

Entanglement entropy of fermions

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I. RÉNYI ENTANGLEMENT ENTROPY FOR FERMIONS

Rényi entanglement entropy is defined by

$$S_N := \frac{1}{1-N} \log \text{tr} [\rho_I^N]. \quad (1.1)$$

Let us consider a fermionic reduced density matrix

$$\rho_I = \int \prod_{i \in I} d\bar{\alpha}_i d\alpha_i d\bar{\beta}_i d\beta_i e^{-\sum_{i \in I} (\bar{\alpha}_i \alpha_i + \bar{\beta}_i \beta_i)} \rho_I(\{\bar{\alpha}_i\}, \{\beta_i\}) |\{\alpha_i\}\rangle \langle\{\bar{\beta}_i\}|. \quad (1.2)$$

From a straightforward calculation we have

$$\text{tr} [\rho_I^N] = \int \prod_{i \in I, n=1, \dots, N} d\bar{\alpha}_{n,i} d\alpha_{n,i} \rho_I(\{-\bar{\alpha}_{1,i}\}, \{\alpha_{1,i}\}) \cdots \rho_I(\{-\bar{\alpha}_{N,i}\}, \{\alpha_{N,i}\}) e^{\sum_{i \in I} (-\bar{\alpha}_{1,i} \alpha_{N,i} + \bar{\alpha}_{2,i} \alpha_{1,i} + \cdots + \bar{\alpha}_{N,i} \alpha_{N-1,i})}. \quad (1.3)$$

Here, $n = 1 \dots, N$ are the replica indices. For a pure state $|\psi\rangle$, the reduced density matrix becomes

$$\rho_I(\{-\bar{\alpha}_i\}_{i \in I}, \{\alpha_i\}_{i \in I}) = \int \prod_{i \notin I} d\bar{\alpha}_i d\alpha_i \psi(\{-\bar{\alpha}_i\}_{i \in I}, \{-\bar{\alpha}_i\}_{i \notin I}) \psi^*(\{\alpha_i\}_{i \in I}, \{\alpha_i\}_{i \notin I}) e^{-\sum_{i \notin I} \bar{\alpha}_i \alpha_i}. \quad (1.4)$$

Then,

$$\text{tr} [\rho_I^N] = \int \prod_{i \in \text{full}, n=1, \dots, N} d\bar{\alpha}_{n,i} d\alpha_{n,i} \psi(\{-\bar{\alpha}_{1,i}\}) \psi^*(\{\alpha_{1,i}\}) \cdots \psi(\{-\bar{\alpha}_{N,i}\}) \psi^*(\{\alpha_{N,i}\}) \quad (1.5)$$

$$e^{-\sum_{i \notin I, n} \bar{\alpha}_{n,i} \alpha_{n,i}} e^{\sum_{i \in I} (-\bar{\alpha}_{1,i} \alpha_{N,i} + \bar{\alpha}_{2,i} \alpha_{1,i} + \cdots + \bar{\alpha}_{N,i} \alpha_{N-1,i})} \quad (1.6)$$

$$= \int \prod_{i \in \text{full}, n=1, \dots, N} d\bar{\alpha}_{n,i} d\alpha_{n,i} \Psi(\{-\bar{\alpha}_{n,i}\}) \Psi^*(\{\alpha_{n,i}\}) e^{-\sum_{i \notin I, n} \bar{\alpha}_{n,i} \alpha_{n,i}} e^{\sum_{i \in I} (-\bar{\alpha}_{1,i} \alpha_{N,i} + \bar{\alpha}_{2,i} \alpha_{1,i} + \cdots + \bar{\alpha}_{N,i} \alpha_{N-1,i})}, \quad (1.7)$$

where we introduced the *replica ground state*

$$\Psi(\{-\bar{\alpha}_{n,i}\}) := \psi(\{-\bar{\alpha}_{1,i}\}) \psi(\{-\bar{\alpha}_{2,i}\}) \cdots \psi(\{-\bar{\alpha}_{N,i}\}), \quad (1.8)$$

$$\Psi^*(\{\alpha_{n,i}\}) := \psi^*(\{\alpha_{N,i}\}) \psi^*(\{\alpha_{N-1,i}\}) \cdots \psi^*(\{\alpha_{1,i}\}). \quad (1.9)$$

$\text{tr} [\rho_I^N]$ can be expressed as the expectation value of the *partial replica permutation operator* T_I on the replica ground state $|\Psi\rangle$. For a while, we ignore site indices. Let $\{f_n\}$ be complex fermions associated with the Grassmann variables $\{\alpha_n\}$. We define the replica permutation operator T so that T satisfies

$$T f_1 T^{-1} = f_N, \quad T f_n T^{-1} = -f_{n-1} \quad (n = 2, \dots, N). \quad (1.10)$$

Note that

$$T^N \sim \begin{cases} 1 & (N : \text{odd}) \\ (-1)^F & (N : \text{even}) \end{cases} \quad (1.11)$$

up to a $U(1)$ phase factor. By introducing real fermions $\{c_n^R, c_n^L\}$ by

$$f_n^\dagger = \frac{c_n^R + i c_n^L}{2}, \quad f_n = \frac{c_n^R - i c_n^L}{2}, \quad (1.12)$$

the permutation operator T is given by

$$T = e^{\frac{\pi}{4} c_N^R c_{N-1}^R} e^{\frac{\pi}{4} c_{N-1}^R c_{N-2}^R} \cdots e^{\frac{\pi}{4} c_2^R c_1^R} \cdot e^{\frac{\pi}{4} c_N^L c_{N-1}^L} e^{\frac{\pi}{4} c_{N-1}^L c_{N-2}^L} \cdots e^{\frac{\pi}{4} c_2^L c_1^L} \quad (1.13)$$

$$= (1 - f_{N-1}^\dagger f_{N-1} - f_N^\dagger f_N - f_{N-1}^\dagger f_N + f_N^\dagger f_{N-1} + 2f_{N-1}^\dagger f_N^\dagger f_N f_{N-1}) \quad (1.14)$$

$$\cdots (1 - f_1^\dagger f_1 - f_2^\dagger f_2 - f_1^\dagger f_2 + f_2^\dagger f_1 + 2f_1^\dagger f_2^\dagger f_2 f_1). \quad (1.15)$$

T is normalized as

$$T^N = \begin{cases} 1 & (N : \text{odd}) \\ (-1)^F & (N : \text{even}) \end{cases} \quad (1.16)$$

(KS: I checked this for $N = 2, 3, 4, 5$ from a direct calculation.) Its matrix element is given by

$$\langle \alpha | T | \beta \rangle \quad (1.17)$$

$$= \int \prod d\gamma_n d\delta_n e^{-\sum_n \gamma_n \delta_n} \langle \alpha | (1 - f_{N-1}^\dagger f_{N-1} - f_N^\dagger f_N - f_{N-1}^\dagger f_N + f_N^\dagger f_{N-1} + 2f_{N-1}^\dagger f_N^\dagger f_N f_{N-1}) \quad (1.18)$$

$$\cdots | \delta \rangle \langle \gamma | (1 - f_1^\dagger f_1 - f_2^\dagger f_2 - f_1^\dagger f_2 + f_2^\dagger f_1 + 2f_1^\dagger f_2^\dagger f_2 f_1) | \beta \rangle \quad (1.19)$$

$$= \int \prod d\gamma_n d\delta_n e^{-\sum_n \gamma_n \delta_n} \langle \alpha | (1 - f_{N-1}^\dagger f_{N-1} - f_N^\dagger f_N - f_{N-1}^\dagger f_N + f_N^\dagger f_{N-1} + 2f_{N-1}^\dagger f_N^\dagger f_N f_{N-1}) \quad (1.20)$$

$$\cdots | \delta \rangle e^{-\gamma_1 \beta_2 + \gamma_2 \beta_1 + \sum_{n=3}^N \gamma_n \beta_n} \quad (1.21)$$

$$= \langle \alpha | (1 - f_{N-1}^\dagger f_{N-1} - f_N^\dagger f_N - f_{N-1}^\dagger f_N + f_N^\dagger f_{N-1} + 2f_{N-1}^\dagger f_N^\dagger f_N f_{N-1}) \quad (1.22)$$

$$\cdots (1 - f_2^\dagger f_2 - f_3^\dagger f_3 - f_2^\dagger f_3 + f_3^\dagger f_2 + 2f_2^\dagger f_3^\dagger f_3 f_2) | -\beta_2, \beta_1, \beta_3, \dots, \beta_N \rangle \quad (1.23)$$

$$= \cdots \quad (1.24)$$

$$= \langle \alpha | -\beta_2, -\beta_3, \dots, -\beta_N, \beta_1 \rangle \quad (1.25)$$

$$= e^{-\sum_{n=1}^{N-1} \alpha_n \beta_{n+1} + \alpha_N \beta_1}. \quad (1.26)$$

