Exact Diagonalization for topological phases driven by interactions

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Thanks

- J. W. F. Venderbos (IFW Dresden → MIT): QAH, FCI
- S. Kourtis (IFW Dresden → Cambridge): FCI, topological pinball liquid
- M. Hohenadler (Univ. Würzburg): fermions on honeycomb
- A. Fischer (IFW Dresden)
- J. van den Brink (IFW Dresden)
Integer Quantum Hall Effect

- transverse conductivity quantized
- Standard for electrical resistance
- is (first) Chern number
- implies edge states

figures: M.E. Cage, Springer 1987; M. Hasan and C. Kane, RMP 82, 3045 (2010); wikipedia

von Klitzing et al., PRL 45, 494 (1980)
Quantum Anomalous Hall States

- Haldane’s proposal: open gaps in graphene by breaking of time reversal symmetry

- Complex hoppings instead of a magnetic field
  F. D. M. Haldane, PRL 61, 2015 (1988)

- Spin-orbit coupling

- Topological features from correlations? S. Raghu et al., PRL 100, 156401 (2008)

- Example: Checkerboard lattice with quadratic band crossing K. Sun et al., PRL 103, (2009)

- Kondo-lattice model on frustrated lattices e.g. I. Martin and C. D. Batista, PRL 101, 156402 (2008)
Spinless fermions on honeycomb

- Mean-field: 2nd-neighbour Coulomb repulsion $V_2$ drives type of bond order that gives QAH S. Raghu et al., PRL 100, 156401 (2008)
- Exact diagonalization: some tendency to QAH

\[
\frac{1}{L^2} \left\langle \left| \sum_{\langle\langle i,j \rangle\rangle} (c_i^\dagger c_j - c_j^\dagger c_i) \right|^2 \right\rangle
\]

... but stronger tendency to charge order.

ED phase diagram:
Fluctuations beyond mean-field

- Systematic improvement over mean field: Quantum fluctuations on more and more bonds
- Used cluster perturbation theory / variational cluster approach: bonds within cluster exact, outside mean field
- QAH disappears for 6 cluster sites

\[
100 \times \frac{(E_{\text{CPT}} - E_0)}{t} \quad |\chi| \quad L = 2 \quad L = 4 \quad L = 6
\]

M. Daghofer & M. Hohenadler, PRB 89, 035103 (2014); N. A. García-Martínez et al. PRB 88, 245123 (2013); T. Duric et al., arXiv:1401.5680
Instead of QAH: partial CDW

- CDW driven by $V_2$ does not ‘fit’ with half filling
- Frustrated on triangular sublattice
- Mean-field: More charge in one sublattice
  A. G. Grushin et al., PRB 87, 085136 (2013)
- ED: No signature of charge imbalance
- Weird: One-particle gap given by $t$, not $V_2$ (or $V_1$)
Partial CDW related to ‘pinball liquid’

- Fermionic analogue to supersolid: CDW + superfluid M. Boninsegni & N. Prokof’ev, PRL 95, 237204 (2005); S. Wessel & M. Troyer, PRL 95, 127205 (2005).
- Here: Two sublattices

(a)

- Black sites account for $2/3$ of electrons, remaining can be distributed in any way on $+$ sites
- Weird properties, topological order?
Another route: Non-coplanar spin patterns

- Spin has to realign itself from site to site:
  \[ t_{ij} = \left( \cos \frac{\theta_i}{2} \cos \frac{\theta_j}{2} + \sin \frac{\theta_i}{2} \sin \frac{\theta_j}{2} e^{-i(\phi_i - \phi_j)} \right) t \]

- Triangular Kondo-lattice model

- Checkerboard Kondo-lattice model


J. W. F. Venderbos, M. Daghofer, J. van den Brink, S. Kumar, PRL 109, 166405 (2012)
Hubbard model

- Classical Kondo-lattice model = mean field for Hubbard
- Non-coplanar Ground state at van-Hove?
- Finite $T$: coplanar
- (also: $d + id$ SC at small $U$)
- Large $U$, Variational Cluster Approach: Quantum fluctuations prefer collinear order
  A. Fischer & M. Daghofer, in preparation
- classical spin/mean field better justified in multi-orbital model
$d$ orbitals in octahedral coordination
$d$ orbitals in octahedral coordination

\[ d \quad \longleftrightarrow \quad e_g \quad \longleftrightarrow \quad t_{2g} \]
$d$ orbitals in octahedral coordination
Mean-field bands in cylinder

- Low-lying $e'_{g}$ electrons: “localized” spin
- $a_{1g}$ levels around $\mu$: itinerant electrons


- Similar situation to Kondo-lattice model
Add inter-site Coulomb repulsion

Insert magnetic flux:

$$t_{i,j} \rightarrow t_{i,j} e^{i \left( \phi_x \frac{j x - i x}{L x} + \phi_y \frac{j y - i y}{L y} \right)}$$

Add inter-site Coulomb repulsion

Insert magnetic flux:

\[ t_{i,j} \rightarrow t_{i,j} e^{i \left( \phi_x \frac{j_x - i_x}{L_x} + \phi_y \frac{j_y - i_y}{L_y} \right)} \]

Add inter-site Coulomb repulsion

\[ \frac{V}{t} = 1 \]

\( t_{i,j} \rightarrow t_{i,j} e^{i \left( \phi_x \frac{jx-i}{L_x} + \phi_y \frac{jy-i}{L_y} \right)} \)

Add one hole to FQH/FCI state on torus: certain number of states expected below gap

Hall Conductivity

\[ \Omega^n(\phi_x, \phi_y) = i L_x L_y \sum_{n' \neq n} \frac{\langle n | \frac{\partial H_{\text{eff}}(\phi_x, \phi_y)}{\partial \phi_x} | n' \rangle \langle n' | \frac{\partial H_{\text{eff}}(\phi_x, \phi_y)}{\partial \phi_y} | n \rangle}{(\epsilon_n - \epsilon_{n'})^2} - (x \leftrightarrow y) \]

Similar for \( \nu = 2/3, 1/5, 2/5, \ldots \) and other models.

