SSH and HH Models: Two Simple Topological Insulators

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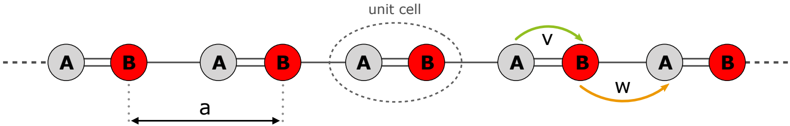
4 Dicember 2019

SISSA

Section 1

Su-Schrieffer-Heeger Model (and extensions)

SSH model



Nearest-neighbours (N.N.) interaction:

$$H = \sum_j \left(v\, c^\dagger_{\mathrm{A},j} c_{\mathrm{B},j} + w\, c^\dagger_{\mathrm{B},j} c_{\mathrm{A},j+1} + \mathrm{h.c.} \right) \qquad N: \text{ number of cells}$$

Chiral symmetry ($\Gamma = P_\mathrm{A} - P_\mathrm{B}$) anticommutes with the Hamiltonian thus ensuring *particle-hole* symmetry on the energy spectrum

SSH model $\rightarrow$ PBCs Reminder

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By using Fourier transform:

$$\mathbb{H}(k) = \mathbf{d}(k) \cdot \boldsymbol{\sigma}, \quad \boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \quad \Rightarrow \quad \varepsilon(k) = |\mathbf{d}(k)|$$

$$\mathbf{d}(k) = (v + w\cos(ka),\ -w\sin(ka),\ 0)$$

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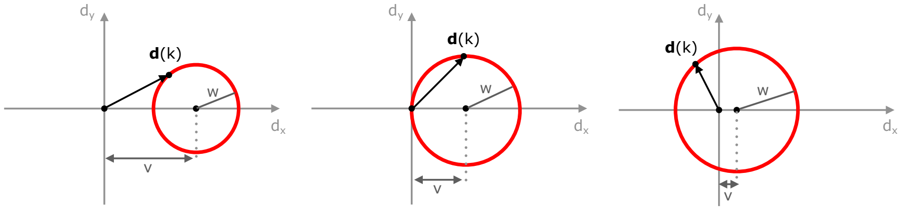
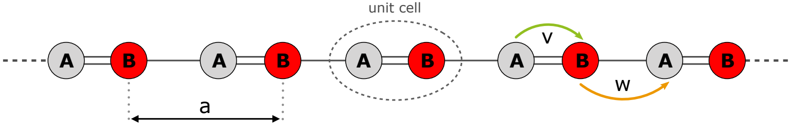


$$\varepsilon(k) = |\mathbf{d}(k)| \quad \Longrightarrow \quad \text{Gap closing at } \mathbf{d}(k) = 0$$

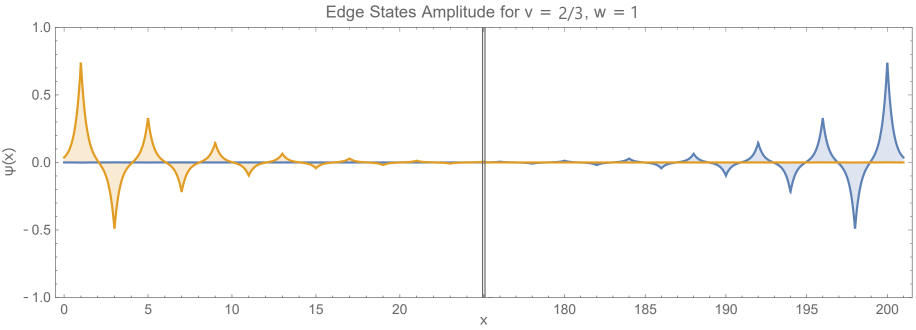
SSH Model $\rightarrow$ Open Boundary Conditions (OBCs)



$$\mathbb{H} = \begin{pmatrix} 0 & v & & & & & & \\ v & 0 & w & & & & & \\ & w & 0 & v & & & & \\ & & v & 0 & w & & & \\ & & & w & 0 & v & & \\ & & & & \ddots & \ddots & \ddots & \\ & & & & & w & 0 & v \\ & & & & & & v & 0 \end{pmatrix}$$

Edge states ($v < w$, $\varepsilon \sim 0$)

- Exponentially localized at the edges ($\xi^{-1} = -\log(v/w)$)
- Exponentially vanishing energy split ($\Delta E \approx e^{-N/\xi}$)
- Edge charge must not change varying the length of the chain



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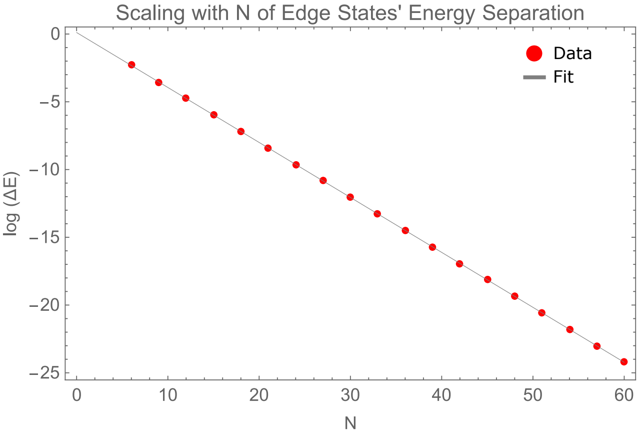

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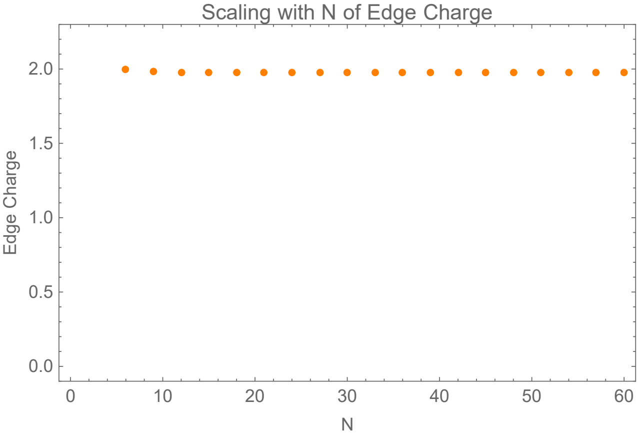
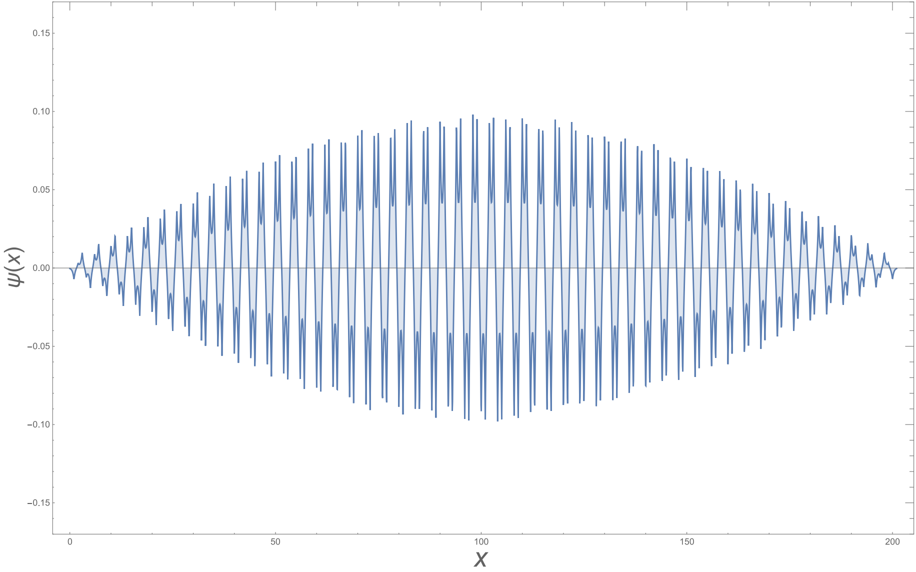


Typical bulk state: very different!