We define the partial N -fold rotation T_I on the interval I by

$$T_I := \prod_{i \in I} e^{\frac{\pi}{4} c_{N,i}^R c_{N-1,i}^R} e^{\frac{\pi}{4} c_{N-1,i}^R c_{N-2,i}^R} \cdots e^{\frac{\pi}{4} c_{2,i}^R c_{1,i}^R} \cdot e^{\frac{\pi}{4} c_{N,i}^L c_{N-1,i}^L} e^{\frac{\pi}{4} c_{N-1,i}^L c_{N-2,i}^L} \cdots e^{\frac{\pi}{4} c_{2,i}^L c_{1,i}^L} \quad (1.27)$$

Then,

$$\langle \Psi | T_I | \Psi \rangle = \text{tr} [T_I | \Psi \rangle \langle \Psi |] \quad (1.28)$$

$$= \int \prod d\bar{\alpha}_{n,i} d\alpha_{n,i} e^{-\sum_{n,i} \bar{\alpha}_{n,i} \alpha_{n,i}} \langle -\bar{\alpha} | T_I | \Psi \rangle \langle \Psi | \alpha \rangle \quad (1.29)$$

$$= \int \prod d\bar{\alpha}_{n,i} d\alpha_{n,i} d\bar{\beta}_{n,i} d\beta_{n,i} e^{-\sum_{n,i} \bar{\alpha}_{n,i} \alpha_{n,i} - \sum_{n,i} \bar{\beta}_{n,i} \beta_{n,i}} \langle -\bar{\alpha} | T_I | \beta \rangle \langle \bar{\beta} | \Psi \rangle \langle \Psi | \alpha \rangle \quad (1.30)$$

$$= \int \prod d\bar{\alpha}_{n,i} d\alpha_{n,i} d\bar{\beta}_{n,i} d\beta_{n,i} e^{-\sum_{n,i} \bar{\alpha}_{n,i} \alpha_{n,i} - \sum_{n,i} \bar{\beta}_{n,i} \beta_{n,i}} \quad (1.31)$$

$$e^{-\sum_{n,i \notin I} \bar{\alpha}_{n,i} \beta_{n,i}} e^{\sum_{i \in I} [\sum_{n=1}^{N-1} \bar{\alpha}_{n,i} \beta_{n+1,i} - \bar{\alpha}_{N,i} \beta_{1,i}]} \langle \bar{\beta} | \Psi \rangle \langle \Psi | \alpha \rangle \quad (1.32)$$

$$= \int \prod d\alpha_{n,i} d\bar{\beta}_{n,i} e^{\sum_{n,i \notin I} \bar{\beta}_{n,i} \alpha_{n,i}} e^{\sum_{i \in I} [\bar{\beta}_{1,i} \alpha_{N,i} - \sum_{n=2}^N \bar{\beta}_{n,i} \alpha_{n-1,i}]} \langle \bar{\beta} | \Psi \rangle \langle \Psi | \alpha \rangle \quad (1.33)$$

$$= \int \prod d\bar{\alpha}_{n,i} d\alpha_{n,i} e^{-\sum_{n,i \notin I} \bar{\alpha}_{n,i} \alpha_{n,i}} e^{\sum_{i \in I} [-\bar{\alpha}_{1,i} \alpha_{N,i} + \sum_{n=2}^N \bar{\alpha}_{n,i} \alpha_{n-1,i}]} \langle -\bar{\alpha} | \Psi \rangle \langle \Psi | \alpha \rangle \quad (1.34)$$

$$= \text{tr} [\rho_I^N]. \quad (1.35)$$

Here we used

$$\int \prod_n d\bar{\alpha}_n d\beta_n e^{-\sum_n \bar{\alpha}_n \alpha_n} e^{-\sum_n \bar{\beta}_n \beta_n} e^{\sum_{n=1}^{N-1} \bar{\alpha}_n \beta_{n+1} - \bar{\alpha}_N \beta_1} \quad (1.36)$$

$$= \int (\beta_2 - \alpha_1) d\beta_1 (\beta_3 - \alpha_2) d\beta_2 \cdots (\beta_N - \alpha_{N-1}) d\beta_{N-1} (-\beta_1 - \alpha_N) d\beta_N e^{-\sum_n \bar{\beta}_n \beta_n} \quad (1.37)$$

$$= \int d\beta_1 (\beta_1 + \alpha_N) d\beta_2 (\beta_2 - \alpha_1) \cdots d\beta_N (\beta_N - \alpha_{N-1}) e^{-\sum_n \bar{\beta}_n \beta_n} \quad (1.38)$$

$$= e^{\bar{\beta}_1 \alpha_N - \sum_{n=2}^N \bar{\beta}_n \alpha_{n-1}}. \quad (1.39)$$

It is useful to introduce a basis of fermions which diagonalizes the permutation operator T . T is written as

$$T f_n^\dagger T^{-1} = f_m^\dagger [U_T]_{mn}, \quad U_T = \begin{pmatrix} 0 & -1 & & \\ & 0 & -1 & \\ & & \cdots & \\ & & & 0 & -1 \\ 1 & & & & 0 \end{pmatrix}. \quad (1.40)$$

The matrix U_T is diagonalized by

$$U_T v_k = -\omega_k v_k, \quad v_k = \frac{1}{\sqrt{N}}(1, \omega_k, \omega_k^2, \dots, \omega_k^{N-1})^T, \quad \omega_k = e^{\frac{\pi i}{N}(2k-1)} \quad (k = 1, \dots, N). \quad (1.41)$$

We introduce new fermions $\psi_k^\dagger (k = 1, \dots, N)$ by

$$\psi_k^\dagger := \frac{1}{\sqrt{N}}(f_1^\dagger + \omega_k f_2^\dagger + \omega_k^2 f_3^\dagger + \dots + \omega_k^{N-1} f_N^\dagger), \quad (1.42)$$

$$T \psi_k^\dagger T^{-1} = -\omega_k \psi_k^\dagger. \quad (1.43)$$

If the pure state $|\psi\rangle$ has the particle number symmetry (Spin^c structure), the Rényi entanglement entropy for the subregion I factorizes into the N number of the partial $U(1)$ rotations

$$\text{tr}[\rho_I^N] = \langle \Psi | T | \Psi \rangle = \prod_{k=-\frac{N-1}{2}, -\frac{N-1}{2}+1, \dots, \frac{N-1}{2}} \langle \psi | U_k | \psi \rangle, \quad (1.44)$$

where $|\psi\rangle$ is the ground state of original single system and

$$U_k | I \rangle = \exp \left[2\pi i \frac{k}{N} \sum_{i \in I} f_i^\dagger f_i \right]. \quad (1.45)$$

II. PARTIAL TIME-REVERSAL TRANSFORMATION (CLASS AI)

There are three types of partial anti-unitary transformations: class AI, AII, and AIII. Here we consider class AI time-reversal twisting. For a class AI TRS defined by

$$\Theta f_i^\dagger \Theta^{-1} = f_j^\dagger [\mathcal{U}_\Theta]_{ji}, \quad \mathcal{U}_\Theta^T = \mathcal{U}_\Theta, \quad (2.1)$$

the partial time-reversal twisting on a subregion I_1 is defined by

$$U_\Theta^{I_1} \rho_I^{\Theta_1} [U_\Theta^{I_1}]^\dagger = \int \prod_{i \in I} d\bar{\gamma}_i d\gamma_i d\bar{\delta}_i d\delta_i e^{-\sum_i (\bar{\gamma}_i \gamma_i + \bar{\delta}_i \delta_i)} \rho_I(\{\bar{\gamma}_i\}, \{\delta_i\}) | \{i\bar{\delta}_i [\mathcal{U}_\Theta]_{ij}\}_{j \in I_1}, \{\gamma_i\}_{i \in I_2}\rangle \langle \{i[\mathcal{U}_\Theta^*]_{ij} \gamma_j\}_{i \in I_1}, \{\bar{\delta}_i\}_{i \in I_2} |, \quad (2.2)$$

where $U_\Theta^{I_1}$ is the unitary part of the time-reversal transformation on I_1 . Here, we consider the quantity

$$S_N^{\Theta_1} := \text{tr}[(\rho_I^{\Theta_1})^N] = \text{tr}[(U_\Theta^{I_1} \rho_I^{\Theta_1} [U_\Theta^{I_1}]^\dagger)^N]. \quad (2.3)$$

Since $S_N^{\Theta_1}$ does not depend on the choice of $U_\Theta^{I_1}$, we can simply set $\mathcal{U}_\Theta = 1$:

$$U_\Theta^{I_1} \rho_I^{\Theta_1} [U_\Theta^{I_1}]^\dagger = \int \prod_{i \in I} d\bar{\gamma}_i d\gamma_i d\bar{\delta}_i d\delta_i e^{-\sum_i (\bar{\gamma}_i \gamma_i + \bar{\delta}_i \delta_i)} \rho_I(\{\bar{\gamma}_i\}, \{\delta_i\}) | \{i\bar{\delta}_i\}_{i \in I_1}, \{\gamma_i\}_{i \in I_2}\rangle \langle \{i\gamma_i\}_{i \in I_1}, \{\bar{\delta}_i\}_{i \in I_2} |. \quad (2.4)$$