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How flat is flat enough?

Parametrize band flatness:

\[ \Delta_{JT}/t \]

\[ \tau_{dd}/t \]

\[ t'/t \]

\[ M \]

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How flat is flat enough?

Parametrize band flatness:

\[ \frac{t_{dd}}{t} - \Delta_{JT}/t \]

\[ M(t'/t) \]

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How flat is flat enough?

Parametrize band flatness:

\[ \frac{-\Delta J_T}{t} \]

\[ \frac{t_{dd}}{t} \]

\[ \Rightarrow \]

\[ M \]

\[ t'/t \]

\[ i_k = 0 \quad 6 \]

\[ 1 \quad 7 \]

\[ 2 \quad 8 \]

\[ (E - E_0)/t \]

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Impact of band flattness: $\nu = 1/3$

Very flat always good, interaction $\gtrsim$ band gap is OK

- $\nu = 1/3$ (band with $C = 1$) $\Rightarrow \bar{n} = 1/6$ (lattice)
- For NN interactions: No state competes with FCI
- Very flat bands make FCI easier
- Not so flat bands: stronger interaction still induces FCI

S. Kourtis et al., PRL 112, 126806 (2014)

Change filling: Competition with CDW

- $\bar{n} = 1/3$ ($\nu = 2/3$): CDW easy
- $\bar{n} = 1/6$ ($\nu = 1/3$): no easy CDW

- Nesting does not favor CDW for $t' > 0.2$
- Very flat bands: FCI
- Nesting: CDW
Where do FCIs differ from FQH states?

- **Flexibility:** Chern number, spin degree of freedom, …
- **No particle-hole symmetry** (see 1/3 vs. 2/3)
  
  A. G. Grushin, T. Neupert, C. Chamon, C. Mudry, PRB 86, 205125 (2012);
  A. M. Läuchli, Z. Liu, E. J. Bergholtz, R. Moessner, PRL 111, 126802 (2013);

- **Role of the lattice?**
  - Mostly a nuisance
  - Argued away after providing nontrivial bands
  - In fact, mostly only one Chern band is kept: band topology remains, band dispersion maybe, lattice is lost
  - Lattice was responsible for CDW
Coexistence of (Landau) charge and topological order

triangular lattice, $\bar{n} = 12/30$

FCI for $\nu = 4/5$?
Coexistence of (Landau) charge and topological order

triangular lattice, $\bar{n} = 12/30$

FCI for $\nu = 4/5$?

15 states instead of 5! $\sigma_{xy} = 2/5$
Signatures of $\nu = 2/5$ FCI and CDW

FCI with $\nu = 2/5$

- Spectral flow: Five states exchange places, $10\pi$ to get back
- (Three groups of such states)
- Hall conductivity $\sigma_{xy} = 2/5$ in each of the 15 states

CDW with $q = K$

- Charge-structure factor $N(q)$ peaked at $K$
- Peaks grow with $V$

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Charge order + fractional $\sigma_{xy}$

- CDW on $1/3$ of the sites
- remaining system: 4 subbands
- lowest band filled to $2/5$ $\Rightarrow$ FCI with $\nu = 2/5$
- Also found for other fillings
- Quite robust: not sensitive to $t_3$ (band dispersion)
Comments on Stability

- **Phase separation vs. “mixed phase”:**
  - ED for small systems: No PS
  - “Non-topological” analogue known (DMRG)
    - C. Hotta & N. Furukawa, PRB 74, 193107 (2006)
    - S. Nishimoto & C. Hotta, PRB 79, 195124 (2009)
  - Bosonic equivalent: supersolid
    - M. Boninsegni & N. Prokof’ev, PRL 95, 237204 (2005)

- **Topological order for given CDW**
  - large-V limit: prune Hilbert space, somewhat larger systems possible:
    - 14 fermions on $6 \times 6$ sites
    - 16 fermions on 90 sites (resp. 6 on 60)
Topological pinball liquid

- strong interaction: $C = \pm 1$ bands mixed
- Supported by frustrated lattice
- Lattice-specific features beyond FQH states
- Here: CDW + topological order

S. Kourtis & M. Daghofer, PRL 113, 216404 (2014)
Advertising break!!!!!

PhD and Postdoc position available

at Institute for Functional Matter and Quantum Technologies,
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ED-based approaches to topological states

■ **(Variational) Cluster-perturbation theory**: "combined ED and mean-field embedding"
  - Spinless fermions on honeycomb: charge fluctuations kill QAH state
  - Hubbard model on triangular lattice: quantum fluctuations prefer collinear spins (with topo. trivial bands)
■ **Kondo-lattice model**:
  - Electron-spin coupling can induce topological band character
  - Orbital degree of freedom can reduce band dispersion \( \Rightarrow \) interactions more important
■ **ED for FCIs**
■ **eigenenergies + fully interacting** \( \sigma_{xy} \)
■ **Beyond FQH physics**: “topological pinball liquid’, CDW + topological order (like supersolid, but with topo. order instead of superfluid)