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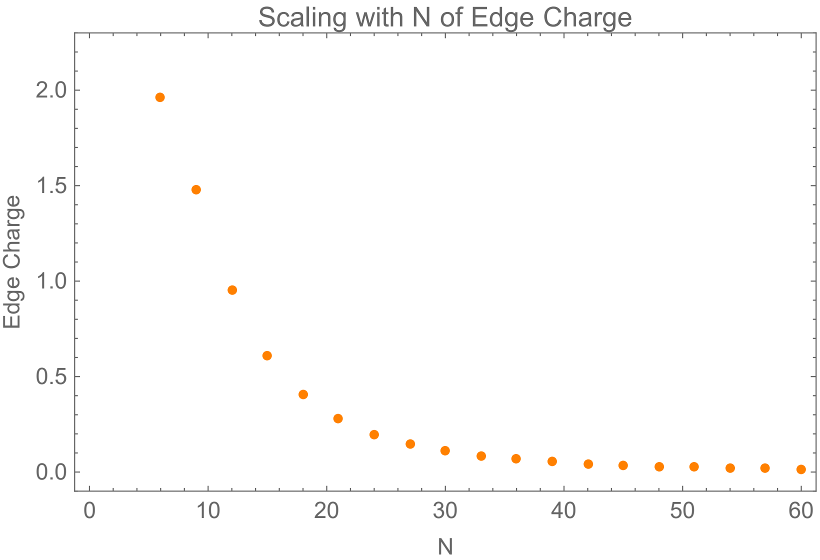
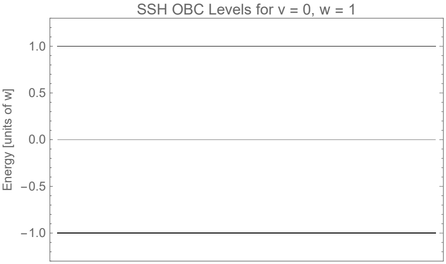
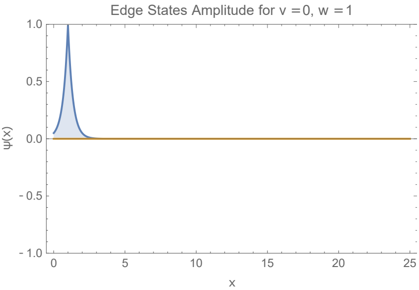


Spanning $v/w \in [0, 2]$





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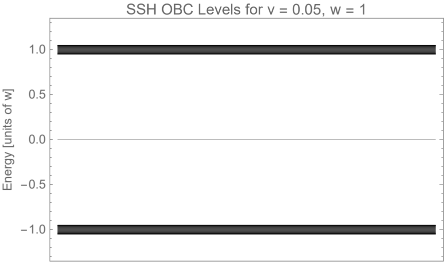

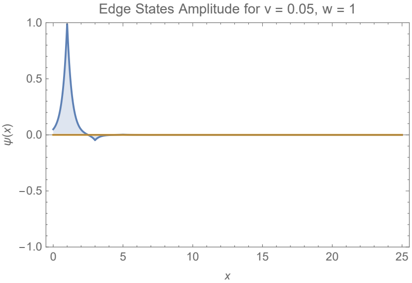

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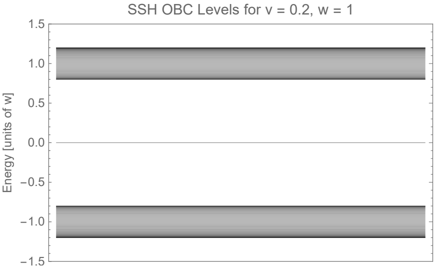

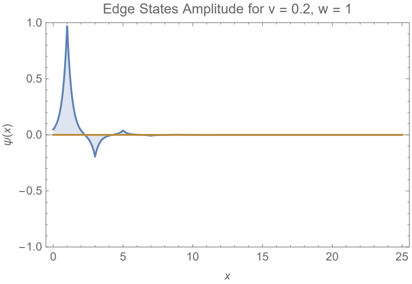

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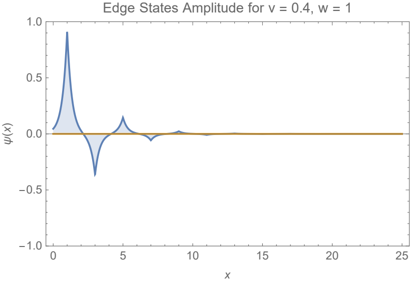

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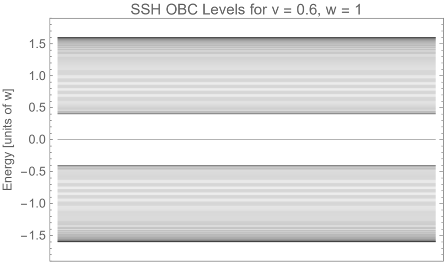

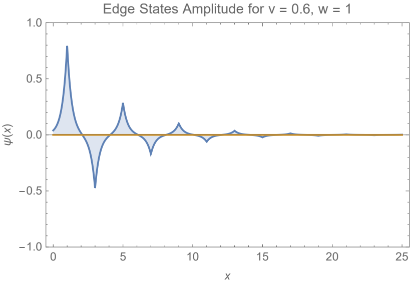

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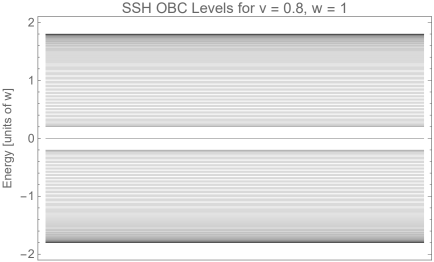
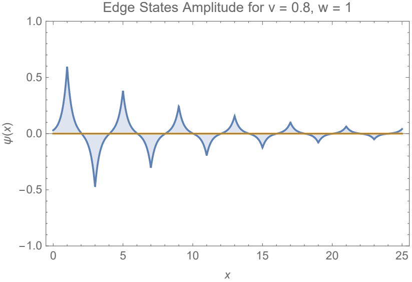
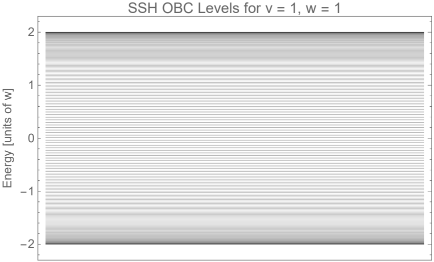
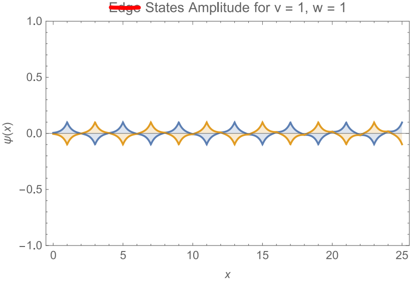




Spanning $v/w \in [0,2] \to$ Closed Gap! Edge States are lost





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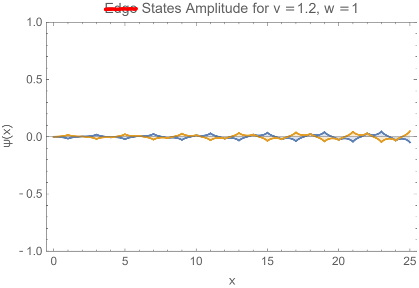
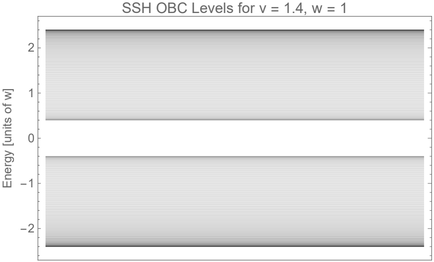
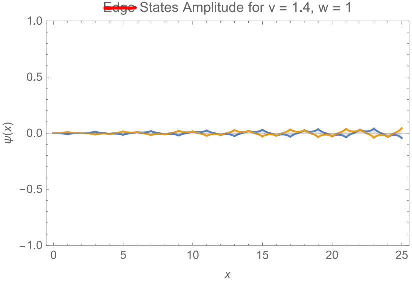
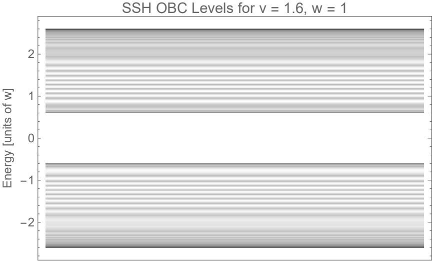


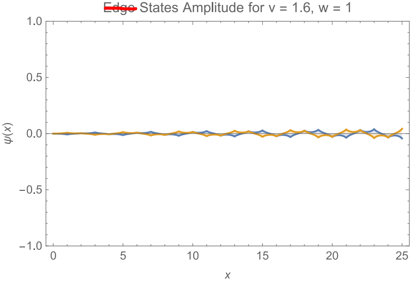
Spanning $v/w \in [0,2] \rightarrow$ Edge States are lost





Spanning $v/w \in [0, 2] \to$ Edge States are lost





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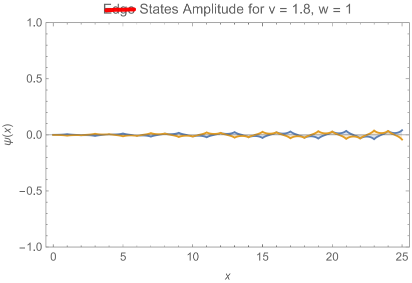