One can show that

$$S_N^{\Theta_1} = \int \prod_{i \in I_1 \cup I_2, n=1, \dots, N} d\bar{\alpha}_{n,i} d\alpha_{n,i} e^{\sum_{i \in I_1} (\sum_{n=1}^{N-1} \bar{\alpha}_{n,i} \alpha_{n+1,i} - \bar{\alpha}_{N,i} \alpha_{1,i})} e^{\sum_{i \in I_2} (\sum_{n=1}^{N-1} \bar{\alpha}_{n+1,i} \alpha_{n,i} - \bar{\alpha}_{1,i} \alpha_{N,i})} \prod_n \rho(\{-\bar{\alpha}_{n,i}\}, \{\alpha_{n,i}\}). \quad (2.5)$$

For a pure state $|\psi\rangle$,

$$S_N^{\Theta_1} = \int \prod_{i,n=1, \dots, N} d\bar{\alpha}_{n,i} d\alpha_{n,i} e^{\sum_{i \in I_1} (\sum_{n=1}^{N-1} \bar{\alpha}_{n,i} \alpha_{n+1,i} - \bar{\alpha}_{N,i} \alpha_{1,i})} e^{\sum_{i \in I_2} (\sum_{n=1}^{N-1} \bar{\alpha}_{n+1,i} \alpha_{n,i} - \bar{\alpha}_{1,i} \alpha_{N,i})} e^{-\sum_{i \notin I_1 \cup I_2} \sum_{n=1}^N \bar{\alpha}_{n,i} \alpha_{n,i}} \quad (2.6)$$

$$\psi(\{-\bar{\alpha}_{1,i}\}) \psi(\{-\bar{\alpha}_{2,i}\}) \dots \psi(\{-\bar{\alpha}_{N,i}\}) \psi^*(\{\alpha_{N,i}\}) \dots \psi^*(\{\alpha_{2,i}\}) \psi^*(\{\alpha_{1,i}\}). \quad (2.7)$$

This can be written as an expectation value of the partial N -fold permutation operator on the replicated ground state $|\Psi\rangle$. Noticing that

$$\langle \alpha | T^{-1} | \beta \rangle = \langle -\alpha_2, -\alpha_3, \dots, -\alpha_N, \alpha_1 | \beta \rangle = e^{\alpha_1 \beta_N - \sum_{n=2}^N \alpha_n \beta_{n-1}}, \quad (2.8)$$

we get

$$S_N^{\Theta_1} = \langle \Psi | T_{I_1}^{-1} T_{I_2} | \Psi \rangle \quad (2.9)$$

with

$$T_{I_1}^{-1} = \prod_{i \in I_1} e^{\frac{\pi}{4} c_{1,i}^R c_{2,i}^R} e^{\frac{\pi}{4} c_{2,i}^R c_{3,i}^R} \dots e^{\frac{\pi}{4} c_{N-1,i}^R c_{N,i}^R} \cdot e^{\frac{\pi}{4} c_{1,i}^L c_{2,i}^L} e^{\frac{\pi}{4} c_{2,i}^L c_{3,i}^L} \dots e^{\frac{\pi}{4} c_{N-1,i}^L c_{N,i}^L}, \quad (2.10)$$

$$T_{I_2} = \prod_{i \in I_2} e^{\frac{\pi}{4} c_{N,i}^R c_{N-1,i}^R} e^{\frac{\pi}{4} c_{N-1,i}^R c_{N-2,i}^R} \dots e^{\frac{\pi}{4} c_{2,i}^R c_{1,i}^R} \cdot e^{\frac{\pi}{4} c_{N,i}^L c_{N-1,i}^L} e^{\frac{\pi}{4} c_{N-1,i}^L c_{N-2,i}^L} \dots e^{\frac{\pi}{4} c_{2,i}^L c_{1,i}^L}. \quad (2.11)$$

If the pure state $|\psi\rangle$ has the particle number conservation symmetry (Spin^c structure), $\langle \Psi | T_{I_1}^{-1} T_{I_2} | \Psi \rangle$ factorizes into the N number of the partial $U(1)$ rotations

$$S_N^{\Theta_1} = \prod_{k=-\frac{N-1}{2}, -\frac{N-1}{2}+1, \dots, \frac{N-1}{2}} \langle \psi | U_k | \psi \rangle, \quad (2.12)$$

$$U_k | I \rangle = \exp \left[-\frac{2\pi i k}{N} \sum_{i \in I_1} f_i^\dagger f_i + \frac{2\pi i k}{N} \sum_{i \in I_2} f_i^\dagger f_i \right]. \quad (2.13)$$

III. MAJORANA CHAIN

A. Jordan-Wigner transformation in (1+1)d

Introducing real fermions

$$f_{n,i}^\dagger = \frac{c_{n,i}^R + i c_{n,i}^L}{2}, \quad f_{n,i} = \frac{c_{n,i}^R - i c_{n,i}^L}{2}, \quad (3.1)$$

we introduce spin 1/2 variables $\{\sigma_{n,i}^\mu\}$ by

$$c_{n,i}^R = -\sigma_{n,1}^x \sigma_{n,2}^x \dots \sigma_{n,i-1}^x \sigma_{n,i}^y, \quad (3.2)$$

$$c_{n,i}^L = \sigma_{n,1}^x \sigma_{n,2}^x \dots \sigma_{n,i-1}^x \sigma_{n,i}^z. \quad (3.3)$$

The following relations hold:

$$(-1)^F = \prod_{n,i} (-i c_{n,i}^L c_{n,i}^R) = \prod_{n,i} \sigma_{n,i}^x, \quad (3.4)$$

$$f_{n,i}^\dagger f_{n,i} = \frac{1 - \sigma_{n,i}^x}{2}, \quad (3.5)$$

$$P_n = \prod_i \sigma_{n,i}^x, \quad (3.6)$$

$$f_{n,i}^\dagger = -\sigma_{n,1}^x \dots \sigma_{n,i-1}^x \sigma_{n,i}^-, \quad \sigma_{n,i}^- = \frac{\sigma_{n,i}^y - i \sigma_{n,i}^z}{2}, \quad (3.7)$$

$$f_{n,i} = -\sigma_{n,1}^x \dots \sigma_{n,i-1}^x \sigma_{n,i}^+, \quad \sigma_{n,i}^+ = \frac{\sigma_{n,i}^y + i \sigma_{n,i}^z}{2}, \quad (3.8)$$

$$i c_{n,i}^L c_{n,i}^R = -\sigma_{n,i}^x, \quad (3.9)$$

$$i c_{n,i}^R c_{n,i+1}^L = -\sigma_{n,i}^z \sigma_{n,i+1}^z, \quad i c_{n,L}^R c_{n,1}^L = P_n \sigma_{n,L}^z \sigma_{n,1}^z, \quad (3.10)$$

$$i c_{n,i}^L c_{n,i+1}^R = \sigma_{n,i}^y \sigma_{n,i+1}^y, \quad i c_{n,L}^L c_{n,1}^R = -P_n \sigma_{n,L}^y \sigma_{n,1}^y. \quad (3.11)$$

1. Majorana chain

$$H_n = \sum_{i=1}^L (f_{n,i}^\dagger f_{n,i} + h.c.) + J \sum_{i=1}^{L-1} (-f_{n,i}^\dagger f_{n,i+1} - f_{n,i} f_{n,i+1} + h.c.) \pm J(-f_{n,L}^\dagger f_{n,1} - f_{n,L} f_{n,1} + h.c.) \quad (3.12)$$

$$= \sum_{i=1}^L i c_{n,i}^L c_{n,i}^R + J \sum_{i=1}^{L-1} i c_{n,i}^R c_{n,i+1}^L \pm J i c_{n,L}^R c_{1,1}^L \quad (3.13)$$

$$= - \sum_{i=1}^L \sigma_{n,i}^x - J \sum_{i=1}^{L-1} \sigma_{n,i}^z \sigma_{n,i+1}^z \pm J i P_n \sigma_{n,L}^z \sigma_{n,1}^z. \quad (3.14)$$

$J = 1$ is the critical point. We introduce new fermions $\psi_k^\dagger (k = 1, \dots, N)$ by

$$\psi_k^\dagger := \frac{1}{\sqrt{N}} (f_1^\dagger + \omega_k f_2^\dagger + \omega_k^2 f_3^\dagger + \dots + \omega_k^{N-1} f_N^\dagger), \quad \omega_k = e^{\frac{2\pi i}{N}(2k-1)}, \quad (3.15)$$

$$T \psi_k^\dagger T^{-1} = -\omega_k \psi_k^\dagger. \quad (3.16)$$

This inverse transformation is

$$f_n^\dagger = \frac{1}{\sqrt{N}} (\bar{\omega}_1^{n-1} \psi_1^\dagger + \bar{\omega}_2^{n-1} \psi_2^\dagger + \dots + \bar{\omega}_N^{n-1} \psi_N^\dagger), \quad (3.17)$$

$$f_n = \frac{1}{\sqrt{N}} (\omega_1^{n-1} \psi_1 + \omega_2^{n-1} \psi_2 + \dots + \omega_N^{n-1} \psi_N). \quad (3.18)$$

$$\sum_n f_{n,i} f_{n,i+1} = \frac{1}{N} \sum_{n,k,l} \omega_k^{n-1} \omega_l^{n-1} \psi_{k,i} \psi_{l,i+1} = \sum_k \psi_{k,i} \psi_{1-k,i+1}. \quad (3.19)$$

IV. DIRAC FERMION (Spin^c)

Model Hamiltonian

$$H(\theta) = - \sum_{i=1}^{L-1} [f_i^\dagger f_{i+1} + h.c.] - e^{i\theta} [f_L^\dagger f_1 + h.c.] \quad (4.1)$$

$$(4.2)$$

A. Bosonization

- Spin^c \leftrightarrow $U(1)$?
- Dirac fermion \leftrightarrow compactified boson ?

