

Spectral flow applied to solid state systems

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Plan

- Review of classical spectral flow
- Laughlin arguments
- η -invariants and finite-volume calculation of indices
- \mathbb{Z}_2 -valued spectral flow
- Application to a topological insulator (Kitaev chain)

Review of spectral flow

\mathcal{H} separable Hilbert space and $\mathbb{B}(\mathcal{H})$ bounded operators

$T \in \mathbb{B}(\mathcal{H})$ Fredholm $\iff \text{Ker}(T), \text{Ker}(T^*)$ finite dimensional

$T = T^*$ Fredholm $\iff 0 \notin \sigma_{\text{ess}}(T)$

$\mathbb{F}_{\text{sa}} = \{T = T^* \text{ Fredholm}\}$ has 3 components which contract to

$$\mathbb{F}_{\text{sa}}^* = \{T \in \mathbb{F}_{\text{sa}} \mid \sigma_{\text{ess}}(T) = \{-1, 1\}\}$$

$$\mathbb{F}_{\text{sa}}^+ = \{T \in \mathbb{F}_{\text{sa}} \mid \sigma_{\text{ess}}(T) = \{1\}\}$$

$$\mathbb{F}_{\text{sa}}^- = \{T \in \mathbb{F}_{\text{sa}} \mid \sigma_{\text{ess}}(T) = \{-1\}\}$$

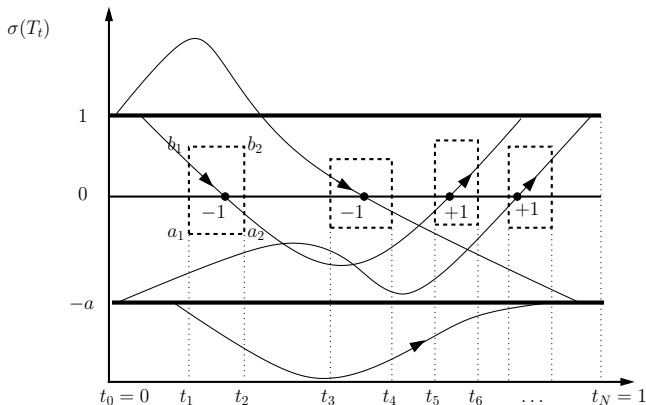
Theorem (Atiyah-Singer 1969)

Homotopy groups of \mathbb{F}_{sa}^ are $\pi_{2n}(\mathbb{F}_{\text{sa}}^*) = 0$ and $\pi_{2n+1}(\mathbb{F}_{\text{sa}}^*) = \mathbb{Z}$*

Aim: spectral flow calculates $\pi_1(\mathbb{F}_{\text{sa}}^*)$

Intuitive notion of spectral flow

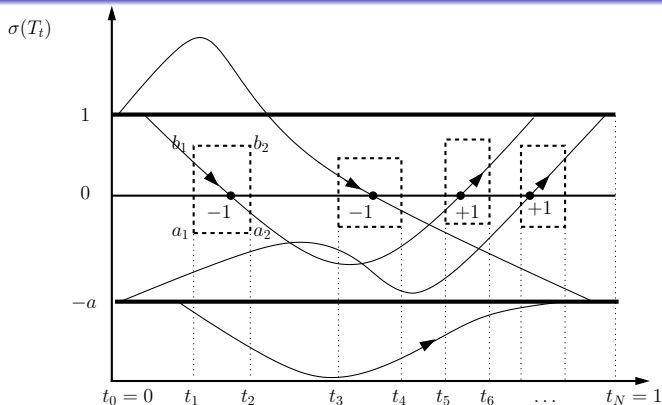
Given path $t \in [0, 1] \mapsto T_t = (T_t)^*$ of self-adjoint Fredholms on \mathcal{H}



Counting of eigenvalues passing 0 works if path analytic (APS)

For continuous paths need to go to "generic position", or:

Phillips' analytic approach (1996)



\exists finite partition $0 = t_0 < t_1 < \dots < t_{N-1} < t_N = 1$ of $[0, 1]$ and $a_n < 0 < b_n$ with $t \in [t_{n-1}, t_n] \mapsto \chi(T_t \in [a_n, b_n])$ continuous. Set:

$$\text{SF}(t \in [0, 1] \mapsto T_t) = \sum_{n=1}^N \text{Tr}_{\mathcal{H}} (\chi(T_{t_{n-1}} \in [a_n, 0]) - \chi(T_{t_n} \in [a_n, 0]))$$

Theorem (Phillips 1996)

$\text{SF}(t \in [0, 1] \mapsto T_t)$ independent of partition and $a_n < 0 < b_n$.