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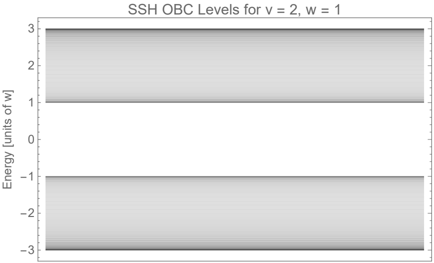
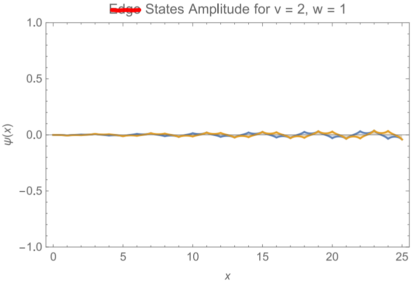




Disorder on Nearest Neighbors

$$\mathbb{H}_R = \begin{pmatrix} 0 & v + r_1 & & & & & \\ v + r_1 & 0 & w + r_1' & & & & \\ & w + r_1' & 0 & v + r_2 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & w + r_{n-1}' & 0 & v + r_n \\ & & & & v + r_n & 0 \end{pmatrix}$$

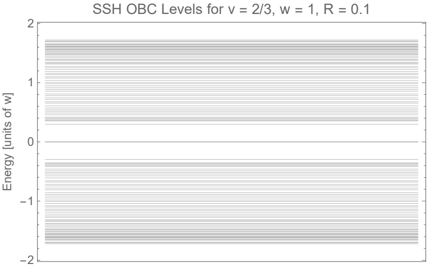
$\{r_i, r_i'\}$ are uniform distributed in $[-R, +R]$

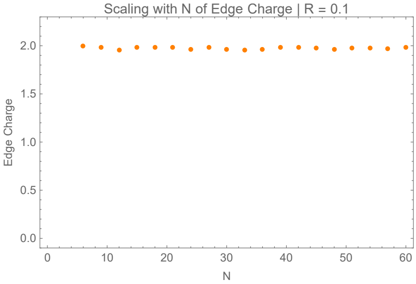
Chiral symmetry is still preserved

The gap vanishes (typically) at $R \approx 2(w - v)$

Edge states are observed also for higher R-values (maybe not topological)

Spanning $R \in [0, 2w]$





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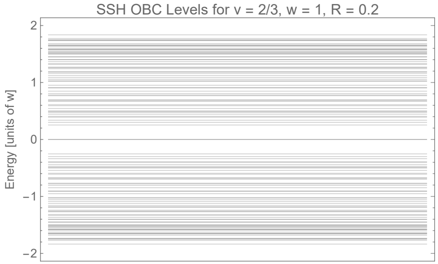
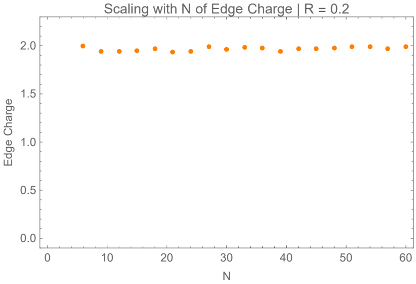
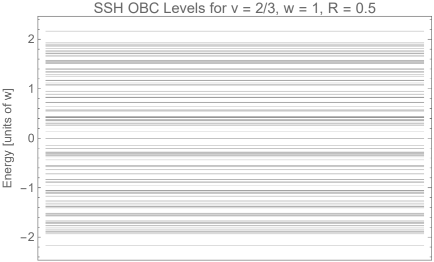
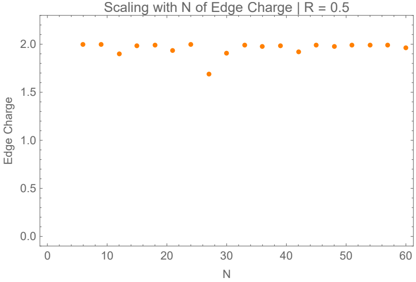


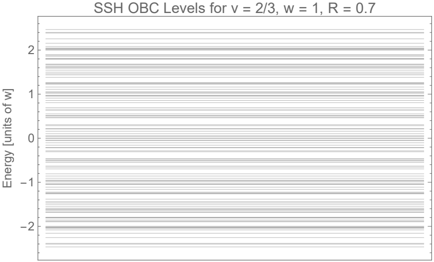


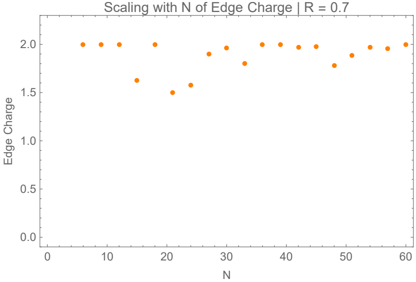
Spanning $R \in [0, 2w]$



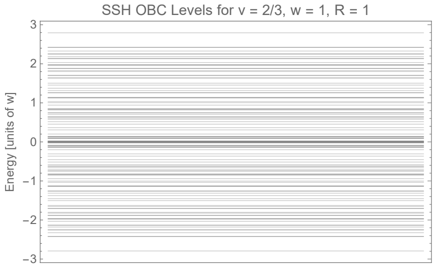


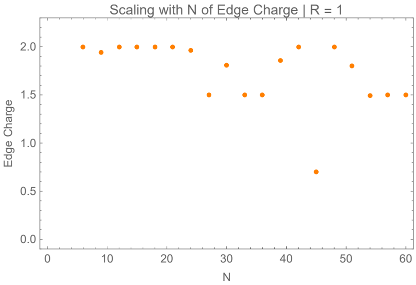
Spanning $R \in [0, 2w] \to$ Gap closes but still edge-like!



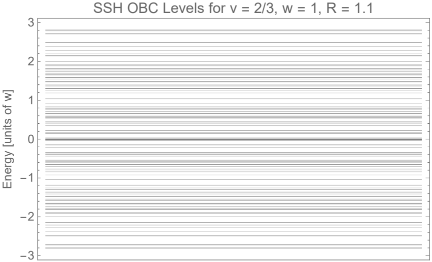


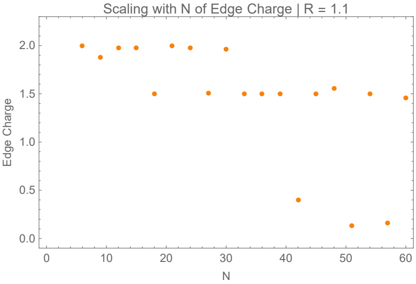
Spanning $R \in [0, 2w] \rightarrow$ Gap closes. Is this still edge-like?





Spanning $R \in [0, 2w] \rightarrow$ Edge character definitely destroyed.





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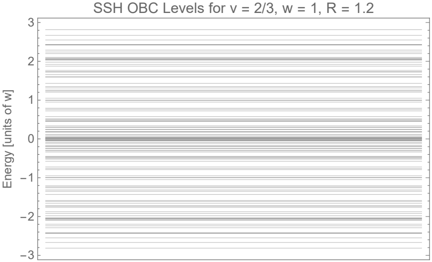
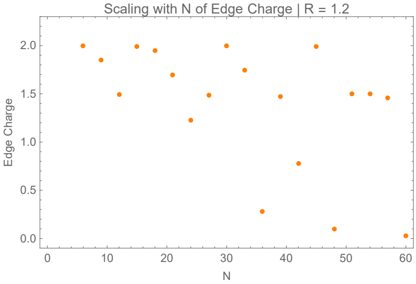
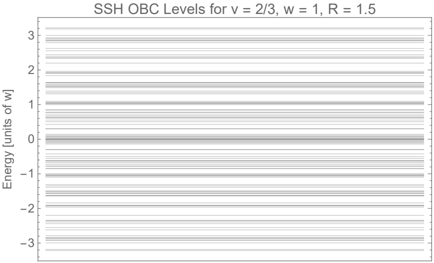
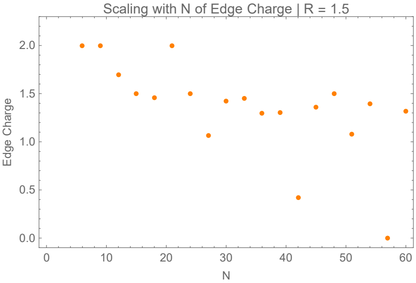




Spanning $R \in [0, 2w] \to$ Edge character definitely destroyed.





