Exact Diagonalization for topological phases driven by interactions

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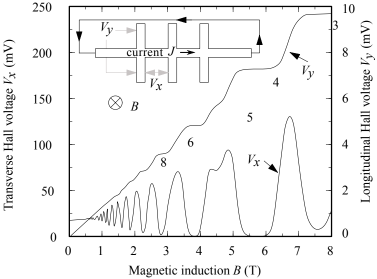
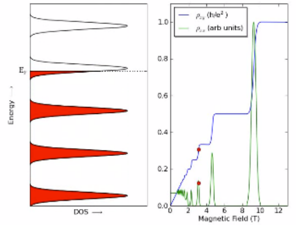
DFG

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)

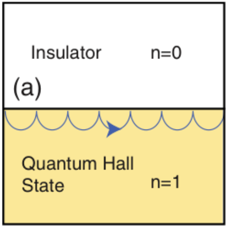
Integer Quantum Hall Effect





von Klitzing *et al.*, PRL **45**, 494 (1980)

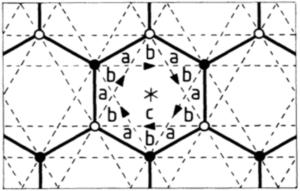
- transverse conductivity quantized
- Standard for electrical resistance
- is (first) Chern number
- implies edge states



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

Quantum Anomalous Hall States

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



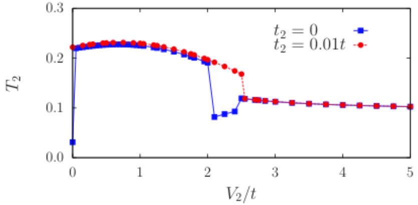
Complex hoppings instead of a magnetic field

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)

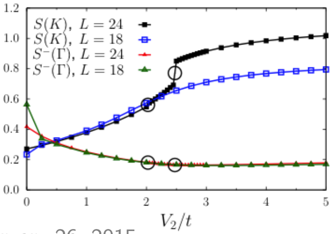
Spinless fermions on honeycomb

- 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

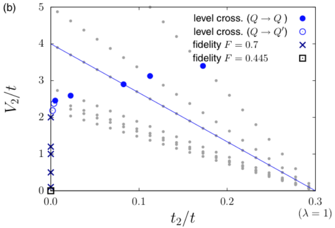


$$\frac{1}{L^2}\left\langle \Big| \sum_{\langle\langle i,j\rangle\rangle} (c_i^\dagger c_j - c_j^\dagger c_i) \Big|^2 \right\rangle$$

- . . . but stronger tendency to charge order.

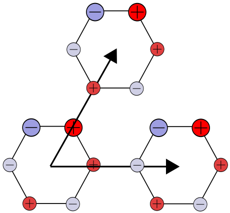


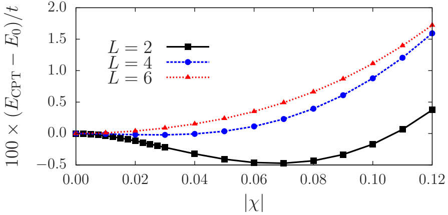
ED phase diagram:



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



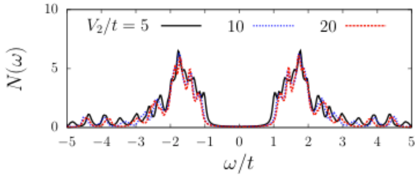


M. Daghofer & M. Hohenadler, PRB **89**, 035103 (2014); N. A. García-Martínez *et al.* PRB **88**, 245123 (2013); T. Duric *et al.*, arXiv:1401.5680

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

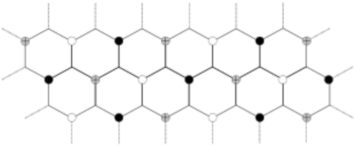
  A. G. Grushin *et al.*, PRB **87**, 085136 (2013)
- ED: No signature of charge imbalance
- Weird: One-particle gap given by t, not V_2 (or V_1)



Partial CDW related to 'pinball liquid'

- 'pinball liquid' known from triangular lattice: CDW + metal/superconductor C. Hotta & N. Furukawa, PRB **74**, 193107 (2006).
- 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)



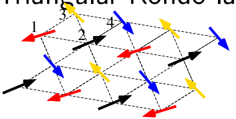
- Black sites account for $2/3$ of electrons, remaining can be distributed in any way on $+$ sites
- Weird properties, topological order?

