Interaction-induced phases in the half-filled Bernevig-Hughes-Zhang model in one dimension

Federico Becca

Entanglement in Strongly Correlated Systems, February 2025

UNIVERSITÀ DEGLI STUDI DI TRIESTE

R. Favata, D. Piccioni, A. Parola, and FB, arXiv:2412.05975

1. Introduction

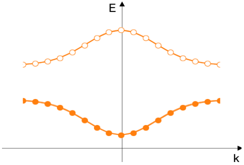
2. The interacting one-dimensional BHZ model
   - The intra-orbital Hubbard U and the nearest-neighbor V repulsions
   - The "atomic limit"
   - The strong-coupling expansion

3. The variational approach

4. Results
   - The $V = 0$
   - The spin-1 Haldane insulator
   - The unexpected gapless insulator
   - The $V > 0$ case
   - The fully gapped CDW
   - The CDW with gapless spin excitations

Topology in the band theory

- **A long time ago in a galaxy far, far away...**



Looking at the band filling:

- Metals
- Insulators

N. Ashcroft and N.D. Mermin, *Solid State Physics*

C. Kittel, *Introduction to Solid State Physics*

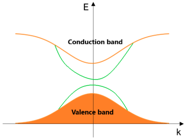
- **...More recently, a large variety of metals and insulators (Mos Eisley Cantina)**

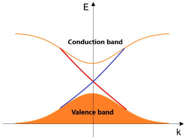
C.L. Kane and E.J. Mele, Phys. Rev. Lett. **95**, 146802 (2005)

B.A. Bernevig, T.L. Hughes, and S.-C. Zhang, Science **314**, 1757 (2006)

D.J. Thouless, M. Kohmoto, M.P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982)

F.D.M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988)

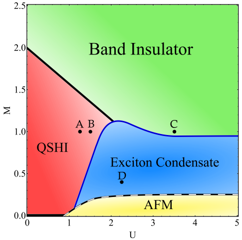


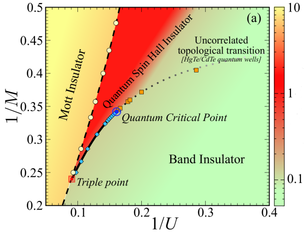


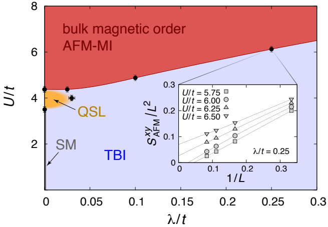
For non-interacting systems:

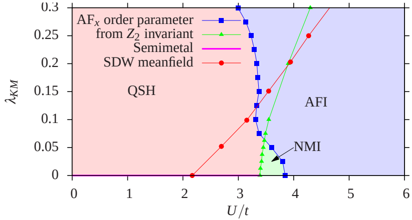
- Topological invariants
- Edge states

Topology and electron-electron interaction (no fractional Hall/Chern insulators)









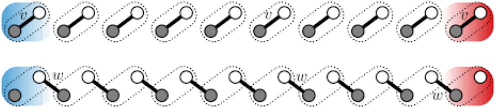
A. Amaricci, J.C. Budich, M. Capone, B. Trauzettel, and G. Sangiovanni, Phys. Rev. Lett. **114**, 185701 (2015)

A. Blason and M. Fabrizio, Phys. Rev. B **102**, 035146 (2020)

M. Hohenadler, T.C. Lang, and F.F. Assaad, Phys. Rev. Lett. **106**, 100403 (2011)

J.C. Budich, R. Thomale, G. Li, M. Laubach, and S.-C. Zhang, Phys. Rev. B 86, 201407 (2012)

- In 1D, the prototypical example is the Su-Schrieffer-Heeger (SSH) model



- The Hubbard-U interaction (spinful model) has been included by several works (even before the "topological era")