Critical Dirac fermion (Spin^c structure):

$$H(\theta) = - \sum_{i=1}^{L-1} [f_i^\dagger f_{i+1} + h.c.] - e^{i\theta} [f_L^\dagger f_1 + h.c.] \quad (4.3)$$

$$= - \frac{1}{2} \sum_{i=1}^{L-1} [i c_i^L c_{i+1}^R - i c_i^R c_{i+1}^L] - \frac{e^{i\theta}}{2} [i c_L^L c_1^R - i c_L^R c_1^L] \quad (4.4)$$

$$= - \frac{1}{2} \sum_{i=1}^{L-1} [\sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z] + \frac{e^{i\theta}}{2} P [\sigma_L^y \sigma_1^y + \sigma_L^z \sigma_1^z] \quad (4.5)$$

$$= - \sum_{i=1}^{L-1} [\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+] + e^{i\theta} P [\sigma_L^+ \sigma_1^- + \sigma_L^- \sigma_1^+]. \quad (4.6)$$

$$(-1)^F = \prod_i (1 - 2f_i^\dagger f_i) = P = \prod_i \sigma_i^x, \quad (4.7)$$

$$T_{I,k} = \exp \left[\frac{2\pi ik}{N} \sum_{i \in I} f_i^\dagger f_i \right] = \exp \left[\frac{\pi ik}{N} |I| - \frac{\pi ik}{N} \sum_{i \in I} \sigma_i^x \right], \quad (4.8)$$

$$T_{I,k}^{-1} = \exp \left[-\frac{2\pi ik}{N} \sum_{i \in I} f_i^\dagger f_i \right] = \exp \left[-\frac{\pi ik}{N} |I| + \frac{\pi ik}{N} \sum_{i \in I} \sigma_i^x \right], \quad (4.9)$$

$$k = -\frac{N-1}{2}, -\frac{N-1}{2} + 1, \dots, \frac{N-1}{2}. \quad (4.10)$$

$$\begin{cases} e^{-2\pi ib f^\dagger f} f^\dagger e^{2\pi ib f^\dagger f} = e^{-2\pi ib} f^\dagger \\ e^{-2\pi ib f^\dagger f} f e^{2\pi ib f^\dagger f} = e^{2\pi ib} f \end{cases} \leftrightarrow \begin{cases} e^{-\pi ib + \pi ib \sigma^x} \sigma^y e^{\pi ib - \pi ib \sigma^x} = \sigma^y \cos(2\pi b) + \sigma^z \sin(2\pi b) \\ e^{-\pi ib + \pi ib \sigma^x} \sigma^z e^{\pi ib - \pi ib \sigma^x} = \sigma^z \cos(2\pi b) - \sigma^y \sin(2\pi b) \end{cases} \quad (4.11)$$

$$\leftrightarrow \begin{cases} e^{-\pi ib + \pi ib \sigma^x} \sigma^+ e^{\pi ib - \pi ib \sigma^x} = e^{-2\pi ib} \sigma^+ \\ e^{-\pi ib + \pi ib \sigma^x} \sigma^- e^{\pi ib - \pi ib \sigma^x} = e^{2\pi ib} \sigma^- \end{cases} \quad (4.12)$$

B. Toeplitz determinant

Let $|\psi\rangle$ be a occupied state

$$|\psi\rangle = \prod_{|k| < k_F} f_k^\dagger |0\rangle \quad (4.13)$$

of complex fermions f_k with momentum $k \in \frac{2\pi n}{L}$, $n \in \mathbb{Z}$, $-\pi/a < k < \pi/a$ with a the lattice constant. In the present section, we do not assume any forms of the dispersion ϵ_k of the complex fermions. What we want to compute is the following expectation value of the sequence of the partial $U(1)$ transformation

$$\left\langle \psi \left| \exp \left[2\pi i b_1 \sum_{x \in I_1} f_x^\dagger f_x + 2\pi i b_2 \sum_{x \in I_2} f_x^\dagger f_x + \dots \right] \right| \psi \right\rangle. \quad (4.14)$$

The above expectation value can be estimated by use of the Fisher-Hartwig theorem.¹ The matrix element of the sequence for momentum basis

$$|n\rangle = \sqrt{\frac{a}{L}} \sum_x |x\rangle e^{2\pi i n x / L} \quad (4.15)$$

is given approximated as

$$\phi_{n-m} = \left\langle n \left| \exp \left[2\pi i b_1 \sum_{x \in I_1} f_x^\dagger f_x + 2\pi i b_2 \sum_{x \in I_2} f_x^\dagger f_x + \dots \right] \right| m \right\rangle \quad (4.16)$$

$$= \frac{a}{L} \sum_x \begin{cases} e^{2\pi i b_j} & (x \in I_j) \\ 1 & \text{otherwise} \end{cases} e^{-i(n-m) \frac{2\pi x}{L}} \quad (4.17)$$

$$\sim \frac{1}{2\pi} \oint_0^{2\pi} d\theta \begin{cases} e^{2\pi i b_j} & (\theta \in I_j) \\ 1 & \text{otherwise} \end{cases} e^{-i(n-m)\theta} \quad \text{for } \frac{a}{L} \ll 1. \quad (4.18)$$

Here, we used the same notations I_j for the intervals in $S^1 = [0, 2\pi]$. The generating function of the Toeplitz matrix

$$T_{k_F}[\phi] = (\phi_{n-m}), \quad -\frac{Lk_F}{2\pi} < n, m < \frac{Lk_F}{2\pi}. \quad (4.19)$$

is given by

$$\phi(\theta) = \begin{cases} e^{2\pi i b_j} & (\theta \in I_j) \\ 1 & \text{otherwise} \end{cases} \quad (4.20)$$

The expectation value (4.14) is given by the determinant of the Toeplitz matrix

$$(4.14) \sim \det T_{k_F}[\phi] \quad (4.21)$$

Notice that the Toeplitz matrix (4.19) is equivalent to

$$T_{k_F}[\phi] = (\phi_{n-m}), \quad 0 < n, m < \frac{Lk_F}{\pi}. \quad (4.22)$$

We can immediately apply the Fisher-Hartwig theorem, which is reviewed in Appendix A, to (4.14).

C. Single interval

Here we consider the partial $e^{2\pi ib}$ transformation and the Rényi entanglement entropy on an interval $[0, \ell]$. The data of generating function of the Toeplitz matrix is

$$e^{V(e^{i\theta})} = e^{i\theta_1 b}, \quad 0 = \theta_0 < \theta_1 = \frac{2\pi\ell}{L}, \quad \alpha_0 = \alpha_1 = 0, \quad \beta_0 = -b, \beta_1 = b. \quad (4.23)$$

There is ambiguity in β_0 and β_1 which arises from

$$\beta_i \mapsto \beta_i + n_i, \quad \sum_i n_i = 0. \quad (4.24)$$

β_i should be chosen to minimize

$$\sum_i (\text{Re } \beta_i)^2. \quad (4.25)$$

If there are multiple minimized points $\{\beta_i\}$, all the minimized points $\{\beta_i\}$ contribute the determinant of the Toeplitz matrix in an equal footing.