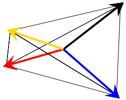
Another route: Non-coplanar spin patterns

- Spin has to realign itself from site to site:

$$t_{ij} = (\cos\frac{\theta_i}{2}\cos\frac{\theta_j}{2} + \sin\frac{\theta_i}{2}\sin\frac{\theta_j}{2}e^{-i(\phi_i-\phi_j)})t$$

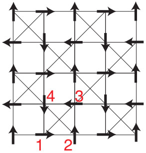
- Triangular Kondo-lattice model

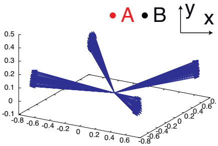




I. Martin and C. D. Batista, PRL **101**, 156402 (2008)

- Checkerboard Kondo-lattice model

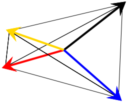




J. W. F. Venderbos, M. Daghofer, J. van den Brink, S. Kumar, PRL **109**, 166405 (2012)

Hubbard model

- Classical Kondo-lattice model = mean field for Hubbard
- Non-coplanar Ground state at van-Hove?



I. Martin & C. D. Batista, PRL **101**, 156402 (2008); R. Nandkishore *et al.*, PRL **108**, 227204 (2012); R. Nandkishore *et al.*, Nat. Phys. **8**, 158 (2012); G.-W. Chern & C. D. Batista, PRL **109**, 156801 (2012).

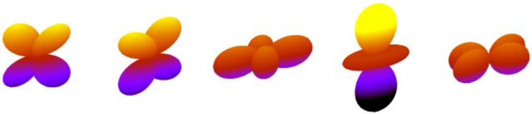
- Finite T: coplanar

  G.-W. Chern & C. D. Batista, PRL **109**, 156801 (2012)
- (also: $d + id$ SC at small U)
- Large U, Variational Cluster Approach: Quantum fluctuations prefer collinear order

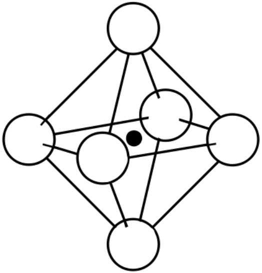
  A. Fischer & M. Daghofer, in preparation
- classical spin/mean field better justified in multi-orbital model