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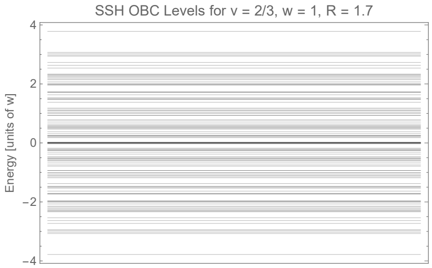
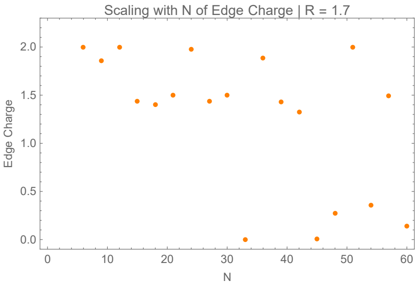
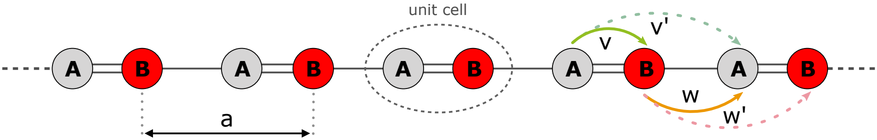




Next-N.N. hoppings



$$\mathbb{H}_{\text{N.N.N.}} = \begin{pmatrix} 0 & v & v' & & & & & \\ v & 0 & w & w' & & & & \\ v' & w & 0 & v & v' & & & \\ & w' & v & 0 & w & w' & & \\ & & v' & w & 0 & v & v' & \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}$$

Next-N.N. hoppings

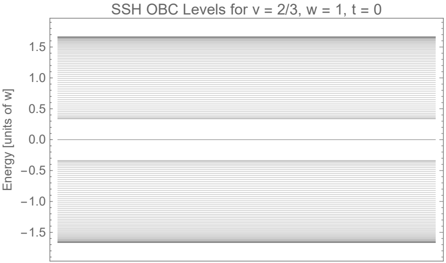
Let's put them all equal and focus on the topological phase:

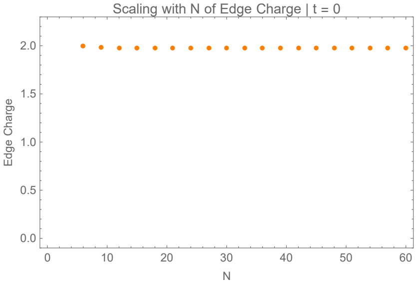
$$v' = w' =: t < v < w$$

$$\Downarrow$$

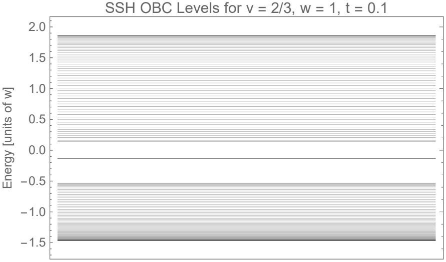
$$\mathbb{H}_{\text{N.N.N.}} = \begin{pmatrix} 0 & v & t & & & & \\ v & 0 & w & t & & & \\ t & w & 0 & v & t & & \\ & t & v & 0 & w & t & \\ & & t & w & 0 & v & t \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}$$

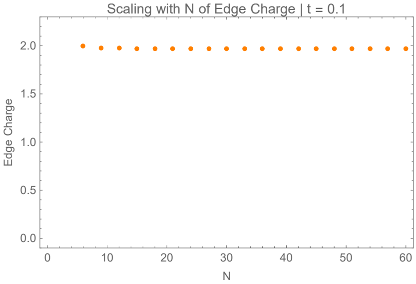
Spanning $t \in [0, w]$



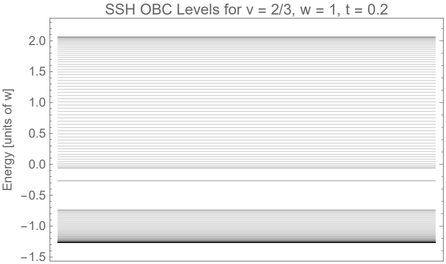


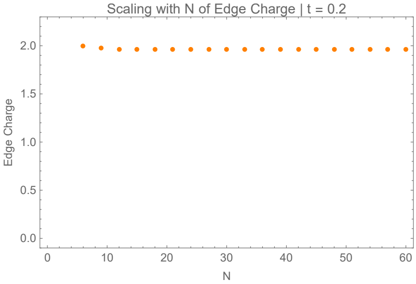
Spanning $t \in [0, w] \to$ Breaking of Chiral Symmetry!





Spanning $t \in [0, w]$





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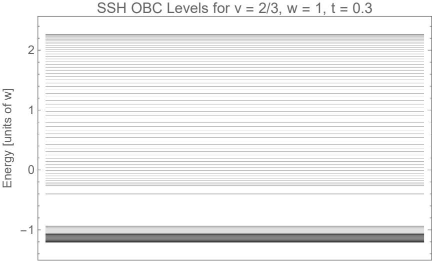
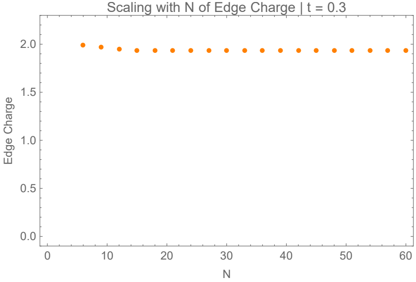
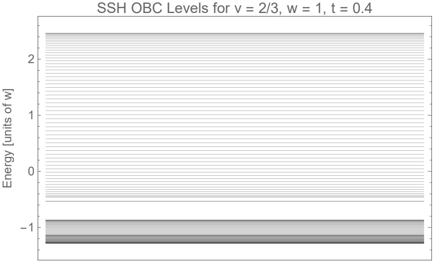
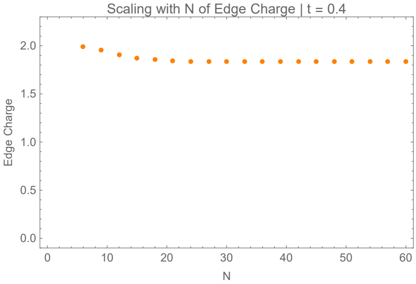




Spanning $t \in [0, w] \rightarrow$ Convergence starts to slow down...





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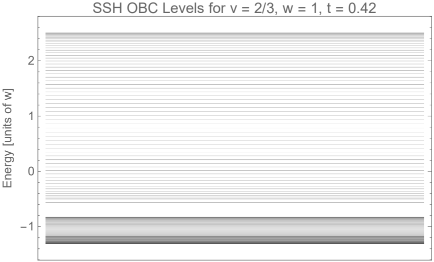
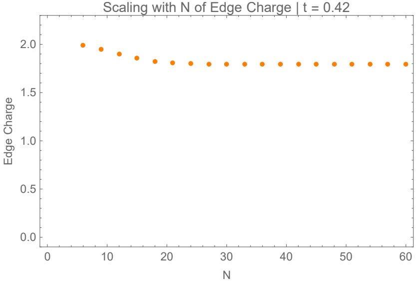
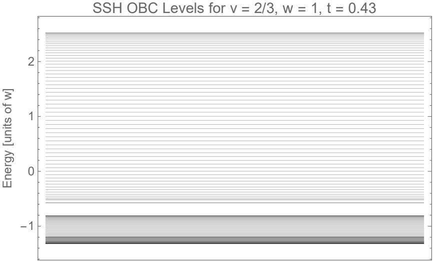
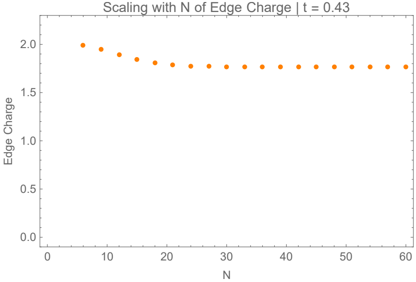