K. Penc and F. Mila, Phys. Rev. B **50**, 11429 (1994)

S. Nishimoto, M. Takahashi, and Y. Ohta, J. Phys. Soc. Jpn. **69**, 1594 (2000)

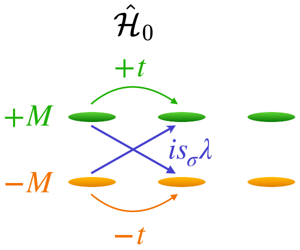
S.R. Manmana, A.M. Essin, R.M. Noack, and V. Gurarie, Phys. Rev. B **86**, 205119 (2012)

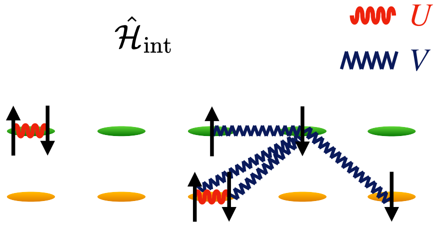
M. Yahyavi, L. Saleem, and B. Hetènyi, J. Phys.: Condens. Matter **30**, 445602 (2018)

...and many more...

- The SSH model is a caricature to describe topological effects

(topological and trivial phases are interchanged by a shift of the unit cell)





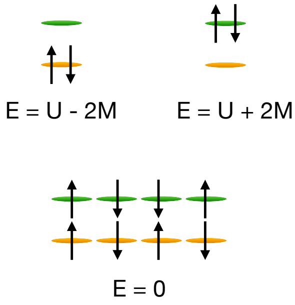
$$\hat{\mathcal{H}}_0 = \sum_{j=1}^{L} \sum_{\eta,\sigma} \left[M\,\eta\,\hat{n}_{j,\eta,\sigma} + \left(t\,\eta\,\hat{c}^\dagger_{j+1,\eta,\sigma}\hat{c}_{j,\eta,\sigma} + i s_\sigma \lambda\,\hat{c}^\dagger_{j+1,\eta,\sigma}\hat{c}_{j,-\eta,\sigma} + \text{h.c.} \right) \right]$$

$$\hat{\mathcal{H}}_{\rm int} = U \sum_{j=1}^{L} \sum_{\eta} \hat{n}_{j,\eta,\uparrow}\hat{n}_{j,\eta,\downarrow} + V \sum_{j=1}^{L} \hat{n}_j \hat{n}_{j+1}$$

Half filling: two electrons per site (in average)

S. Barbarino, G. Sangiovanni, and J.C. Budich, Phys. Rev. B **99**, 075158 (2019)

- **Six states with two electrons on a site**



- **For $U > 2M$, the ground state is 4-fold degenerate**
- **With the inter-orbital interaction $U' = U$, the ground state is unique**
- **No Hund's coupling, for simplicity**

- **Time reversal**

$$\hat{c}^{\dagger}_{j,\eta,\sigma} \Longrightarrow s_{\sigma} \hat{c}^{\dagger}_{j,\eta,\bar{\sigma}}$$

- **Particle-hole transformation with orbital flip**

$$\hat{c}^{\dagger}_{j,\eta,\sigma} \Longrightarrow \hat{c}_{j,-\eta,\sigma}$$

DIII class of the 10-fold way
[Z_2 in 1D]

- **Spin-flip with a sign depending on the orbital**

$$\hat{c}^{\dagger}_{j,\eta,\sigma} \Longrightarrow \eta \hat{c}^{\dagger}_{j,\eta,\bar{\sigma}}$$

- $U(1)$ **spin rotations**

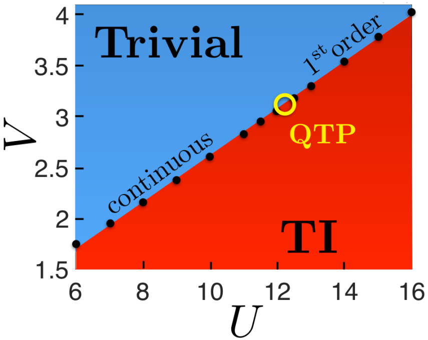
$$\hat{c}^{\dagger}_{j,\eta,\sigma} \Longrightarrow e^{is_{\sigma}\theta} \hat{c}^{\dagger}_{j,\eta,\sigma}$$