It is a homotopy invariant when end points are kept fixed.

It satisfies concatenation and normalization:

$$\text{SF}(t \in [0, 1] \mapsto T + (1 - 2t)P) = -\dim(P) \quad \text{for } TP = P$$

Theorem (Lesch 2004)

Homotopy invariance, concatenation, normalization characterize SF

Theorem (Perera 1993, Phillips 1996)

SF on loops establishes isomorphism $\pi_1(\mathbb{F}_{\text{sa}}^*) = \mathbb{Z}$

Theorem (Phillips 1996, based on Avron-Seiler-Simon 1994)

Let $T_1 = U^* T_0 U$ invertible with U unitary and $[U, T_0]$ compact

$$\text{SF}(t \in [0, 1] \mapsto (1-t)T_0 + tT_1) = -\text{Ind}(PUP|_{P\mathcal{H}}), \quad P = \chi(T_0 > 0)$$

Example: Laughlin argument 1981

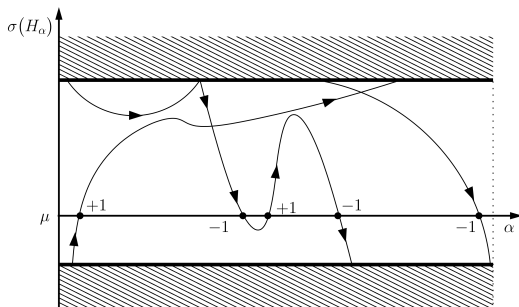
Theorem (Macris 2002, De Nittis, S-B 2016)

H disordered Harper-like operator on $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^L$ with $\mu \in \text{gap}$

H_α Hamiltonian with extra flux $\alpha \in [0, 1]$ through 1 cell of \mathbb{Z}^2

Then $T_\alpha = H_\alpha - \mu \in \mathbb{F}_{\text{sa}}^*$ and with $P = \chi(H_\alpha \leq \mu)$, $U = \frac{X_1 + iX_2}{|X_1 + iX_2|}$

$$\text{SF}\left(\alpha \in [0, 1] \mapsto H_\alpha \text{ through } \mu\right) = -\text{Ind}(PUP) = -\text{Ch}(P)$$



\mathbb{Z}_2 invariant for QSH by spectral flow

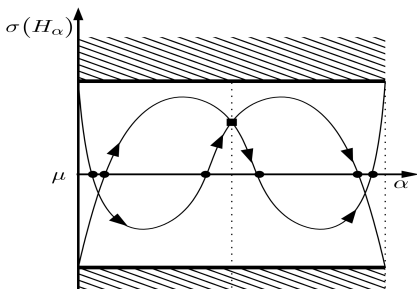
TRS implemented by a real unitary S_{tr} with $S_{\text{tr}}^2 = -\mathbf{1}$

$$S_{\text{tr}}^* \overline{H_\alpha} S_{\text{tr}} = H_{-\alpha} = U^* H_{1-\alpha} U$$

Both for $\alpha = 0$ (no flux) and $\alpha = \frac{1}{2}$ (half flux) one has TRS

Theorem (De Nittis, S-B 2016)

$\text{Ind}_2(PUP) = \dim(\ker(PUP)) \bmod 2 = 1$, namely non-trivial QSH
 $\implies H_{\frac{1}{2}}$ has Kramers pair bound state in gap



Spectral flow in a BdG-Hamiltonian

Flux tube in two-dimensional BdG Hamiltonian

$$S_{\text{ph}}^* \overline{H_\alpha} S_{\text{ph}} = -H_{-\alpha} \quad , \quad S_{\text{ph}}^2 = \pm \mathbf{1}$$