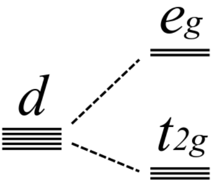
d orbitals in octahedral coordination

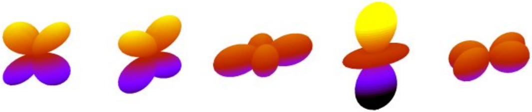
-



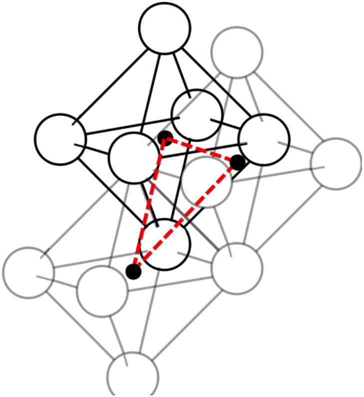
d orbitals in octahedral coordination

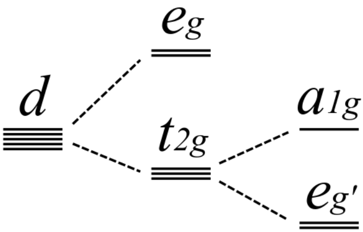


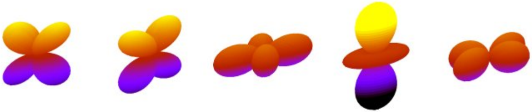




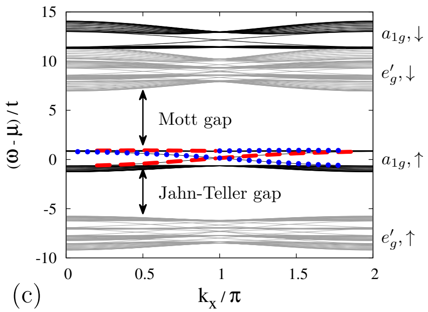
d orbitals in octahedral coordination







Mean-field bands in cylinder



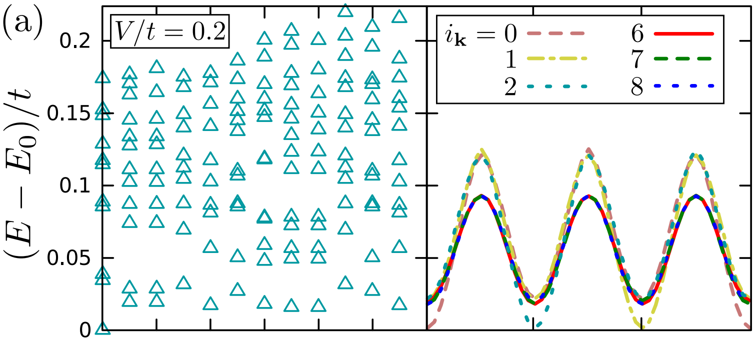
- Low-lying e'_g electrons: "localized" spin
- a_{1g} levels around μ: itinerant electrons

J. W. F. Venderbos, S. Kourtis, J. van den Brink, M. Daghofer, PRL **108**, 126405 (2012), S. Kourtis, J. W. F. Venderbos, M. Daghofer, PRB **86**, 235118 (2012)

- Similar situation to Kondo-lattice model

I. Martin and C. D. Batista, PRL **101**, 156402 (2008); Y. Akagi and Y. Motome, JPSJ **79**, 083711 (2010); Y. Kato *et al.*, PRL **105**, 266405 (2010)

Add inter-site Coulomb repulsion



Insert magnetic flux:

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

J. W. F. Venderbos, S. Kourtis, J. van den Brink, M. Daghofer, PRL **108**, 126405 (2012); S. Kourtis, J. W. F. Venderbos, M. Daghofer, PRB **86**, 235118 (2012)

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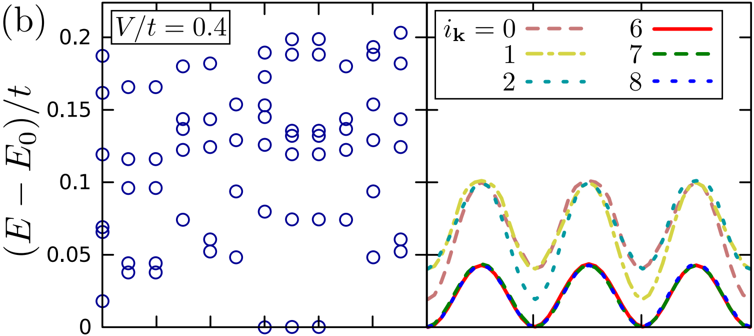