- **Translation and inversion with a sign depending on the orbital**

$$\hat{c}^{\dagger}_{j,\eta,\sigma} \Longrightarrow \hat{c}^{\dagger}_{j+1,\eta,\sigma}$$
$$\hat{c}^{\dagger}_{j,\eta,\sigma} \Longrightarrow \eta \hat{c}^{\dagger}_{L+2-j,\eta,\sigma}$$

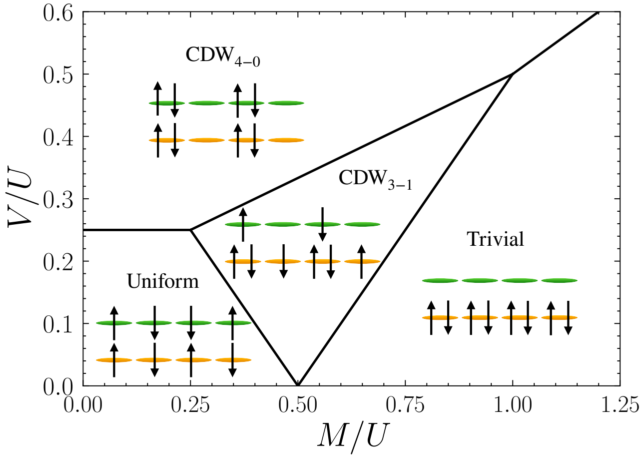
DMRG ($L = 36$ OBC) calculations for $M = 0$

- One topological phase
- One "Trivial" (CDW) phase



S. Barbarino, G. Sangiovanni, and J.C. Budich, Phys. Rev. B **99**, 075158 (2019)

- $t = \lambda = 0$


CDW$_{4-0}$
CDW$_{3-1}$
Uniform
Trivial
V/U
M/U
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.00
0.25
0.50
0.75
1.00
1.25

$$\hat{S}^{\alpha}_{j,\eta} = \frac{1}{2} \sum_{\sigma,\sigma'} \hat{c}^{\dagger}_{j,\eta,\sigma} \tau^{\alpha}_{\sigma,\sigma'} \hat{c}_{j,\eta,\sigma'} \qquad \hat{\mathbf{S}}_j = \hat{\mathbf{S}}_{j,+} + \hat{\mathbf{S}}_{j,-}$$

- The CDW_{3-1} phase has a 2×2^L degeneracy

$$\mathcal{H}_{CDW_{3-1}} = J_{3-1} \sum_{j=1}^{L} \left[\hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_{j+1} - \frac{1}{4} \right]$$

spin-1/2 Heisenberg model (gapless)

- The "Uniform" phase has a 2^{2L} spin degeneracy

$$\mathcal{H}_U = J \sum_{j=1}^{L} \sum_{\eta} \left[\hat{\mathbf{S}}_{j,\eta} \cdot \hat{\mathbf{S}}_{j+1,\eta} - \frac{1}{4} \right] + J' \sum_{j=1}^{L} \sum_{\eta} \left[\hat{\mathbf{S}}_{j,\eta} \cdot \hat{\mathbf{S}}_{j+1,-\eta} - \frac{1}{4} \right]$$

spin-1 Heisenberg model (gapped)

S.R. White, Phys. Rev. B **53**, 52 (1996)

- **For the CDW_{3-1} Heisenberg model**

$$J_{3-1} = \frac{2\lambda^2}{U - 2M + 3V} + \frac{2\lambda^2}{U + 2M - 5V}$$

- **For the "Uniform" Heisenberg model**

$$\begin{aligned} J &= \frac{4t^2}{U - V} \\ J' &= \frac{2\lambda^2}{U - V - 2M} + \frac{2\lambda^2}{U - V + 2M} \end{aligned}$$

White's arguments are rigorous for $\lambda = t\sqrt{1 - \frac{4M^2}{(U-V)^2}}$

S.R. White, Phys. Rev. B **53**, 52 (1996)

$$|\Psi_{\rm var}\rangle = \mathcal{J}_{\rm s}\mathcal{J}_{\rm d}\mathcal{P}_{\{S^z=0\}}|\Phi_0\rangle$$