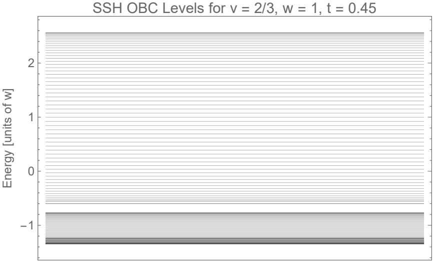


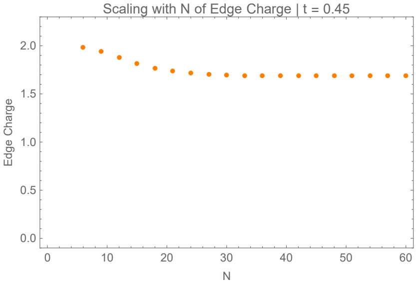
Spanning $t \in [0, w]$



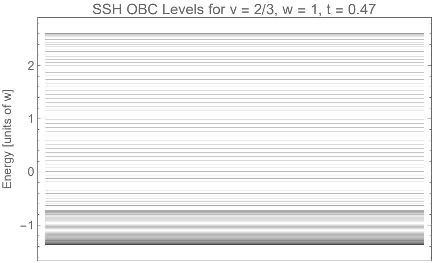


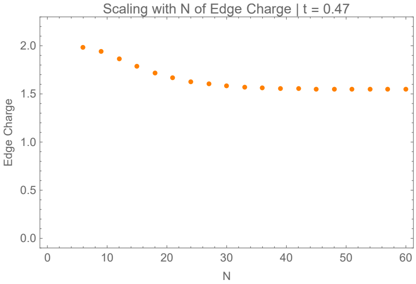
Spanning $t \in [0, w]$



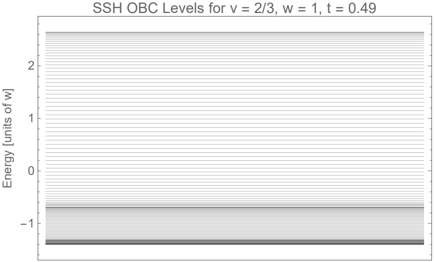


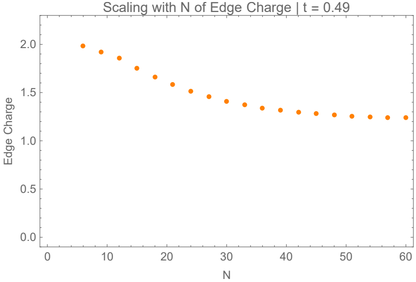
Spanning $t \in [0, w]$



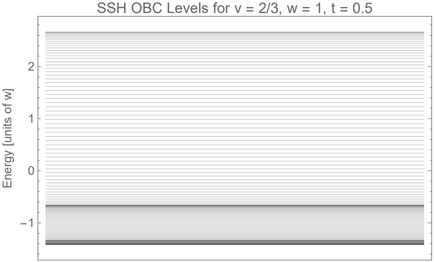


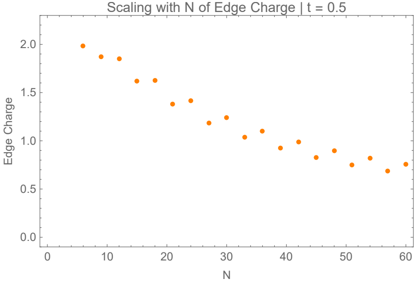
Spanning $t \in [0, w] \to$ Extremely long tales in the bulk!



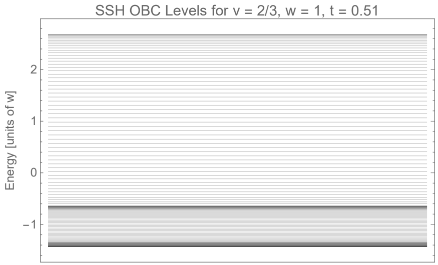


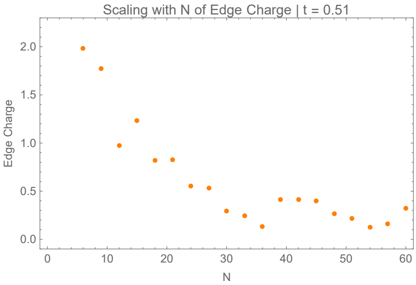
Spanning $t \in [0, w] \rightarrow$ Edge character definitely broken.





Spanning $t \in [0, w] \rightarrow$ Edge character definitely broken.





Disorder on N.N.N. hoppings

Let's consider random next-nearest neighbors (N.N.N.) hoppings:

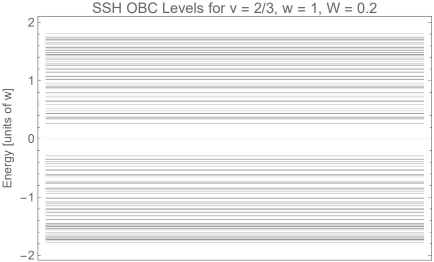
$$\{t_i\} \in [-W, +W]$$

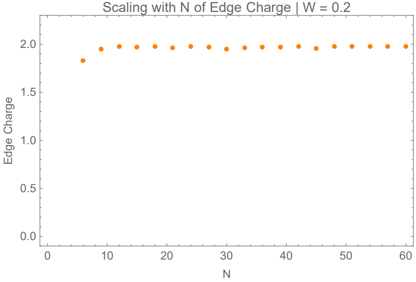
$$W < v < w$$

$$\Downarrow$$

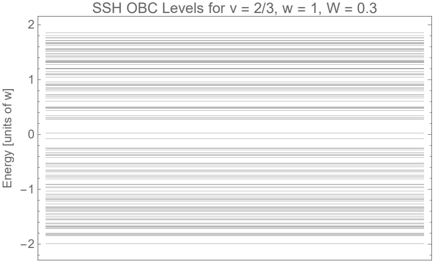
$$\mathbb{H}_W = \begin{pmatrix} 0 & v & t_1 & & & & \\ v & 0 & w & t_2 & & & \\ t_1 & w & 0 & v & t_3 & & \\ & t_2 & v & 0 & w & t_4 & \\ & & t_3 & w & 0 & v & t_5 \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}$$

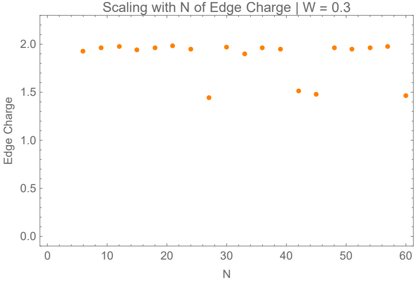
Spanning $W \in [0, w/2]$



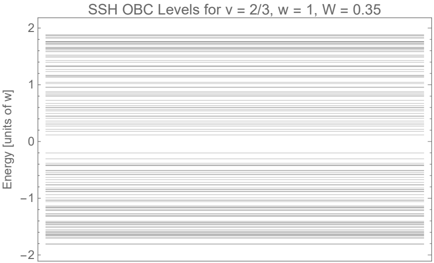


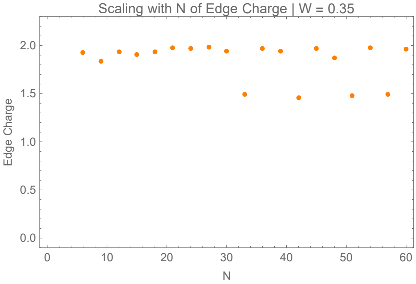
Spanning $W \in [0, w/2] \rightarrow$ Already large deviations!



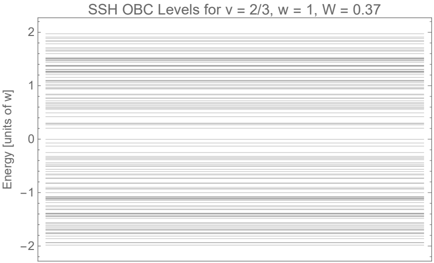


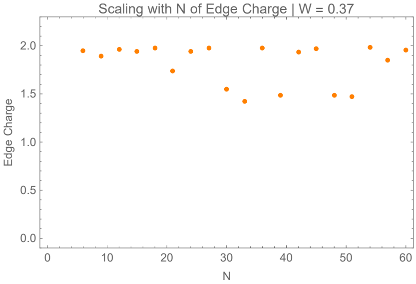
Spanning $W \in [0, w/2]$



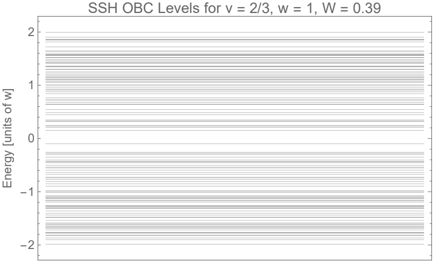


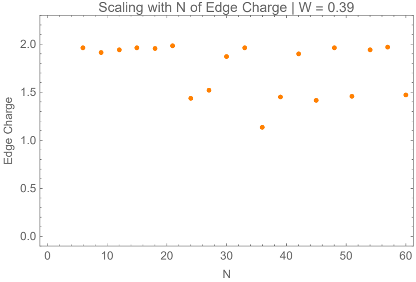
Spanning $W \in [0, w/2]$



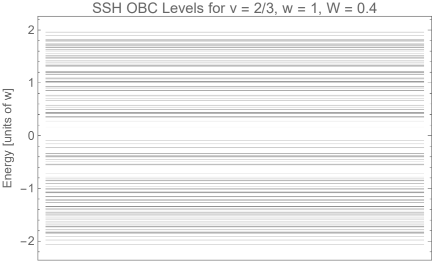


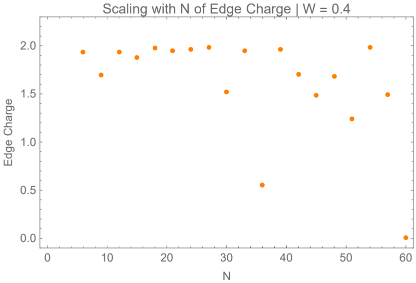
Spanning $W \in [0, w/2]$



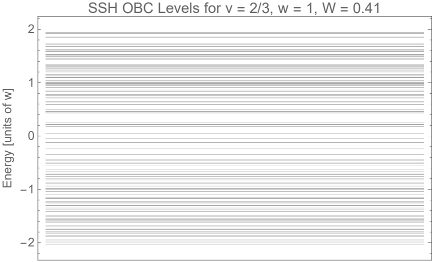


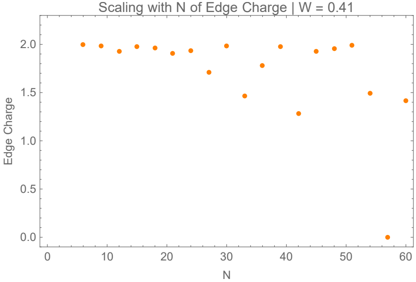
Spanning $W \in [0, w/2] \rightarrow$ Edge character is broken.