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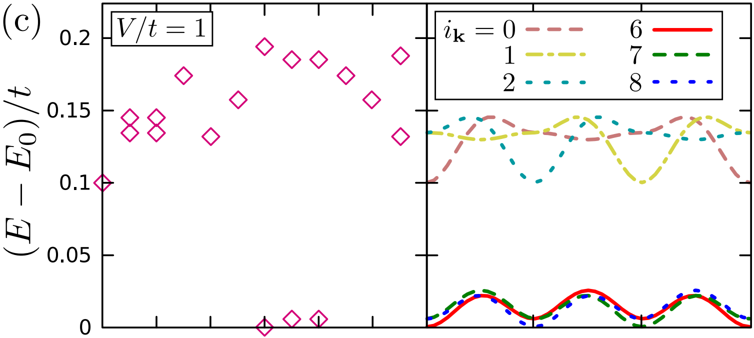

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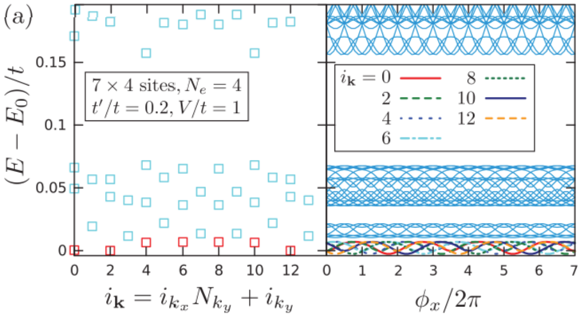
J. W. F. Venderbos, S. Kourtis, J. van den Brink, M. Daghofer, PRL **108**, 126405 (2012); S. Kourtis, J. W. F. Venderbos, M. Daghofer, PRB **86**, 235118 (2012)

Level Statistics for one added hole

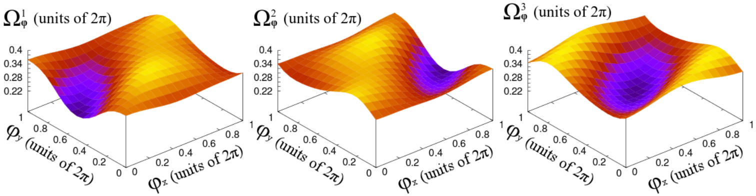


Add one hole to FQH/FCI state on torus: certain number of states expected below gap

B. A. Bernevig and N. Regnault, PRB 85, 075128 (2012); S. Kourtis, J. W. F. Venderbos, M. Daghofer, PRB **86**, 235118 (2012)

Hall Conductivity

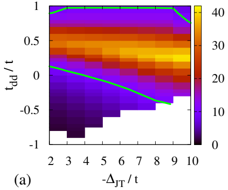
$$\Omega^n(\phi_x,\phi_y) = iL_xL_y \sum_{n'\neq n} \frac{\langle n|\frac{\partial H_{\text{eff}}(\phi_x,\phi_y)}{\partial \phi_x}|n'\rangle\langle n'|\frac{\partial H_{\text{eff}}(\phi_x,\phi_y)}{\partial \phi_y}|n\rangle}{(\epsilon_n-\epsilon_{n'})^2} - (x \leftrightarrow y)$$



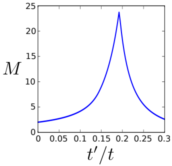
Similar for $\nu = 2/3,\ 1/5,\ 2/5,\ \ldots$ and other models.

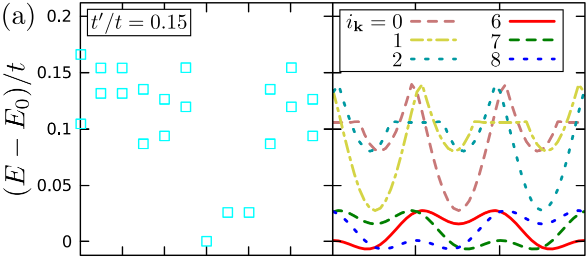
How flat is flat enough?