- The Slater determinant is constucted from an auxiliary (quadratic) Hamiltonian

$$\hat{\mathcal{H}}_{\rm aux} = \hat{\mathcal{H}}_{\rm band} + \hat{\mathcal{H}}_{\rm CDW} + \hat{\mathcal{H}}_{\rm AF}$$

$$\begin{aligned}
\hat{\mathcal{H}}_{\rm band} &= \sum_{j=1}^{L}\sum_{\eta,\sigma}\Big[\tilde{M}\,\eta\,\hat{n}_{j,\eta,\sigma} + \tilde{\lambda}_{0,\sigma}\hat{c}^{\dagger}_{j,\eta,\sigma}\hat{c}_{j,-\eta,\sigma} \\
&+ \sum_{k=1,2}(\tilde{t}_k\,\eta\hat{c}^{\dagger}_{j+k,\eta,\sigma}\hat{c}_{j,\eta,\sigma} + \text{h.c.}) + (\tilde{\lambda}_{k,\eta,\sigma}\,\hat{c}^{\dagger}_{j+k,\eta,\sigma}\hat{c}_{j,-\eta,\sigma} + \text{h.c.})\Big] \\
\hat{\mathcal{H}}_{\rm CDW} &= \Delta\sum_{j=1}^{L}(-1)^j\,\hat{n}_j \qquad (1) \\
\hat{\mathcal{H}}_{\rm AF} &= h\sum_{j=1}^{L}(-1)^j\sum_{\eta}\eta(\hat{c}^{\dagger}_{j,\eta,\uparrow}\hat{c}_{j,\eta,\downarrow} + \text{h.c.})
\end{aligned}$$

- A density-density term

$$\mathcal{J}_{\rm d} = \exp\left(\frac{1}{2}\sum_{i,j}\sum_{\alpha,\beta} v_{i,j}^{\alpha,\beta}\,\hat{n}_{i,\alpha}\hat{n}_{j,\beta}\right)$$

- A spin-spin term

$$\mathcal{J}_{\rm s} = \exp\left(\frac{1}{2}\sum_{i,j}\sum_{\alpha,\beta} u_{i,j}^{\alpha,\beta}\,\hat{S}^z_{i,\alpha}\hat{S}^z_{j,\beta}\right)$$

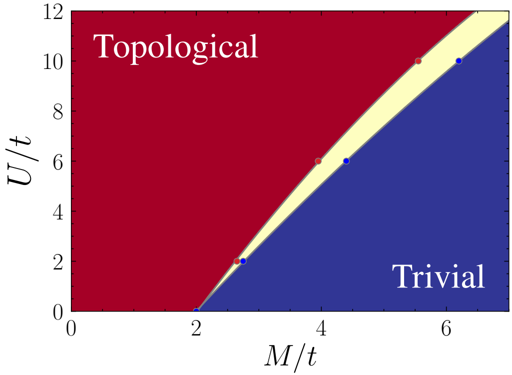
$u_{i,j}^{\alpha,\beta}$ and $v_{i,j}^{\alpha,\beta}$ are variational parameters depending on $|i-j|$

$u_{i,j}^{1,2} = u_{i,j}^{2,1}$ and $v_{i,j}^{1,2} = v_{i,j}^{2,1}$

$u_{i,j}^{1,1} = u_{i,j}^{2,2}$ and $v_{i,j}^{1,1} = v_{i,j}^{2,2}$

- Projection onto the subspace with $S^z_{\rm tot} = 0$

The phase diagram for $V = 0$ (with $\lambda = t$)