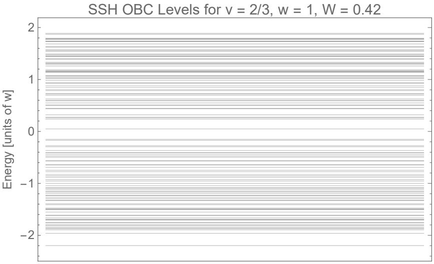


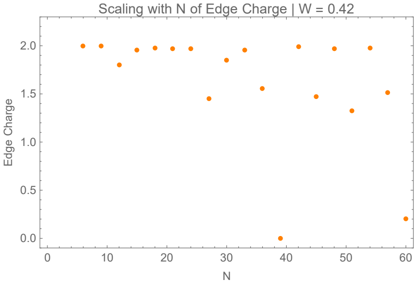
Spanning $W \in [0, w/2] \rightarrow$ Edge character is broken.



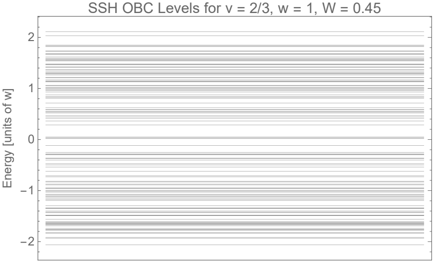


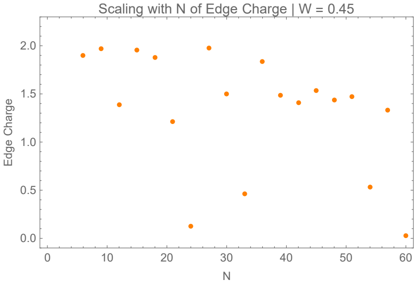
Spanning $W \in [0, w/2] \to$ Edge character is broken.





Spanning $W \in [0, w/2] \rightarrow$ Edge character is broken.





Conclusions

The edge-character of highest occupied and lowest unoccupied states seems to be:

- extremely robust when chiral symmetry is preserved so we infer that the edge states are somehow *protected* by $\{\Gamma, H\} = 0$, at least as far as the gap remains opened.;
- untouched when chiral symmetry is broken by fixed N.N.N. hoppings until the closure of the gap;
- noticeably fragile when the N.N.N. hoppings are disordered, proving that without some special "protection" a disordered perturbation is quite efficient at destroying edge character.

Section 2

Hofstadter-Harper Model

HH model

$$H = -\sum_{i,j}\sum_{k,l} t_{(k,l)\to(i,j)}\, c^{\dagger}_{ij} c_{kl}$$

$$t_{(k,l)\to(i,j)} = t\Big(\delta_{ik}\big(\delta_{j+1,l} + \delta_{j-1,l}\big) + \delta_{jl}\big(\delta_{i+1,k} + \delta_{i-1,k}\big)\Big)$$

Introducing a magnetic field corresponds to the "**Peierls substitution**":

$$t_{(k,l)\to(i,j)} \quad \longmapsto \quad t_{(k,l)\to(i,j)} \exp\left(-\, i\,\frac{e}{\hbar c}\int_{\mathbf{R}_{kl}}^{\mathbf{R}_{ij}} \mathbf{A}\cdot d\mathbf{r}\right)$$

HH model

For $\mathbf{B} = B\hat{z}$ and fixing $\mathbf{A} = \big(0, Bx, 0\big)$ (*Landau gauge*):

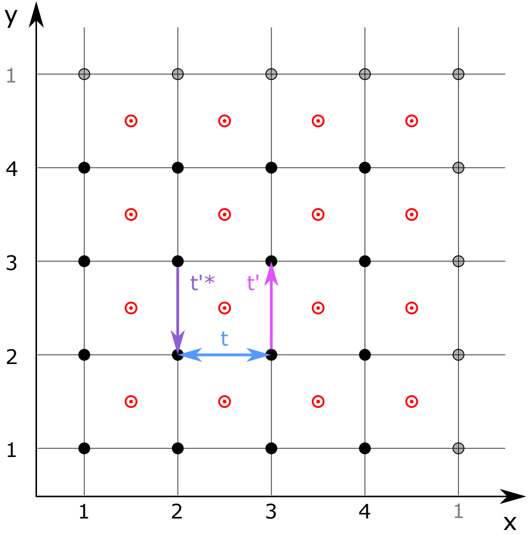
$$t'(x) = t\exp(-2\pi i\alpha x/a), \qquad \alpha = \Phi/\Phi_0, \quad a: \text{ lattice spacing}$$

$$\Phi = a^2 B: \text{ magnetic flux}, \qquad \Phi_0 = \frac{hc}{e}: \text{ quantum of magnetic flux}$$

$$t_{(k,l)\to(i,j)} \mapsto \Bigg(\delta_{ik}\big((t_i')^*\delta_{j+1,l} + t_i'\delta_{j-1,l}\big) + t\,\delta_{jl}\big(\delta_{i+1,k} + \delta_{i-1,k}\big)\Bigg)$$

$$t_i' = t'(x = ia)$$

HH model



Translational symmetries

$\hat{y}-$translational invariance is always conserved.

$\hat{x}-$translational invariance is (partially) broken because of the dependence of t' on the x lattice position.

However if $\alpha = P/Q$, with P and Q coprime integers:

$$t'(x + nQa) = t \exp\left(-2\pi i \frac{P}{Q}\frac{x}{a} - 2\pi i n P\right) = t'(x),$$

We get an expanded unit cell made of Q atoms in the x-direction and one atom in the y-direction.

Bloch theorem on $\hat{y}$

Imposing PBCs on $\hat{y}$ we get:

$$c_{lm} = \frac{1}{\sqrt{N_y}} \sum_{k_y} e^{-ik_y ma} c_{lk_y}, \qquad k_y = \frac{2\pi}{aN_y} m, \qquad m = 0,\, 1,\, \ldots,\, N_y - 1$$

$$H = -\sum_{k_y, i} t \left(2\cos\left(k_y a - 2\pi\alpha i\right) c^{\dagger}_{ik_y} c_{ik_y} + \left(c^{\dagger}_{ik_y} c_{i+1,k_y} + c^{\dagger}_{i+1,k_y} c_{ik_y} \right) \right)$$

$$H = \sum_{k_y} H_{k_y} \qquad \Longrightarrow \qquad N_x^{at} \times N_x^{at} - \text{block diagonal form!}$$

Ready-to-guess spectrum properties

1. Chiral symmetry:

$$\mathcal{E} = \{(i,j) \text{ such that } (-1)^{i+j} = +1\}$$
$$\mathcal{O} = \{(i,j) \text{ such that } (-1)^{i+j} = -1\}$$
$$\Gamma = P_{\mathcal{E}} - P_{\mathcal{O}}$$
$$\text{OBC} \to \{H,\Gamma\} = 0$$
$$\text{PBC} \to \{H,\Gamma\} = 0 \;\; \text{for even } N_x,\ N_y$$
$$\{H,\Gamma\} = 0 \;\; \to \;\; S\big(H(\alpha)\big) = -S\big(H(\alpha)\big)$$

2. Symmetry under $B \mapsto -B$: $S\big(H(\alpha)\big) = S\big(H(-\alpha)\big)$
3. For $n \in \mathbb{Z}$:

$$t'(x = ja; \alpha) = t'(x = ja; \alpha + n) \;\; \to \;\; S\big(H(\alpha)\big) = S\big(H(\alpha + n)\big)$$