1. Partial $e^{2\pi ib}$ transformation, $b \neq 1/2$.

For $b \neq 1/2$, β is fixed to be $|\beta| < 1/2$, thus we assume $-1/2 < b < 1/2$. The partial $e^{2\pi ib}$ transformation is given by

$$Z(b) := \langle \psi | e^{2\pi ib \sum_{0 \leq x \leq \ell} f_x^\dagger f_x} | \psi \rangle \quad (4.26)$$

$$\cong \left[2 \sin \left(\frac{\pi\ell}{L} \right) \right]^{-2b^2} \cdot \left(\frac{Lk_F}{\pi} \right)^{-2b^2} \cdot e^{2ik_F \ell b} \cdot [G(1+b)G(1-b)]^2, \quad (4.27)$$

where $G(z)$ is the Barnes G-function

$$G(1+z) = (2\pi)^{z/2} \exp \left(-\frac{z + (1+\gamma)z^2}{2} \right) \prod_{r=1}^{\infty} \left[\left(1 + \frac{z}{r} \right)^r e^{\frac{z^2}{2r} - z} \right]. \quad (4.28)$$

The logarithm of the partial $e^{2\pi ib}$ transformation is

$$\log Z(b) = \log \langle \psi | e^{2\pi ib \sum_{0 \leq x \leq \ell} f_x^\dagger f_x} | \psi \rangle \quad (4.29)$$

$$\cong -2b^2 \log \left[\frac{Lk_F}{\pi} \cdot 2 \sin \left(\frac{\pi\ell}{L} \right) \right] + 2ik_F \ell b + 2 \log [G(1+b)G(1-b)]. \quad (4.30)$$

The pure imaginary part is a trivial contribution from the fermi sea. In fact, this can be removed by the redefinition the $U(1)$ charge operator as

$$Z'(b) := \langle \psi | e^{2\pi ib \sum_{0 \leq x \leq \ell} (f_x^\dagger f_x - \nu)} | \psi \rangle, \quad (4.31)$$

with ν the filling number per a site. In the present case, ν is given by

$$\nu = \frac{N_F}{L/a} = \frac{2k_F/(2\pi/L)}{L/a} = \frac{k_F a}{\pi}, \quad (4.32)$$

where N_F is the total fermion number of the fermi sea. Then,

$$-2\pi i b \nu \sum_{0 \leq x \leq \ell} = -2\pi i b \frac{k_F a}{\pi} \cdot \frac{\ell}{a} = -2i b k_F \ell, \quad (4.33)$$

which cancels the pure imaginary part of $\log Z(b)$.

2. Partial $(-1)^F$ transformation

Let us consider the partial fermion parity flip on a single interval $I = [0, \ell]$

$$Z((-1)_I^F) = \langle \psi | e^{\pi i \sum_{0 \leq x \leq \ell} f_x^\dagger f_x} | \psi \rangle. \quad (4.34)$$

We have two minima $b = \pm 1/2$, both of which contribute $Z((-1)_I^F)$. This is something like zero modes in the partition function. We have that

$$Z((-1)_I^F) = \sum_{b=\pm 1/2} Z(b) \quad (4.35)$$

$$= 2 \cos(k_F \ell) \cdot \left[2 \sin\left(\frac{\pi \ell}{L}\right) \right]^{-1/2} \cdot \left(\frac{L k_F}{\pi}\right)^{-1/2} \cdot [G(1/2)G(3/2)]^2. \quad (4.36)$$

3. Rényi entanglement entropy

The Rényi entanglement entropy is

$$S_n = \frac{1}{1-n} \sum_{k=-\frac{n-1}{2}, \dots, \frac{n-1}{2}} \ln Z(b = k/n) \quad (4.37)$$

$$= \frac{n+1}{6n} \log \left[\frac{L k_F}{\pi} \cdot 2 \sin\left(\frac{\pi \ell}{L}\right) \right] + \frac{2}{1-n} \sum_{k=-(n-1)/2}^{(n-1)/2} \log [G(1+k/n)G(1-k/n)] \quad (4.38)$$

$$= \frac{n+1}{6n} \log \left[\frac{L k_F}{\pi} \cdot 2 \sin\left(\frac{\pi \ell}{L}\right) \right] + \frac{4}{1-n} f(n), \quad (4.39)$$

where $f(n)$ is given as

$$f(n_o) = \frac{n_o^2 - 1}{n_o} \left(\frac{1}{12} - \log A \right) + \frac{\log n_o}{12 n_o} + \sum_{k=1}^{(n_o-1)/2} \left[(k/n_o) \log \Gamma(k/n_o) - (k/n_o) \log \Gamma(1 - k/n_o) \right] \quad (4.40)$$

$$f(n_e) = \frac{n_e^2 + 1/2}{n_e} \left(\frac{1}{12} - \log A \right) - \frac{\log(n_e/2)}{24 n_e} + \sum_{k=1/2}^{(n_e-1)/2} \left[(k/n_e) \log \Gamma(k/n_e) - (k/n_e) \log \Gamma(1 - k/n_e) \right] \quad (4.41)$$

for odd (even) integers n_o (n_e). A is the Glaisher–Kinkelin constant. Note that the Rényi entanglement entropy S_n satisfies

$$S_n(\ell) = S_n(L - \ell). \quad (4.42)$$

D. Smooth kink adding operator

Let us consider the expectation value of the operator adding a one kink by

$$O = \langle \psi | e^{2\pi i \sum_x x/L} | \psi \rangle. \quad (4.43)$$

The corresponding generating function of the Toeplitz matrix is

$$\psi(\theta) = e^{i\theta}. \quad (4.44)$$

The Toeplitz determinant is zero since O is nothing but the momentum shift

$$O f_k^\dagger O^{-1} = f_{k+2\pi/L}. \quad (4.45)$$

Thus, there is no overlap

$$\langle \psi | O | \psi \rangle = 0. \quad (4.46)$$

E. Smooth function without winding

next, let us consider the expectation value of the operator parametrized by a smooth function $V : S^1 \rightarrow \mathbb{C}^\times$ without winding number.

$$O[V] = \langle \psi | e^{\sum_x V(2\pi x/L) f_x^\dagger f_x} | \psi \rangle. \quad (4.47)$$

The generating function of the Toeplitz matrix is

$$\psi(\theta) = e^{V(\theta)}. \quad (4.48)$$

This has no singularity. The Toeplitz determinant is given as

$$\langle \psi | O[V] | \psi \rangle = \exp \left[\sum_k k V_k V_{-k} \right] = \exp \left[\frac{1}{2\pi} \oint_0^{2\pi} d\theta V(\theta) (-i\partial_\theta) V(\theta) \right] \quad (4.49)$$

with V_k the Fourier component of $V(\theta)$,

$$V_k = \frac{1}{2\pi} \oint_0^{2\pi} d\theta V(\theta) e^{-ik\theta}. \quad (4.50)$$

V. (2+1)D CHERN INSULATOR

As an application of the formula, we estimate the entanglement entropy associated with a disc region for the Chern insulator with a single right-mover chiral mode. We employ the bulk-boundary correspondence: the reduced density matrix ρ_D of a disc region is given by the thermal state of the physical edge excitations

$$\rho_D = \frac{e^{-\frac{\xi}{v} H}}{\text{tr} e^{-\frac{\xi}{v} H}}, \quad (5.1)$$

$$H = \frac{2\pi v}{L} \sum_{m \in \mathbb{Z} + \frac{1}{2}} m : \gamma_m^\dagger \gamma : - \frac{1}{24}, \quad (5.2)$$

where the edge excitations are written by the bulk fermions as

$$\gamma^\dagger \left(\frac{L\phi}{2\pi} \right) \sim (e^{-\phi/2 - \pi i/4} \psi_1^\dagger(r, \phi) + e^{\phi/2 + \pi i/4} \psi_2^\dagger(r, \phi)) e^{-\int^r dr' m(r')}, \quad (5.3)$$

and $L = |\partial D|$. The partial $U_{b,D} = e^{-2\pi i b \sum_{x \in D} \psi_x^\dagger \psi_x}$ transformation induces the U_b action on the edge CFT. We get

$$\langle \psi | U_{b,D} | \psi \rangle \sim \frac{\text{tr} [e^{-2\pi i b \tilde{Q}} e^{-\frac{\xi}{v} H}]}{\text{tr} e^{-\frac{\xi}{v} H}}, \quad \tilde{Q} = \sum_{m \in \mathbb{Z} + \frac{1}{2}} : \gamma_m^\dagger \gamma_m :. \quad (5.4)$$

This is the partition function of the free Dirac fermions. We have

$$\langle \psi | U_{b,D} | \psi \rangle \sim \frac{Z_{\frac{1}{2}, b+\frac{1}{2}}(\frac{i\xi}{L})}{Z_{\frac{1}{2}, \frac{1}{2}}(\frac{i\xi}{L})} = \frac{Z_{\frac{1}{2}-b, \frac{1}{2}}(\frac{iL}{\xi})}{Z_{\frac{1}{2}, \frac{1}{2}}(\frac{iL}{\xi})}. \quad (5.5)$$

For $b \neq 1/2$, the numerator is approximated by the unique vacuum state as

$$Z_{\frac{1}{2}-b, \frac{1}{2}}(\frac{iL}{\xi}) \sim \exp \left[-\frac{2\pi L}{\xi} \left(\frac{1}{2}b^2 - \frac{1}{24} \right) \right], \quad \left(-\frac{1}{2} < b < \frac{1}{2} \right). \quad (5.6)$$

Thus,

$$\langle \psi | U_{b,D} | \psi \rangle \sim \exp \left[-\frac{2\pi L}{\xi} \cdot \frac{1}{2}b^2 \right], \quad \left(-\frac{1}{2} < b < \frac{1}{2} \right). \quad (5.7)$$