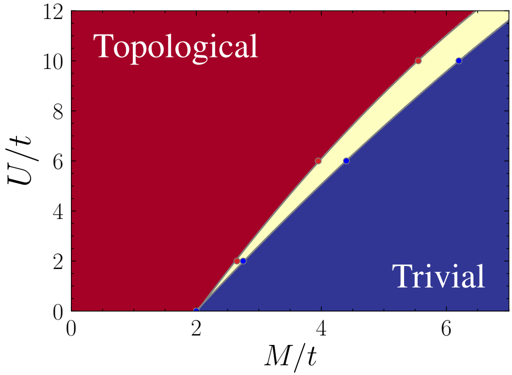


- No transition from the topological phase when increasing U

  The spin-1 Haldane state is connected to the non-interacting topological state

- An intermediate phase intrudes between topological and trivial phases

  This is an insulator with gapless spin excitation



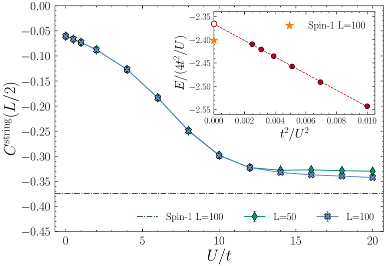
- In the topological region: $h > 0$

The spin-spin Jastrow factor prevents the instauration of a true magnetic order (no TR symmetry breaking because of $\mathcal{P}_{\{S^z=0\}}$)

D. Piccioni, C. Apostoli, FB, G. Mazzola, A. Parola, S. Sorella, and G.E. Santoro, Phys. Rev. B **108**, 104417 (2023)

- In the intermediate phase: $\tilde{\lambda}_{0,\sigma} = is_\sigma \lambda_0$

It breaks both η-PH and I+ηsign symmetries

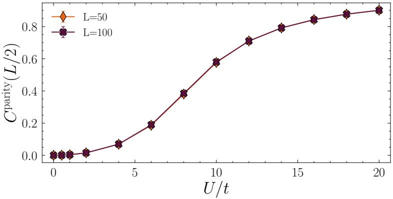


$$C^{\rm string}(r) = \frac{1}{L}\sum_{j=1}^{L} \langle \hat{S}^z_j \exp\left\{ i\pi \sum_{l=j+1}^{j+r-1} \hat{S}^z_l \right\} \hat{S}^z_{j+r} \rangle$$

M. den Nijs and K. Rommelse, Phys. Rev. B **40**, 4709 (1989)

U=0: Finite (trivial and topological)

F. Anfuso and A. Rosch, Phys. Rev. B **75**, 144420 (2007)

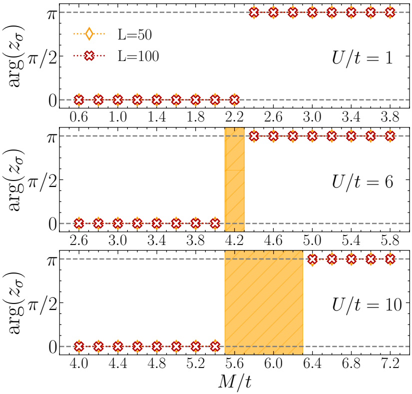


$$C^{\rm parity}(r) = \frac{1}{L}\sum_{j=1}^{L} \langle \exp\left\{ i\pi \sum_{l=j+1}^{j+r} (\hat{n}_l - 2) \right\} \rangle$$

A. Montorsi and M. Roncaglia, Phys. Rev. Lett. **109**, 236404 (2012)

L. Barbiero, A. Montorsi, and M. Roncaglia, Phys. Rev. B **88**, 035109 (2013)

U=0: Finite (trivial) and zero (topological)



$$z_\sigma = \langle \exp \left\{ i \frac{2\pi}{L} \sum_{j=1}^{L} j \hat{n}_{j,\sigma} \right\} \rangle$$

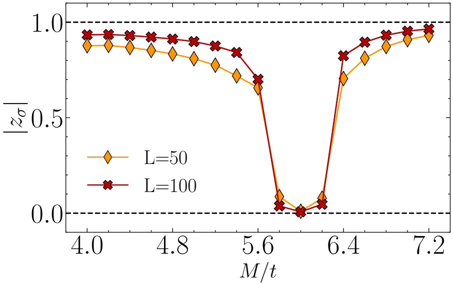
In the non-interacting limit:

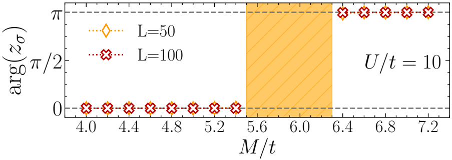
$$z_\sigma = (-1)^{N-1} \exp \left\{ \int_0^{2\pi} dq \langle \partial_q u_{q,\sigma} | u_{q,\sigma} \rangle \right\}$$