Then $S_{\text{ph}}^* \overline{H_\alpha} S_{\text{ph}} = -U^* H_{1-\alpha} U$ so that

$$\sigma(H_\alpha) = -\sigma(H_{-\alpha}) = -\sigma(H_{1-\alpha})$$

PHS only for $\alpha = 0, \frac{1}{2}, 1$ and thus $\text{Ind}_2(H_{\frac{1}{2}})$ well-defined

Theorem (De Nittis, S-B 2016)

$$\text{Ind}(PUP) \bmod 2 = \text{Ind}_2(H_{\frac{1}{2}})$$

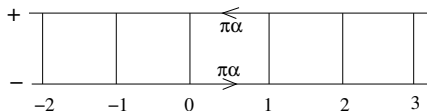
or: odd Chern number implies existence of zero mode at defect

These zero modes are Majorana fermions (Read-Green 2000)

Worth noting: $S_{\text{ph}}^2 = -\mathbf{1} \implies \text{Ind}(PUP) \text{ even} \implies \text{no zero mode}$

Laughlin arguments in other dimensions (in preparation with Carey)

$d = 1$: chiral spectral flow in SSH leads to bound state of $H_{\frac{1}{2}}$



On $\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^L$ with $d \geq 3$: insert non-abelian Wu-Yang monopole

$$A = \frac{i}{2} \frac{[D, \gamma]}{D^2} \quad , \quad D = \sum_{j=1}^d \gamma_j X_j$$

into non-abelian translations (say without magnetic field):

$$S_k^\alpha = e^{i\nabla_k^\alpha} = U^\alpha(X) S_k \quad , \quad \nabla_k^\alpha = i\partial_k + \alpha A_k$$

Then study (chiral) spectral flow for $H_\alpha = P(S_1^\alpha, \dots, S_d^\alpha)$

Spectral flow and η -invariant

$B = B^*$ invertible operator on \mathcal{H} with compact resolvent. Then

$$\eta(B) = \text{Tr}(B|B|^{-s-1})|_{s=0} = \frac{1}{\Gamma(\frac{s+1}{2})} \int_0^\infty dt t^{\frac{s-1}{2}} \text{Tr}(B e^{-tB^2}) \Big|_{s=0}$$

provided it exists! If $\dim(\mathcal{H}) < \infty$, then $\eta(B) = 2 \text{Sig}(B)$

Proposition

Given $D > 0$ and A bounded, and B with η -invariant

$$B = \begin{pmatrix} D & A \\ A^* & -D \end{pmatrix} \implies \eta(B) = 0$$

Proposition (Corollary of result in Getzler, 1993)

$\lambda \in [0, 1] \mapsto B(\lambda) - B(0) \in \mathcal{L}^1$, $B(0)$ and $B(1)$ have η -invariants

$$\eta(B(1)) - \eta(B(0)) = 2 \text{SF}(\lambda \in [0, 1] \mapsto B(\lambda))$$

η -Invariant for chiral Hamiltonian

Chiral Hamiltonian $H = \begin{pmatrix} 0 & A \\ A^* & 0 \end{pmatrix}$ in $d = 1$ on $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^{2N}$

Introduce operator with compact resolvent:

$$B = (\kappa X + iH)J = \begin{pmatrix} \kappa X & -iA \\ iA^* & -\kappa X \end{pmatrix}, \quad J = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}$$

Proposition (in preparation with Loring)

If $[H, X]$ bounded, $\eta(B)$ exists

Use path $\lambda \in [0, 1] \mapsto H(\lambda)$ splitting H on $\ell^2(\mathbb{N}_+) \oplus \ell^2(\mathbb{N}_-)$

Leads to path $\lambda \in [0, 1] \mapsto B(\lambda)$ with $B(0) = B$ and

$$B(1) = \begin{pmatrix} \kappa X_+ & -iA_+ \\ iA_+^* & -\kappa X_+ \end{pmatrix} \oplus \begin{pmatrix} \kappa X_- & -iA_- \\ iA_-^* & -\kappa X_- \end{pmatrix}$$

Thus $\eta(B(1)) = 0$ by above proposition!