The Rényi entanglement entropy is

$$S_N \sim \frac{1}{1-N} \sum_{k=-\frac{N-1}{2}, \dots, \frac{N-1}{2}} \left[-\frac{2\pi L}{\xi} \cdot \frac{1}{2} \left(\frac{k}{N} \right)^2 \right] \quad (5.8)$$

$$= \frac{N+1}{24N} \cdot \frac{2\pi L}{\xi}. \quad (5.9)$$

The Von Neumann Entanglement entropy is

$$S = \lim_{N \rightarrow 1} S_N = \frac{1}{12} \cdot \frac{2\pi L}{\xi}. \quad (5.10)$$

VI. (3+1)D TOPOLOGICAL INSULATOR

Let us consider the three-ball entanglement entropy of the $(3+1)d$ insulator

$$H = \sum_k \psi_k^\dagger \left[\left(\frac{k^2}{2m} - \mu \right) \tau_z + v \tau_x \boldsymbol{\sigma} \cdot \mathbf{k} \right] \psi_k. \quad (6.1)$$

The partial $U(1)$ transformation is approximated as

$$\langle \psi | U_{a,D} | \psi \rangle \sim \frac{\text{tr} \left[e^{-2\pi i a Q} e^{-\frac{\xi}{v} H} \right]}{\text{tr} e^{-\frac{\xi}{v} H}}, \quad (6.2)$$

$$H = \frac{v}{R} \sum_{n \in \mathbb{Z}, n > 0} \sum_{m=-(n-\frac{1}{2}), \dots, n-\frac{1}{2}} [2n \chi_{n,m}^\dagger \chi_{n,m} + 2n \chi_{-n,m} \chi_{-n,m}^\dagger], \quad (6.3)$$

$$Q = \sum_{n \in \mathbb{Z}, n > 0} \sum_{m=-(n-\frac{1}{2}), \dots, n-\frac{1}{2}} [\chi_{n,m}^\dagger \chi_{n,m} - \chi_{-n,m} \chi_{-n,m}^\dagger], \quad (6.4)$$

where R is the radius of the three-ball D . A direct calculation shows

$$\langle \psi | U_{a,D} | \psi \rangle \sim \frac{\prod_{n=1}^{\infty} (1 + e^{-2\pi i a} q^n)^{2n} (1 + e^{2\pi i a} q^n)^{2n}}{\prod_{n=1}^{\infty} (1 + q^n)^{2n} (1 + q^n)^{2n}} \quad (q = e^{-2\xi/R}) \quad (6.5)$$

$$\sim \exp \left[-2(2\xi/R)^{-2} \{ \text{Li}_3(-e^{-2\pi i a}) + \text{Li}_3(-e^{2\pi i a}) \} - 3(2\xi/R)^{-2} \zeta(3) - \frac{1}{3} \log |\cos(\pi a)| \right]. \quad (6.6)$$

The Rényi entanglement entropy is

$$S_N \sim \frac{1}{1-N} \sum_{k=-\frac{N-1}{2}, \dots, \frac{N-1}{2}} \left[-2(2\xi/R)^{-2} \{ \text{Li}_3(-e^{-2\pi i k/N}) + \text{Li}_3(-e^{2\pi i k/N}) \} - 3(2\xi/R)^{-2} \zeta(3) - \frac{1}{3} \log |\cos(\pi k/N)| \right] \quad (6.7)$$

$$= \frac{1}{1-N} \sum_{k=0}^{N-1} \left[-\frac{R^2}{\xi^2} \text{Li}_3(e^{\pi i/N} e^{2\pi i k/N}) - \frac{3\zeta(3)}{4} \frac{R^2}{\xi^2} - \frac{1}{3} \log \sin \left(\frac{\pi}{N} \left(k + \frac{1}{2} \right) \right) \right] \quad (6.8)$$

$$= \frac{3}{4} \zeta(3) \frac{1+N+N^2}{N^2} \frac{R^2}{\xi^2} - \frac{1}{3} \log 2. \quad (6.9)$$

The Von Neumann Entanglement entropy is

$$S = \lim_{N \rightarrow 1} S_N = \frac{9}{4} \zeta(3) \frac{R^2}{\xi^2} - \frac{1}{3} \log 2. \quad (6.10)$$

Here we used

$$\sum_{k=0}^{N-1} \text{Li}_s(z e^{2\pi i k/N}) = N^{1-s} \text{Li}_s(z^N), \quad \text{Li}_3(-1) = -\frac{3}{4} \zeta(3), \quad (6.11)$$

$$\sum_{k=0}^{N-1} \log \sin\left(\frac{\pi}{N} \left(k + \frac{1}{2}\right)\right) = -(N-1) \log 2. \quad (6.12)$$

Appendix A: Toeplitz determinant and Fisher-Hartwig theorem

The symbols of Fisher-Hartwig (FH) class have the following form¹

$$f(z) = e^{V(z)} z^{\sum_{j=0}^m \beta_j} \prod_{j=0}^m |z - z_j|^{2\alpha_j} g_{z_j, \beta_j}(z) z_j^{-\beta_j}, \quad z = e^{i\theta}, \quad 0 \leq \theta \leq 2\pi, \quad (A1)$$

for some $m = 0, 1, 2, \dots$, where

$$z_j = e^{i\theta_j}, \quad j = 0, 1, \dots, m, \quad 0 = \theta_0 < \theta_1 < \dots < \theta_m < 2\pi, \quad (A2)$$

$$g_{z_j, \beta_j}(z) = g_{\beta_j}(z) = \begin{cases} e^{i\pi\beta_j}, & 0 \leq \arg z < \theta_j, \\ e^{-i\pi\beta_j}, & \theta_j \leq \arg z < 2\pi, \end{cases} \quad (A3)$$

$$\text{Re } \alpha_j > -\frac{1}{2}, \quad \beta_j \in \mathbb{C}, \quad j = 0, 1, \dots, m, \quad (A4)$$

and $V(e^{i\theta})$ is a sufficiently smooth function on S^1 . Note that $e^{V(e^{i\theta})}$ has no winding number.

Let $\{n_j\}_{j=0, \dots, m}$ be a set of integers with $\sum_j n_j = 0$, and let $f(z; \hat{\beta})$ denote the Fisher-Hartwig (FH) symbol obtained by replacing β_j with $\hat{\beta}_j = \beta_j + n_j$ and $e^{V(z)}$ by $(\prod_j z_j^{n_j}) e^V = e^{V+i\sum_j n_j \theta_j}$. Then, $f(z; \hat{\beta})$ gives another FH representation for $f(z)$,

$$f(z) = f(z; \hat{\beta}), \quad \hat{\beta}_j = \beta_j + n_j, \quad \sum_j n_j = 0. \quad (A5)$$

Given β , we call

$$O_\beta = \{\hat{\beta}_j = \beta_j + n_j, \sum_j n_j = 0\} \quad (A6)$$

the *orbit* of β . We consider the discrete minimization problem

$$F_\beta = \min_{\hat{\beta} \in O_\beta} \sum_j (\text{Re } \hat{\beta}_j)^2. \quad (A7)$$

Let

$$\mathcal{M}_\beta = \{\hat{\beta} \in O_\beta \mid \sum_j (\text{Re } \hat{\beta}_j)^2 = F_\beta\}. \quad (A8)$$

We say \mathcal{M}_β is *non-degenerate* if $\alpha_j \pm \hat{\beta}_j \neq -1, -2, \dots$ for all j and all $\hat{\beta} \in \mathcal{M}_\beta$.

Theorem Suppose \mathcal{M}_β is non-degenerate. Then, as $n \rightarrow \infty$,

$$D_n(f) = \sum_{\hat{\beta} \in \mathcal{M}_\beta} \left[R_n(f(\hat{\beta})) (1 + o(1)) \right], \quad (A9)$$

Note that this is the **sum of minima**, not the product.