4. By using Cauchy-Schwarz inequality: $S\big(H(\alpha)\big) \subset [-4t, +4t]$

Rational values of $\alpha \Rightarrow$ Bloch theorem on $\hat{x}$

With PBCs in both the directions:
(N_x : number of cells in the $x-$direction, $q = 1, 2, \ldots, Q$):

$$c^q_{lk_y} = \frac{1}{\sqrt{N_x}} \sum_{k_x} e^{-ik_x lQa} c^q_{k_x k_y} \qquad k_x = \frac{2\pi}{QaN_x} k \qquad k = 0,\, 1 \ldots N_x - 1$$

$$H = \sum_{k_x, k_y} H_{\mathbf{k}=(k_x,k_y)} \qquad \mathrm{BZ} = \{k_x \in [0, 2\pi/(Qa)],\;\; k_y \in [0, 2\pi/a]\}$$

$$(H_\mathbf{k})_{qq'} = -t\big(2\cos\left(k_y a - 2\pi\alpha q\right)\delta_{qq'} + \delta_{q,q+1} + \delta_{q,q-1}\big) \quad q, q' \in 2 \ldots Q-1$$

$$(H_\mathbf{k})_{11} = -2t\cos\left(k_y a - 2\pi\alpha\right) \qquad (H_\mathbf{k})_{QQ} = -2t\cos\left(k_y a - 2\pi\alpha Q\right)$$

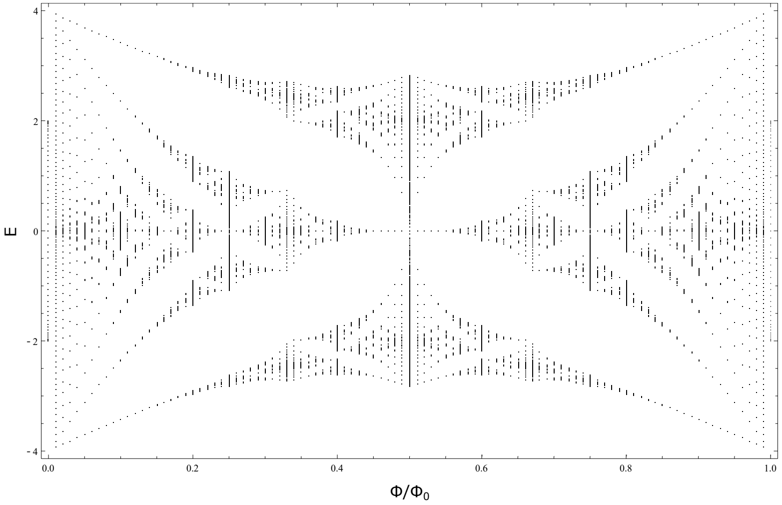
$$(H_\mathbf{k})_{1Q} = \big((H_\mathbf{k})_{Q1}\big)^* = -te^{ik_x Qa}$$

We computed the spectrum of H, diagonalizing each block H_{k_x,k_y}. We set $\alpha = 1/100, 2/100, 3/100, \ldots$

Trick: the spectrum of H_{k_y} is equal to that of $H_{k_y+2\pi/(Qa)}$;
thus, we can limit the computation to: $k_y \in [0, 2\pi/(Qa)]$.

Hofstader butterfly

Resulting energy scheme (for $N_x = N_y = 100$):

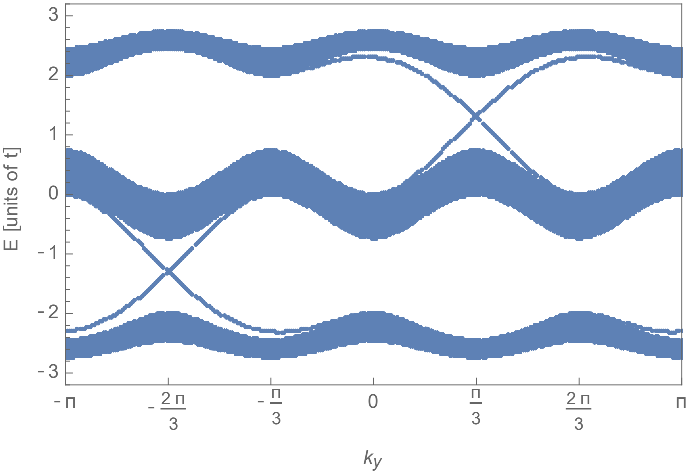


Self-similarity properties!

OBCs on $\hat{x}$ ($\alpha = 1/3$)

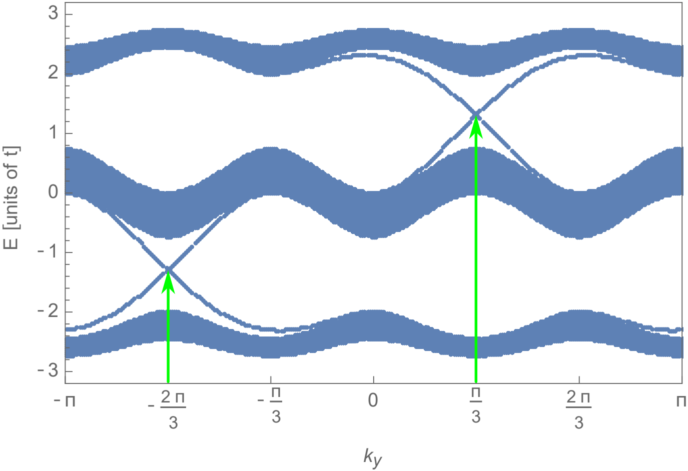
OBCs along **x** and PBCs along **y**.

Diagonalizing H_{k_y} we get, for $N_x = 150$, $N_y = 300$, $t_1 = t_2$:



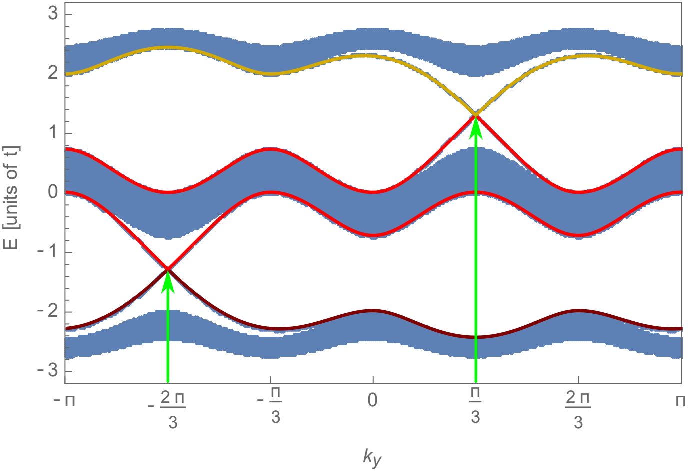
Edge states ($\alpha = 1/3$)

A pair of edge states is found in each of the two band gaps, for $k_y = -2\pi/3$, $k_y = \pi/3$.



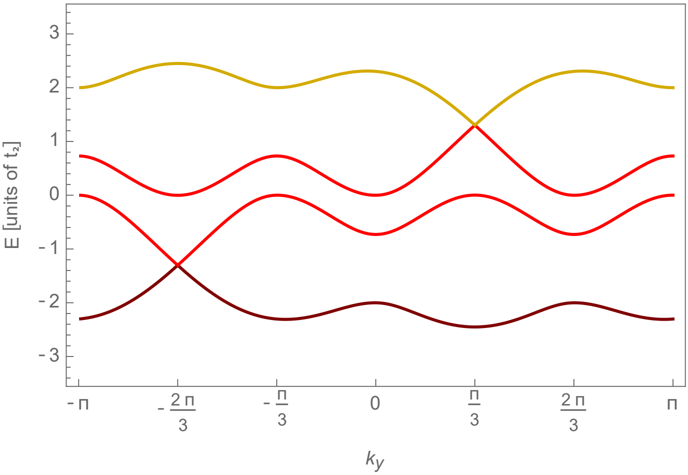
Edge states ($\alpha = 1/3$)

Colors corresponding to $\nu = 1$, $\nu = 2$, $\nu = 3$.

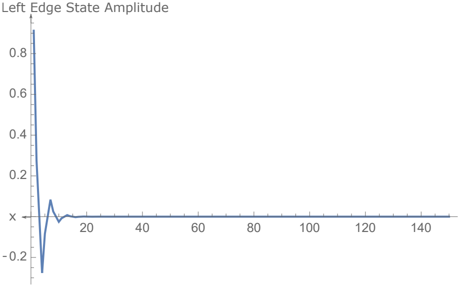


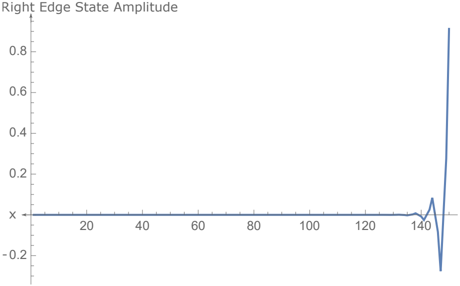
Edge states ($\alpha = 1/3$)

Colors corresponding to $\nu = 1$, $\nu = 2$, $\nu = 3$.