- **A real value of z_σ is guaranteed by either the η-PH or the I+ηsign symmetry**
- **For $L \to \infty$, $|z_\sigma| = 1$ for a fully gapped insulator with fixed S^z_{tot}**

R. Resta and S. Sorella, Phys. Rev. Lett. **82**, 370 (1999)

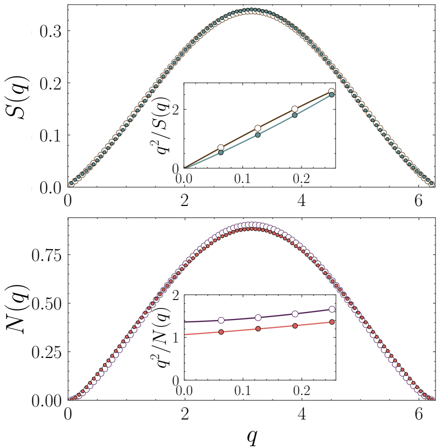
I. Gilardoni, FB, A. Marrazzo, and A. Parola, Phys. Rev. B **106**, L161106 (2022) $\Longrightarrow$ **Many-body marker for Z_2 topological insulators in 2D**





- **A real value of z_σ is guaranteed by either the η-PH or the I+ηsign symmetry**

$\Longrightarrow$ The intermediate phase breaks η-PH and I+ηsign symmetries



$U = 10$

$M/t = 5.9$

DMRG empty points

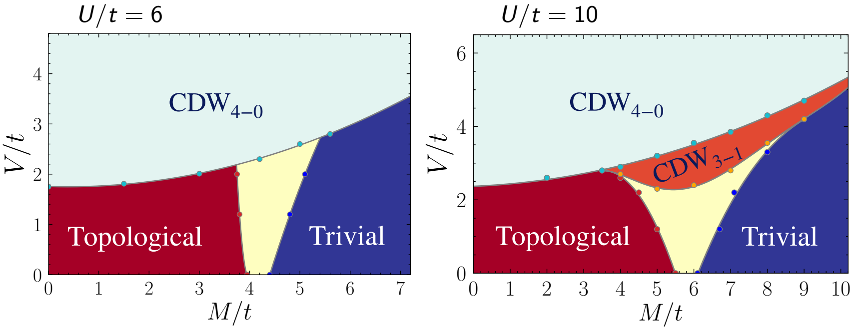
$$N(q) = \frac{1}{L} \sum_{j=1}^{L} e^{iqr} \langle \hat{n}_j \hat{n}_{j+r} \rangle$$

$$S(q) = \frac{1}{L} \sum_{j=1}^{L} e^{iqr} \langle \hat{S}^z_j \hat{S}^z_{j+r} \rangle$$

- $S(q) \approx q \implies$ gapless spin excitations
- $S(q) \approx q^2 \implies$ gapped spin excitations

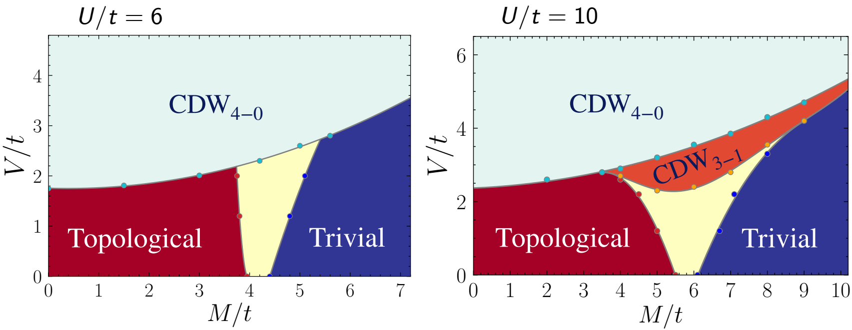
(similar for $N(q)$ and density excitations)

R.P. Feynman and M. Cohen, Phys. Rev. **102**, 1189 (1956)



