\ldots$ ($l=12$)
$\frac{S}{N} \geq \frac{\ln 2}{2} = 0.346\ldots$ ($b=\frac{4}{2}$)

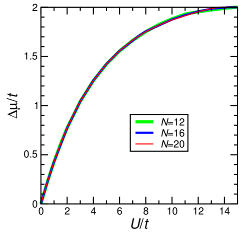


Sawtooth chain: exact diagonalization

Hubbard model at $t' = \sqrt{2}\,t$

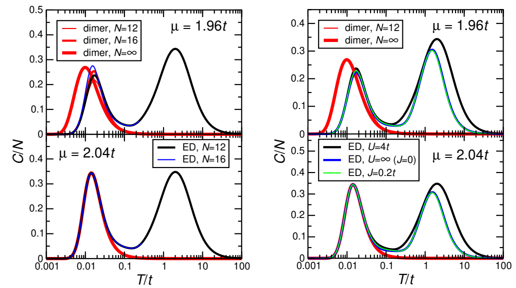
Hole density $n_h = 2\,N - n$ at $U = 4\,t$ — **Charge gap** $\Delta\mu = E\left(\frac{N}{2}+1\right) - 2\,E\left(\frac{N}{2}\right) + E\left(\frac{N}{2}-1\right)$





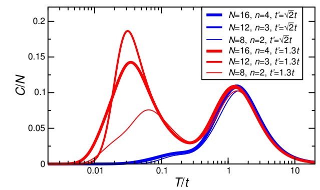
Grand-canonical specific heat C at $t' = \sqrt{2}\,t$

$U = 4\,t$ $\qquad$ $N = 12$



- degenerate ground states ⇒ additional low-temperature peak for $\mu \approx 2\,t$

Canonical specific heat C at $n = N/4$
$U = \infty$ ($t-J$ model with $J = 0$)



- low-temperature peak disappears for $t' = \sqrt{2}\,t$
- distortion $t' \neq \sqrt{2}\,t$ stabilizes low-temperature peak

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