$$R_n(f) = E(e^V, \alpha_0, \dots, \alpha_m, \beta_0, \dots, \beta_m, \theta_0, \dots, \theta_m) \cdot n^{\sum_j (\alpha_j^2 - \beta_j^2)} e^{nV_0} (1 + o(1)), \quad V_0 = \frac{1}{2\pi} \int_0^{2\pi} V(e^{i\theta}) d\theta, \quad (\text{A10})$$

$$E(e^V, \alpha_0, \dots, \alpha_m, \beta_0, \dots, \beta_m, \theta_0, \dots, \theta_m) \quad (\text{A11})$$

$$= E(e^V) \prod_{j=0}^m [b_+(z_j)^{-\alpha_j + \beta_j} b_-(z_j)^{-\alpha_j - \beta_j}] \quad (\text{A12})$$

$$\cdot \prod_{0 \leq j < k \leq m} \left[|z_j - z_k|^{2(\beta_j \beta_k - \alpha_j \alpha_k)} \left(\frac{z_k}{z_j e^{i\pi}} \right)^{\alpha_j \beta_k - \alpha_k \beta_j} \right] \cdot \prod_{j=0}^m \frac{G(1 + \alpha_j + \beta_j) G(1 + \alpha_j - \beta_j)}{G(1 + 2\alpha_j)}. \quad (\text{A13})$$

$$b_+(z) = e^{\sum_{k=1}^{\infty} V_k z^k}, \quad b_-(z) = e^{\sum_{k=-1}^{-\infty} V_k z^k}, \quad (\text{A14})$$

$$E(e^V) = e^{\sum_{k=1}^{\infty} k V_k V_{-k}}, \quad V_k = \text{Fourier coefficient of } V(e^{i\theta}), \quad (\text{A15})$$

$$G(z) = \text{Barnes G-function}, \quad (\text{A16})$$

$$G(1 + z) = (2\pi)^{z/2} \exp\left(-\frac{z + (1 + \gamma)z^2}{2}\right) \prod_{k=1}^{\infty} \left[\left(1 + \frac{z}{k}\right)^k e^{\frac{z^2}{2k} - z} \right]. \quad (\text{A17})$$

$$\ln G(1 + z) = \frac{z}{2} \log(2\pi) - \frac{z + (1 + \gamma)z^2}{2} + \sum_{r=1}^{\infty} \left[r \log(1 + z/r) + \frac{z^2}{2r} - z \right] \quad (\text{A18})$$

$$= \frac{z}{2} - \frac{z + (1 + \gamma)z^2}{2} + \sum_{k=2}^{\infty} (-1)^k \frac{\zeta(k)}{k+1} z^{k+1}, \quad (\text{A19})$$

For $\alpha_j = 0$,

$$E(e^V, \{\alpha_j = 0\}, \{\beta_j\}, \{\theta_j\}) \quad (\text{A20})$$

$$= E(e^V) \prod_{j=0}^m [b_+(z_j)^{\beta_j} b_-(z_j)^{-\beta_j}] \cdot \prod_{0 \leq j < k \leq m} |z_j - z_k|^{2\beta_j \beta_k} \cdot \prod_{j=0}^m [G(1 + \beta_j) G(1 - \beta_j)]. \quad (\text{A21})$$

Here we used $G(1) = 1$. Moreover, if $e^{V(z)}$ is constant, we have that

$$E(e^V = \text{const.}, \{\alpha_j = 0\}, \{\beta_j\}, \{\theta_j\}) = \prod_{0 \leq j < k \leq m} |z_j - z_k|^{2\beta_j \beta_k} \cdot \prod_{j=0}^m [G(1 + \beta_j) G(1 - \beta_j)], \quad (\text{A22})$$

That is to say,

$$R_n(f) = \prod_{0 \leq j < k \leq m} |z_j - z_k|^{2\beta_j \beta_k} \cdot \prod_{j=0}^m [G(1 + \beta_j) G(1 - \beta_j)] \cdot n^{\sum_j (\alpha_j^2 - \beta_j^2)} e^{nV_0} (1 + o(1)) \quad (\text{A23})$$

$$= \prod_{0 \leq j < k \leq m} [2 - 2 \cos(\theta_j - \theta_k)]^{\beta_j \beta_k} \cdot \prod_{j=0}^m [G(1 + \beta_j) G(1 - \beta_j)] \cdot n^{\sum_j (\alpha_j^2 - \beta_j^2)} e^{nV_0} (1 + o(1)). \quad (\text{A24})$$

$$\mathbf{1.} \quad \sum_{k=-\frac{n-1}{2}, \dots, \frac{n-1}{2}} \ln G(1 + k/n)$$

Let

$$f(n) := \sum_{k=-\frac{n-1}{2}, \dots, \frac{n-1}{2}} \ln G(1 + k/n) \quad (\text{A25})$$

$$= -\frac{(1 + \gamma)(n^2 - 1)}{24n} + \sum_{r=1}^{\infty} \left[\frac{n^2 - 1}{24nr} + r \log \left[\left(\frac{1}{nr} \right)^n \left(n \left(r - \frac{1}{2} \right) + \frac{1}{2} \right)_n \right] \right], \quad (\text{A26})$$

where

$$(a)_n = a(a+1)\cdots(a+n) = \frac{\Gamma(a+n)}{\Gamma(a)}. \quad (\text{A27})$$

Some examples (by Mathematica):

$$f(1) = 0, \quad (\text{A28})$$

$$f(2) = \frac{1}{16} \left(-36 \log(A) + 3 + 4 \log \left(\Gamma \left(\frac{1}{4} \right) \right) - 4 \log \left(\Gamma \left(\frac{3}{4} \right) \right) \right), \quad (\text{A29})$$

$$f(3) = \frac{1}{36} \left(-96 \log(A) + 8 + \log(3) + 12 \log \left(\Gamma \left(\frac{1}{3} \right) \right) - 12 \log \left(\Gamma \left(\frac{2}{3} \right) \right) \right), \quad (\text{A30})$$

$$f(4) = \frac{1}{96} \left(-396 \log(A) + 33 - \log(2) + 12 \log \left(\Gamma \left(\frac{1}{8} \right) \right) + 36 \log \left(\Gamma \left(\frac{3}{8} \right) \right) - 36 \log \left(\Gamma \left(\frac{5}{8} \right) \right) - 12 \log \left(\Gamma \left(\frac{7}{8} \right) \right) \right), \quad (\text{A31})$$

$$f(5) = \frac{1}{60} \left(\log(5) - 12 \left(24 \log(A) - 2 + \log \left(\frac{\Gamma(\frac{4}{5})}{\Gamma(\frac{1}{5})} \right) - 2 \log \left(\Gamma \left(\frac{2}{5} \right) \right) + 2 \log \left(\Gamma \left(\frac{3}{5} \right) \right) \right) \right), \quad (\text{A32})$$

$$f(6) = \frac{1}{144} \left[-876 \log(A) + 73 - \log(3) + 36 \log \left(\Gamma \left(\frac{1}{4} \right) \right) - 36 \log \left(\Gamma \left(\frac{3}{4} \right) \right) + 12 \log \left(\Gamma \left(\frac{1}{12} \right) \right) \right. \quad (\text{A33})$$

$$\left. + 60 \log \left(\Gamma \left(\frac{5}{12} \right) \right) - 60 \log \left(\Gamma \left(\frac{7}{12} \right) \right) - 12 \log \left(\Gamma \left(\frac{11}{12} \right) \right) \right], \quad (\text{A34})$$

$$f(7) = \frac{1}{84} \left(\log(7) - 12 \left(48 \log(A) - 4 + \log \left(\frac{\Gamma(\frac{6}{7})}{\Gamma(\frac{1}{7})} \right) - 2 \log \left(\Gamma \left(\frac{2}{7} \right) \right) - 3 \log \left(\Gamma \left(\frac{3}{7} \right) \right) + 3 \log \left(\Gamma \left(\frac{4}{7} \right) \right) + 2 \log \left(\Gamma \left(\frac{5}{7} \right) \right) \right) \right). \quad (\text{A35})$$

These suggests the following general expressions

$$f(n_o) = \frac{n_o^2 - 1}{n_o} \left(\frac{1}{12} - \log A \right) + \frac{\log n_o}{12n_o} + \sum_{k=1}^{(n_o-1)/2} \left[(k/n_o) \log \Gamma(k/n_o) - (k/n_o) \log \Gamma(1 - k/n_o) \right] \quad (\text{A36})$$

$$f(n_e) = \frac{n_e^2 + 1/2}{n_e} \left(\frac{1}{12} - \log A \right) - \frac{\log(n_e/2)}{24n_e} + \sum_{k=1}^{n_e/2} \left[\frac{k-1/2}{n_e} \log \Gamma \left(\frac{k-1/2}{n_e} \right) - \frac{k-1/2}{n_e} \log \Gamma \left(1 - \frac{k-1/2}{n_e} \right) \right] \quad (\text{A37})$$

$$= \frac{n_e^2 + 1/2}{n_e} \left(\frac{1}{12} - \log A \right) - \frac{\log(n_e/2)}{24n_e} + \sum_{k=1/2}^{(n_e-1)/2} \left[(k/n_e) \log \Gamma(k/n_e) - (k/n_e) \log \Gamma(1 - k/n_e) \right]. \quad (\text{A38})$$

where $n_o(n_e)$ represents an odd (even) integer, and A is the Glaisher–Kinkelin constant $A \cong 1.28243$. Recall that $\zeta'(-1, 0) = 1/12 - \ln A$.