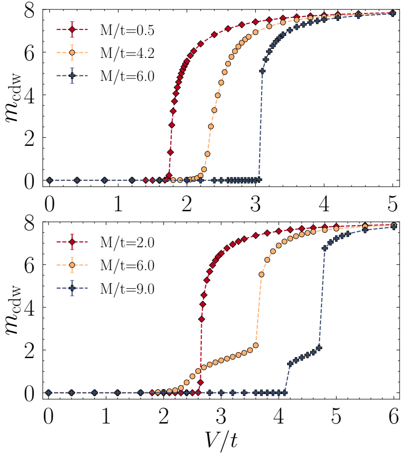
- A fully gapped CDW (CDW_{4-0}) for large V
- A CDW with gapless spin excitations (CDW_{3-1}) for intermediate V

The phase diagram for $V > 0$ (with $\lambda = t$)



- In the CDW$_{4-0}$ phase: $\Delta > 0$
- In the CDW$_{3-1}$ phase: $\Delta > 0$ and $h > 0$

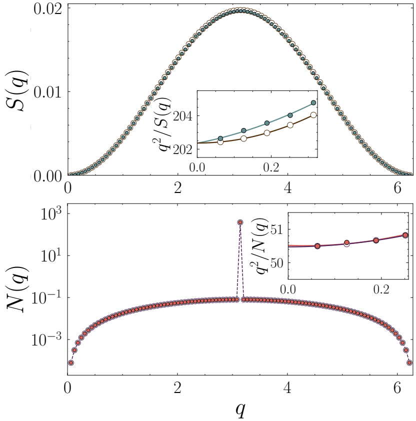
The spin-spin Jastrow factor prevents the instauration of a true magnetic order (no TR symmetry breaking because of $\mathcal{P}_{\{S^z=0\}}$)



$U/t = 6$

$U/t = 10$

$$m_{\rm cdw} = \lim_{L\to\infty} |\tilde{N}(L/2) - \tilde{N}(L/2-1)| \qquad \tilde{N}(r) = \frac{1}{L}\sum_{j=1}^{L} \langle \hat{n}_j \hat{n}_{j+r} \rangle$$



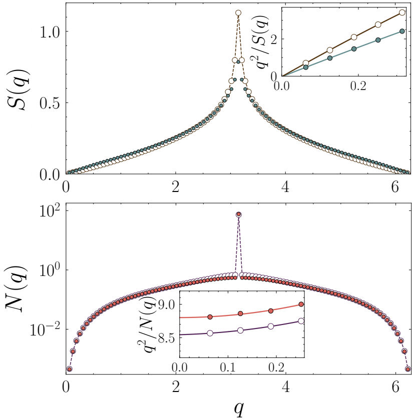
$V/t = 5$

$U/t = 10$

$M/t = 6$

DMRG empty points

- $S(q)$ **without singularities** $\Longrightarrow$ **the spin sector is fully gapped**
- $N(q) \approx q^2$ **and** $N(\pi) \propto L \Longrightarrow$ **CDW order**



$V/t = 3$

$U/t = 10$

$M/t = 6$

DMRG empty points

- $S(q) \approx q$ **for small** q**'s and** $S(\pi) \propto \ln(L) \Longrightarrow$ **gapless spin-1/2 model**
- $N(q) \approx q^2$ **and** $N(\pi) \propto L \Longrightarrow$ **CDW order**

- **The 1D BHZ model has a rich phase diagram with several phases**

- **The spin-1 Haldane state is connected to the non-interacting topological state**

- **Is the intermediate phase also obtained within a perturbative approach?**

  Either weak- or strong-coupling limits

  Is it an excitonic insulator?

A. Blason and M. Fabrizio, Phys. Rev. B **102**, 035146 (2020)

I. Pasqua, A. Blason, and M. Fabrizio, arXiv:2407.08794

- **The Jastrow-Slater wave function describes very well the phase diagram**

- **Next step: 2D BHZ model**

  Role of the Hund (Ising or Heisenberg) coupling

  Antiferromagnetic order and excitonic insulator?

A. Amaricci, J.C. Budich, M. Capone, B. Trauzettel, and G. Sangiovanni, Phys. Rev. Lett. **114**, 185701 (2015)