Finite-volume calculation of index

$$\eta(B) = 2 \text{SF}(\lambda \in [0, 1] \mapsto B(\lambda))$$

Calculation: spectral flow equal to $\text{Ind}(\Pi A \Pi)$ where Π Hardy

Moreover, signature stabilizes for finite volume approximation of B

Theorem (with Loring, in preparation)

Let B_Λ restriction of B to $\ell^2([- \Lambda, \Lambda]) \otimes \mathbb{C}^{2N}$

If $\frac{1}{\Lambda}$ and $\kappa > 0$ sufficiently small,

$$\frac{1}{2} \text{Sig}(B_\Lambda) = \text{Ind}(\Pi A \Pi)$$

Similar results for all d , but K -theoretic proofs (fuzzy spheres)

Symmetries can be implemented and lead to Pfaffians

Basics on skew-adjoint Fredholm operators

$\mathcal{H}_{\mathbb{R}}$ real Hilbert space with complexification $\mathcal{H}_{\mathbb{C}} = \mathcal{H}_{\mathbb{R}} \oplus i\mathcal{H}_{\mathbb{R}}$

$T \in \mathbb{B}(\mathcal{H}_{\mathbb{R}})$ extends to complex linear operator (e.g. for spectrum)

$T^* = -T$ skew-adjoint $\implies \sigma(T) = \overline{\sigma(T)} \subset i\mathbb{R}$

$T^* = -T$ Fredholm $\iff 0 \notin \sigma_{\text{ess}}(T)$

Theorem (Atiyah Singer 1969)

$\mathbb{F}_{\text{sk}} = \{ T = -T^* \text{ Fredholm} \}$ has two connected components distinguished by: $\text{Ind}_2(T) = \dim(\text{Ker}(T)) \bmod 2$

Homotopy groups satisfy $\pi_n(\mathbb{F}_{\text{sk}}) = \pi_{n+8}(\mathbb{F}_{\text{sk}})$ and are given by

n	0	1	2	3	4	5	6	7
$\pi_n(\mathbb{F}_{\text{sk}})$	\mathbb{Z}_2	\mathbb{Z}_2	0	$2\mathbb{Z}$	0	0	0	\mathbb{Z}

Aim: define \mathbb{Z}_2 -valued spectral flow calculating $\pi_1(\mathbb{F}_{\text{sa}}^*)$

Note: $\text{SF}(t \in [0, 1] \mapsto T_t \in \mathbb{F}_{\text{sk}}) = 0$

Start with example in $\mathcal{H}_{\mathbb{R}} = \mathbb{R}^2$

$$T_t = (2t - 1) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \tilde{T}_t = |2t - 1| \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

Spectra identical $\sigma(T_t) = \sigma(\tilde{T}_t) = \{(1 - 2t)i, (2t - 1)i\}$, but

$$\tilde{T}_t(s) = |2ts - 1| \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \in \mathbb{F}_{\text{sk}}$$

homotopy of paths with $\tilde{T}_t(1) = \tilde{T}_t$ and $\tilde{T}_t(0)$ constant

No such homotopy for T_t !

Obstruction is change of orientation of eigenfunctions:

$$T_1 = A^* T_0 A \quad A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Then $\text{sgn}(\det(A)) < 0$

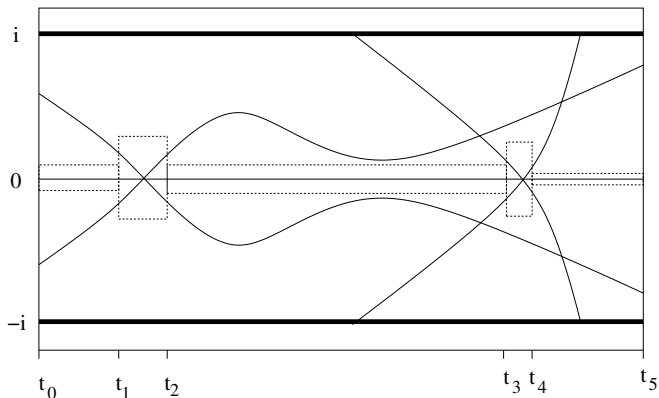
Definition

$\dim(\mathcal{H}_{\mathbb{R}}) < \infty$ and $T_0, T_1 \in \mathbb{F}_{\text{sk}}$ with nullity $\dim(\mathcal{H}_{\mathbb{R}}) \bmod 2$