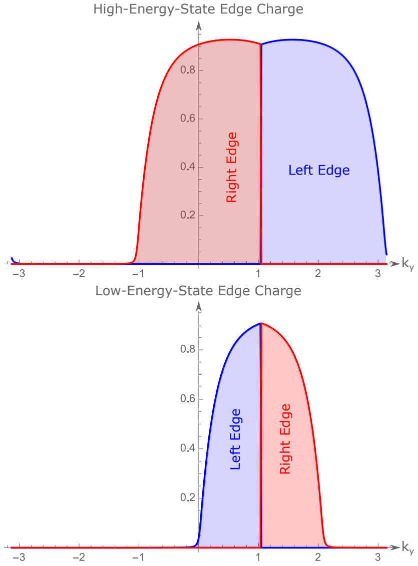


Edges ($\alpha = 1/3$) $\rightarrow$ Amplitude at exact crossing ($k_y = \pi/3$)



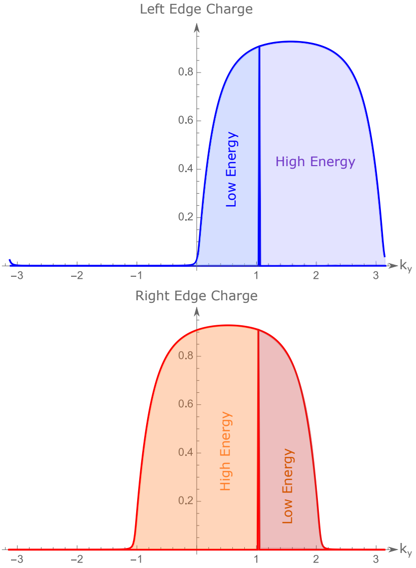


Edge states ($\alpha = 1/3$) $\rightarrow$ Edge charge accross the BZ



Do they really pertain to a band?

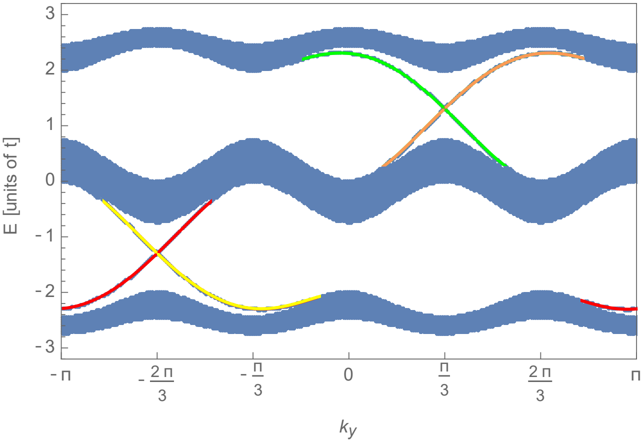
Edge states ($\alpha = 1/3$) $\rightarrow$ Edge charge accross the BZ



Do they really pertain to a band??

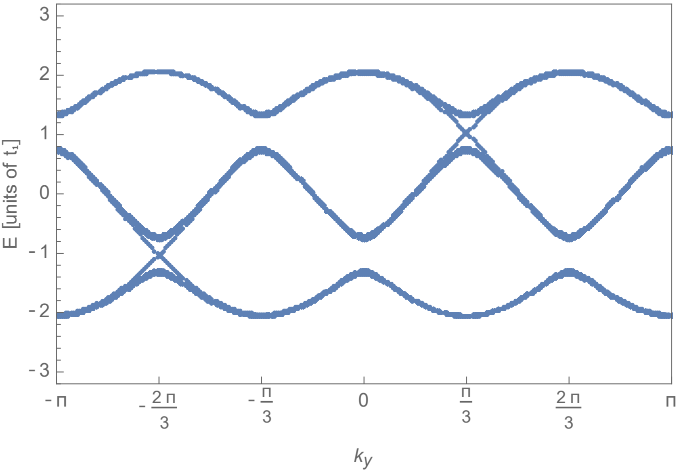
Edge states really cross the gap!

The actual physical way to define the dispersion of an edge state is to impose that its wavefunction varies continuosly with k_y.
So the edge states **do not** pertain to the bands they originate from, but instead they are pure gap-crossing levels.

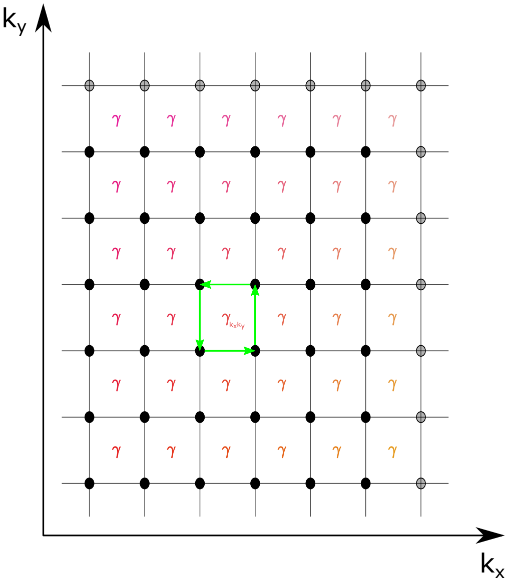


Robustness of Edge States $\rightarrow \alpha = 1/3$ and $t_2/t_1 = 0.2$

As a final comment we notice that the number and k_y-position of the edge states is robust under variation of the hoppings $\rightarrow$ topological invariants?



Chern Numbers (Numerical)



Chern Numbers (Numerical)

$$C^{\nu} = -\frac{1}{2\pi} \sum_{\mathbf{k}} \mathrm{Im} \Bigg[\log \Bigg(\langle u^{\nu}(k_x, k_y) | u^{\nu}(k_x + \delta_x, k_y) \rangle$$

$$\times \langle u^{\nu}(k_x + \delta_x, k_y) | u^{\nu}(k_x + \delta_x, k_y + \delta_y) \rangle$$

$$\times \langle u^{\nu}(k_x + \delta_x, k_y + \delta_y) | u^{\nu}(k_x, k_y + \delta_y) \rangle$$

$$\times \langle u^{\nu}(k_x, k_y + \delta_y) | u^{\nu}(k_x, k_y) \rangle \Bigg) \Bigg]$$

$$\text{for } \alpha = 1/3 \quad \Longrightarrow \quad C^1 = 1, \;\; C^2 = -2, \;\; C^3 = 1$$

Chern Numbers (Analytical)

Chern numbers can be computed analytically[1] (non-trivial!). Consider the Diophantine equation:

$$\nu = Q s_\nu + P t_\nu, \qquad s_\nu, t_\nu \in \mathbb{Z}$$

Unique solution for $|t_\nu| \leq Q/2$. Then:

$$C^\nu = t_\nu - t_{\nu-1}, \qquad t_0 = 0$$

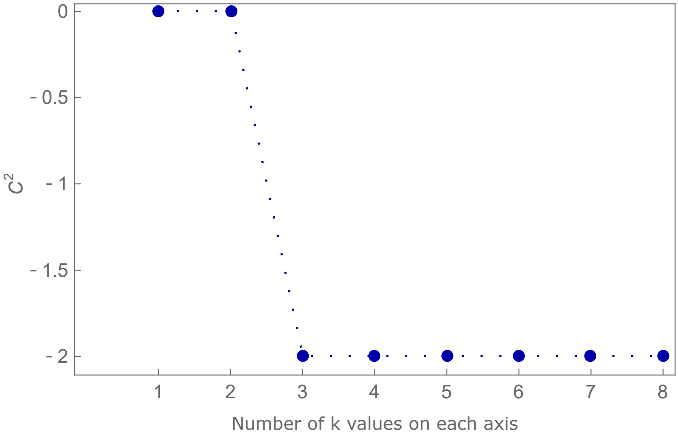
For example $\alpha = 1/3$:

$$C^1 = 1, \;\; C^2 = -2, \;\; C^3 = 1 \;\; \Rightarrow \;\; \text{Identical to our numerical results!}$$

[1] E. Fradkin: "Field Theories of Condensed Matter Physics", 2^{nd} Edition

Chern number convergence

Let's see how the Chern number for the $\nu = 2$ band converges as we increase the number of cells on each axis ($N_x = N_y$)



Chern Number $\Leftrightarrow$ Number of Edge States (?)

In conclusion for each band we may regard the number of edge states as a topological invariant of the system, and in the case we addressed it corresponds to the modulus of the Chern number (if we assign each edge state to the band it originates from) or twice the modulus of the difference of the Chern numbers of the adjacent bands (if we assign each edge state to the gap it crosses):

$$\begin{aligned} |C^\nu| \; &\equiv \; \#\{\text{Edge States from the } \nu\text{-th band}\} \\ &\qquad \text{or} \\ \left|C^\nu - C^{\nu-1}\right| \; &\equiv \; 2 \times \#\{\text{Edge States crossing} \\ &\qquad \text{the gap between the } \nu\text{-th} \\ &\qquad \text{and the } (\nu-1)\text{-th band}\} \end{aligned}$$

Nevertheless for some values of α the rule does not work and we did not find a definitive answer in literature $\quad\Longrightarrow\quad$ OPEN QUESTION?

Thanks for your attention!