Parametrize band flatness:



$\Rightarrow$





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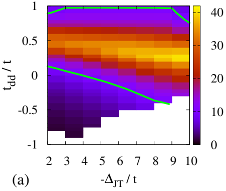

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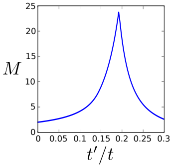

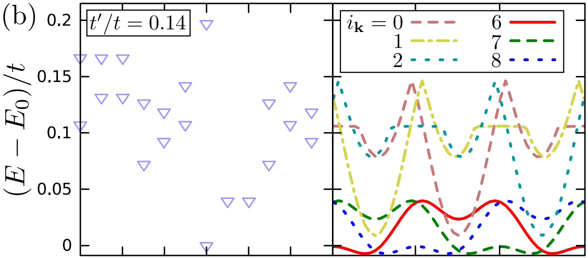

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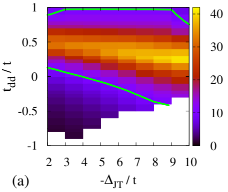

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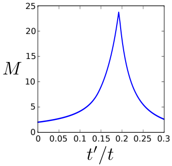
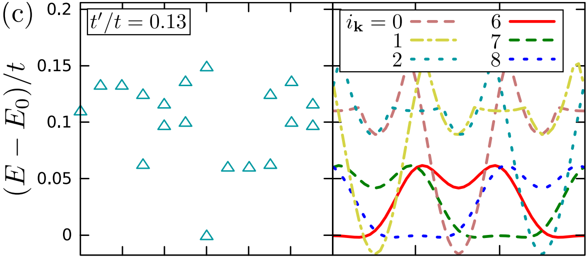
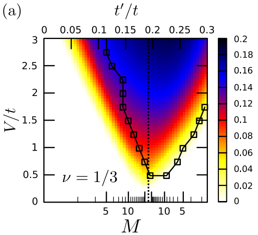




Impact of band flattness: $\nu = 1/3$



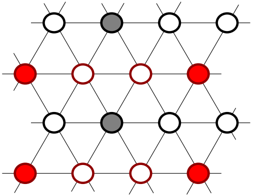
Very flat always good, interaction $\gtrsim$ band gap is OK

- $\nu = 1/3$ (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

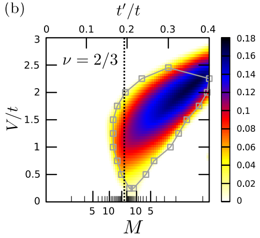
  S. Kourtis *et al.*, PRL **112**, 126806 (2014)

S. Kourtis, J. W. F. Venderbos, M. Daghofer, PRB **86**, 235118 (2012)

Change filling: Competition with CDW



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



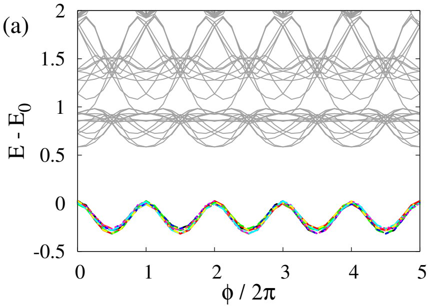
- Nesting does not favor CDW for $t' > 0.2$
- Very flat bands: FCI
- Nesting: CDW

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); S. Kourtis, J. W. F. Venderbos, M. Daghofer, PRB **86**, 235118 (2012)
- 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

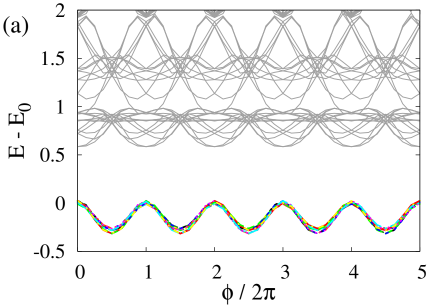
triangular lattice, $\bar{n} = 12/30$

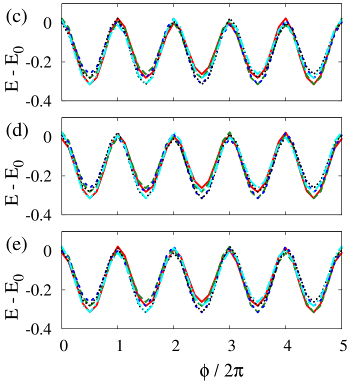


FCI for $\nu = 4/5$?