If $T_1 = A^* T_0 A$ for some invertible A , then

$$\text{SF}_2(T_0, T_1) = \text{sgn}(\det(A)) \in \mathbb{Z}_2$$

Now similar as Phillips: path $t \mapsto T_t \in \mathbb{F}_{\text{sk}}$ with $\text{Ind}_2(T_t) = 0$



Definition of \mathbb{Z}_2 -valued spectral flow

For $a > 0$ set $Q_a(t) = \chi(T_t \in (-ia, ia))$

\exists finite partition $0 = t_0 < t_1 < \dots < t_{N-1} < t_N = 1$ and $a_n > 0$

- $t \in [t_{n-1}, t_n] \mapsto Q_{a_n}(t)$ continuous and constant finite rank
- $\|Q_{a_n}(t) - Q_{a_n}(t')\| < \epsilon \quad \forall t, t' \in [t_{n-1}, t_n]$
- $\|\pi(T_t) - \pi(T_{t'})\|_{\mathcal{Q}} < \epsilon \quad \forall t, t' \in [t_{n-1}, t_n]$

for some $\epsilon \leq \frac{1}{5}$

$V_n : \text{Ran}(Q_{a_n}(t_{n-1})) \rightarrow \text{Ran}(Q_{a_n}(t_n))$ orthogonal projection,
namely $V_n v = Q_{a_n}(t_n) v$. Check: V_n is a bijection.

Define $T_t^{(a)} = Q_a(t) T_t Q_a(t) + R_t$ with R_t lifting kernel

Definition

$$\text{SF}_2(t \in [0, 1] \mapsto T_t) = \sum_{n=1}^N \text{SF}_2(T_{t_{n-1}}^{(a_n)}, V_n^* T_{t_n}^{(a_n)} V_n) \text{ mod } 2$$

Basic properties

Theorem

$SF_2(t \in [0, 1] \mapsto T_t \in \mathbb{F}_{sk})$ independent of partition and $a_n > 0$.

It is a homotopy invariant when end points are kept fixed.

It satisfies concatenation.

It satisfies a normalization (later).

SF_2 has characterizing properties of SF, but *no* "spectral flowing"

Theorem

SF_2 on loops establishes isomorphism $\pi_1(\mathbb{F}_{sk}) = \mathbb{Z}_2$

Reformulation

$J \in \mathbb{B}(\mathcal{H}_{\mathbb{R}})$ complex structure $\iff J^* = -J$ and $J^2 = -\mathbf{1}$

Theorem

J_0, J_1 complex structures with $\|\pi(J_0) - \pi(J_1)\|_{\mathcal{Q}} < 1$. Then

$$\text{SF}_2(t \in [0, 1] \mapsto tJ_0 + (1-t)J_1 \in \mathbb{F}_{\text{sk}}) = \frac{1}{2} \dim(\text{Ker}(J_0 + J_1)) \bmod 2$$

Proof: Both sides are homotopy invariants... \square

Theorem

For above partition of path $t \in [0, 1] \mapsto T_t$, set $J_n = T_{t_n} |T_{t_n}|^{-1}$

Then

$$\text{SF}_2(t \in [0, 1] \mapsto T_t) = \left(\sum_{n=1}^N \frac{1}{2} \dim(\text{Ker}(J_{n-1} + J_n)) \right) \bmod 2$$