Coexistence of (Landau) charge and topological order

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



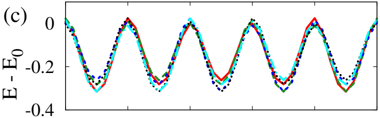


FCI for $\nu = 4/5$?

15 states instead of 5! $\sigma_{xy} = 2/5$

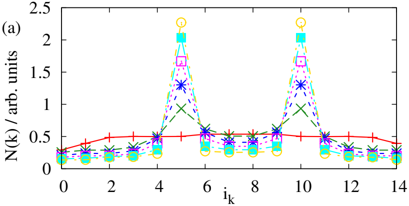
Signatures of $\nu = 2/5$ FCI and CDW

FCI with $\nu = 2/5$



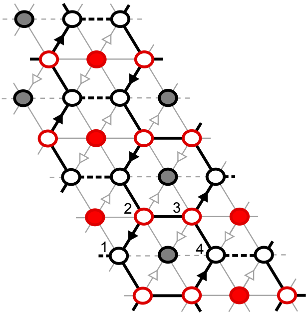
- Spectral flow: Five states exchange places, 10π to get back
- (Three groups of such states)
- Hall conductivity $\sigma_{xy} = 2/5$ in each of the 15 states

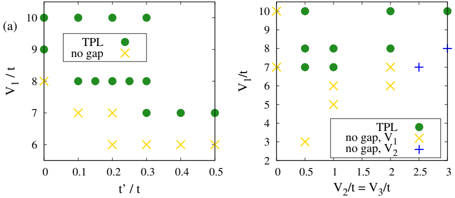
CDW with $\mathbf{q} = K$



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

Charge order + fractional σ_{xy}

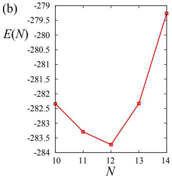




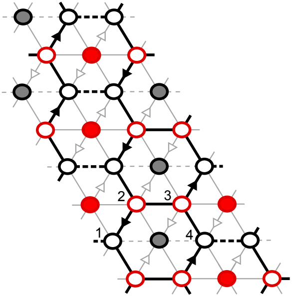
- CDW on $1/3$ of the sites
- remaining system: 4 subbands
- lowest band filled to $2/5 \Rightarrow$ FCI with $\nu = 2/5$
- Also found for other fillings
- Quite robust: not sensitive to t_3 (band dispersion)

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); S. Wessel & M. Troyer, PRL **95**, 127205 (2005).
- Topological order for given CDW
  - large-V limit: prune Hilbert space, somewhat larger systems possible:
    - 14 fermions on 6×6 sites
    - 16 fermions on 90 sites (resp. 6 on 60)



Topological pinball liquid



S. Kourtis & M. Daghofer, PRL **113**, 216404 (2014)

- strong interaction: $C = \pm 1$ bands mixed
- Supported by frustrated lattice
- Lattice-specific features beyond FQH states
- Analogous to supersolid: CDW + superfluid M. Boninsegni & N. Prokof'ev, PRL **95**, 237204 (2005); S. Wessel & M. Troyer, PRL **95**, 127205 (2005).
- Fermionic counterpart "pinball liquid": CDW + metal/superconductor C. Hotta & N. Furukawa, PRB **74**, 193107 (2006).
- Here: CDW + topological order

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FMQ

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 ⇒ interactions more important
- ED for FCIs
- eigenenergies + fully interacting σ_{xy}
- Beyond FQH physics: "topological pinball liquid", CDW + topological order (like supersolid, but with topo. order instead of superfluid)