For classical spectral flow similar with index of pairs of projections

An index formula and canonical example

Theorem

J complex structure, $O = (O^*)^{-1}$ orthogonal with $[O, J]$ compact

$$\text{SF}_2(t \in [0, 1] \mapsto (1 - t)J + tO^*JO) = \dim \text{Ker}(POP|_{P\mathcal{H}}) \bmod 2$$

where $P = \chi(iJ > 0)$ Hardy

Example:

$$\mathcal{H}_{\mathbb{R}} = L^2_{\mathbb{R}}(\mathbb{S}^1) \otimes \mathbb{R}^2 \text{ and } \mathcal{H}_{\mathbb{C}} = L^2_{\mathbb{C}}(\mathbb{S}^1) \otimes \mathbb{C}^2$$

$$\text{Fourier } \mathcal{F} : \mathcal{H}_{\mathbb{C}} \rightarrow \ell^2_{\mathbb{C}}(\mathbb{Z}) \otimes \mathbb{C}^2$$

$$J = \mathcal{F}^* \hat{J} \mathcal{F} \text{ where } \hat{J} = i \text{sgn}(X) \otimes \mathbf{1}_2 + |0\rangle\langle 0| \otimes i\sigma_2$$

$O = (O(k))_{k \in \mathbb{S}^1}$ fibered with 2×2 rotation matrix $O(k)$ by k

$$\text{SF}_2(t \in [0, 1] \mapsto (1 - t)J + tO^*JO) = 1 = \dim \text{Ker}(POP|_{P\mathcal{H}_{\mathbb{C}}})$$

Skew-adjoint Fredholm = gapped BdG

Fermionic quadratic Hamiltonian $\mathbf{H} = (a \ a^*)H\begin{pmatrix} a \\ a^* \end{pmatrix}$ on $\mathcal{F}_-(\mathcal{H})$

BdG Hamiltonian $H \in \mathbb{B}(\mathcal{H} \oplus \mathcal{H})$ satisfies even PHS

$$\sigma_1^* \overline{H} \sigma_1 = -H \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Then Majorana representation:

$$H_{\text{Maj}} = C^* H C = -\overline{H_{\text{Maj}}} = iT, \quad C = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}$$

Then: $\overline{\overline{T}} = T$ and $T^* = -T$ and

$T \in \mathbb{F}_{\text{sk}} \iff 0$ in gap of H

Thus: paths of BdG's have a \mathbb{Z}_2 -valued spectral flow

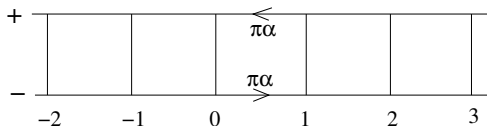
Kitaev chain with flux (disorder suppressed)

Here $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ and with shift S and $\mu \in \mathbb{R}$:

$$\begin{aligned}
 H &= \frac{1}{2} \begin{pmatrix} S + S^* + 2\mu & i(S - S^*) \\ i(S - S^*) & -(S + S^* + 2\mu) \end{pmatrix} \\
 &= S_0 + S_0^* + \mu \mathbf{1} \otimes \sigma_3, \quad S_0 = S \otimes \frac{1}{2} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix}
 \end{aligned}$$

Insert flux: $H_\alpha = S_\alpha + S_\alpha^* + \mu \mathbf{1} \otimes \sigma_3$

$$S_\alpha = S_0 + |1\rangle\langle 0| \otimes \frac{1}{2} \begin{pmatrix} e^{-i\pi\alpha} - 1 & i(e^{-i\pi\alpha} - 1) \\ i(e^{i\pi\alpha} - 1) & -(e^{i\pi\alpha} - 1) \end{pmatrix}$$



Spectral flow and bound states at defect

Proposition

For $|\mu| < 1$,

$$\text{SF}_2(\alpha \in [0, 1] \mapsto H_\alpha) = 1$$

Time-reversal symmetry $\sigma_3 \overline{H} \sigma_3 = H$, hence in CAZ Class BDI

Also holds for half flux: $\sigma_3 \overline{H_{\frac{1}{2}}} \sigma_3 = H_{\frac{1}{2}}$

Proposition

For $|\mu| < 1$, $H_{\frac{1}{2}}$ has odd number of evenly degenerate zero modes:

$$\frac{1}{2} \dim_{\mathbb{C}}(\text{Ker}_{\mathbb{C}}(H_{\frac{1}{2}})) \bmod 2 = 1$$

Proof: Symmetry $\sigma(H_\alpha) = \sigma(H_{1-\alpha})$ and above Proposition