Appendix B: Backup

$$\ln[G(1+z)G(1-z)] = (1+\gamma)z^2 - \sum_{k=1}^{\infty} \frac{\zeta(2k+1)}{k+1} z^{2k+2}. \quad (\text{B1})$$

$$\ln G(1+z) = \frac{z(1-z)}{2} + \frac{z}{2} \ln 2\pi + z \ln \Gamma(z) - \int_0^z dx \ln \Gamma(x), \quad (\text{B2})$$

$$G(1+z) = \Gamma(z)G(z), \quad G(1) = 1. \quad (\text{B3})$$

Some useful formulae:²

$$\ln G(1+z) = z \ln \Gamma(z) + \zeta'(-1) - \zeta'(-1, z) \quad (\text{B4})$$

$$= z(\zeta'(0, z) - \zeta'(0)) + \zeta'(-1) - \zeta'(-1, z), \quad (\text{B5})$$

Here, $\zeta(s, a)$ is the Hurwitz zeta function which is defined by the analytic continuation of

$$\zeta(s, a) = \sum_{n=0}^{\infty} \frac{1}{(n+a)^s}, \quad \text{Re } s > 1, \text{Re } a > 0. \quad (\text{B6})$$

$$\zeta'(t, z) = \frac{d}{dt} \zeta(t, z), \quad (\text{B7})$$

$$\zeta'(-1) = \zeta'(-1, 0) = 2 \int_0^{\infty} dx \frac{x \ln x}{e^{2\pi x} - 1} = \frac{1}{12} - \ln A, \quad \zeta'(0) = -\frac{1}{2} \ln(2\pi), \quad (\text{B8})$$

$$\zeta'(-1, z) = \frac{z^2}{2} \ln z - \frac{z^2}{4} - \frac{z}{2} \ln z + 2z \int_0^{\infty} dx \frac{\tan^{-1}(x/z)}{e^{2\pi x} - 1} + \int_0^{\infty} dx \frac{x \ln(x^2 + z^2)}{e^{2\pi x} - 1}, \quad \text{Re } z > 0. \quad (\text{B9})$$

Here, A is the Glaisher–Kinkelin constant $A \cong 1.28243$. We will use

$$\sum_{p=0}^{q-1} \zeta(s, a + p/q) = q^s \zeta(s, qa), \quad \frac{\partial}{\partial a} \zeta(s, a) = -s \zeta(s+1, a). \quad (\text{B10})$$

The former one is shown as

$$\zeta(s, qa) = \sum_{n=0}^{\infty} \frac{1}{(qa+n)^s} = q^{-s} \sum_{n=0}^{\infty} \frac{1}{(a+n/q)^s} = q^{-s} \sum_{p=0}^{q-1} \sum_{n'=0}^{\infty} \frac{1}{(a+p/q+n')^s} = q^{-s} \sum_{p=0}^{q-1} \zeta(s, a+p/q). \quad (\text{B11})$$

At integer $s = n$,

$$\zeta(-n, a) = -\frac{B_{n+1}(a)}{n+1}. \quad (\text{B12})$$

The following may be useful

$$\ln G(1+z) = z \ln \Gamma(1+z) - z \ln z + \zeta'(-1) - \zeta'(-1, z), \quad (\text{B13})$$

$$a. \quad \zeta'(-1, z)$$

$$\left. \frac{d}{ds} \right|_{s \rightarrow -1} \sum_{k=-\frac{n-1}{2}, \dots, \frac{n-1}{2}} \zeta(s, k/n) = \left. \frac{d}{ds} \right|_{s \rightarrow -1} \sum_{k=0}^{n-1} \zeta\left(s, -\frac{n-1}{2n} + \frac{k}{n}\right) \quad (\text{B14})$$

$$= \left. \frac{d}{ds} \right|_{s \rightarrow -1} n^s \zeta\left(s, -\frac{n-1}{2}\right) \quad (\text{B15})$$

$$= \frac{1}{n} \left[\ln(n) \zeta\left(-1, -\frac{n-1}{2}\right) + \zeta'\left(-1, -\frac{n-1}{2}\right) \right]. \quad (\text{B16})$$

Here,

$$\zeta\left(-1, -\frac{n-1}{2}\right) = \begin{cases} -(n^2-1)/8 + \zeta(-1) & (n : \text{odd}) \\ -(n^2+2n-4)/8 + \zeta(-1, 1/2) & (n : \text{even}) \end{cases} \quad (\text{B17})$$

One can use

$$\zeta'(1-2k, 1/2) = -\frac{B_{2k} \ln 2}{4^k k} - \frac{(2^{2k-1}-1)\zeta'(-2k+1)}{2^{2k-1}}, \quad (\text{B18})$$

$$\zeta'(-1, 1/2) = -\frac{B_2 \ln 2}{4} - \frac{\zeta'(-1)}{2} = \frac{1}{2} \ln A - \frac{1}{24} (1 + \ln 2), \quad (\text{B19})$$

$$\zeta(-1) = -\frac{1}{12}, \quad \zeta(-1, 1/2) = \frac{1}{24}. \quad (\text{B20})$$

b. $z\zeta'(0, z)$

$$\left. \frac{d}{ds} \right|_{s \rightarrow 0} \sum_{k=-\frac{n-1}{2}, \dots, \frac{n-1}{2}} (k/n) \zeta(s, k/n) = \left. \frac{d}{ds} \right|_{s \rightarrow 0} \sum_{k=0}^{n-1} \left(-\frac{n-1}{2n} + \frac{k}{n} \right) \zeta \left(s, -\frac{n-1}{2n} + \frac{k}{n} \right). \quad (\text{B21})$$

The first part is given by

$$-\frac{n-1}{2n} \left. \frac{d}{ds} \right|_{s \rightarrow 0} \sum_{k=0}^{n-1} \zeta \left(s, -\frac{n-1}{2n} + \frac{k}{n} \right) = -\frac{n-1}{2n} \zeta \left(0, \frac{n-1}{2} \right) = \frac{1}{4n} (n-1)(n-2). \quad (\text{B22})$$

The second part is

$$\left. \frac{d}{ds} \right|_{s \rightarrow 0} \sum_{k=1}^{n-1} \frac{k}{n} \zeta \left(s, -\frac{n-1}{2n} + \frac{k}{n} \right) \quad (\text{B23})$$

c. Approach from z^{2k+2}

$$f(n, k) := \sum_{r=-\frac{n-1}{2}, \dots, \frac{n-1}{2}} (r/n)^{2k+2} = n^{-2k-2} \left(\zeta \left(-2k-2, \frac{1-n}{2} \right) - \zeta \left(-2k-2, \frac{1-n}{2} + n \right) \right). \quad (\text{B24})$$

$$f(1, k) = 1, \quad \left. \frac{d}{dn} f(n, k) \right|_{n \rightarrow 1} = -2(k+1) \zeta(-2k-1) = B_{2k+2}. \quad (\text{B25})$$

A lesson is that z^{2k+2} is replaced by the Bernoulli numbers B_{2k+2} .

$$\left[\frac{1}{n-1} \cdot \sum_{r=-\frac{n-1}{2}, \dots, \frac{n-1}{2}} \sum_{k=1}^{\infty} \frac{\zeta(2k+1)}{k+1} (r/n)^{2k+2} \right] \Big|_{n \rightarrow 1} = \sum_{k=1}^{\infty} \frac{\zeta(2k+1)}{k+1} B_{2k+2}. \quad (\text{B26})$$

This does not converge...

d. $z \ln \Gamma(1+z)$

$$\ln \Gamma(1+z) = -\gamma z + \int_0^{\infty} \frac{e^{-zt} - 1 + zt}{t(e^t - 1)} dt \quad (\text{B27})$$

$$= \int_0^{\infty} \frac{e^{-zt} - ze^{-t} - 1 + z}{t(e^t - 1)} dt. \quad (\text{B28})$$

Then,

$$\sum_{k=-\frac{n-1}{2}, \dots, \frac{n-1}{2}} (k/n) \left[\frac{e^{-zt} - ze^{-t} - 1 + z}{t(e^t - 1)} \right]_{z \rightarrow k/n} \quad (\text{B29})$$

$$= \frac{e^{-t}}{12n(e^t - 1)t(e^{t/n} - 1)^2} \cdot \left[-2(n^2 - 1)e^{\frac{t}{n} + t} + (n^2 - 1)e^{\frac{2t}{n} + t} + 2(n^2 - 1)e^{t/n} - (n^2 - 1)e^{\frac{2t}{n}} \right. \quad (\text{B30})$$

$$\left. + (n^2 - 1)e^t - n^2 + 6(n-1)e^{\frac{(n+1)t}{2n}} - 6(n-1)e^{\frac{3(n+1)t}{2n}} - 6(n+1)e^{\frac{(n+3)t}{2n}} + 6(n+1)e^{\frac{3n+1}{2n}t} + 1 \right] \quad (\text{B31})$$

$$=: f(t, n). \quad (\text{B32})$$

We have

$$f(t, 1) = 0, \quad \left. \frac{d}{dn} f(t, n) \right|_{n \rightarrow 1} = \frac{e^{-t} (e^{2t} (6t - 8 \sinh(t) + 4 \cosh(t) - 3) - 1)}{6 (e^t - 1)^3 t}, \quad (\text{B33})$$

$$\int_0^\infty \left[\left. \frac{d}{dn} f(t, n) \right|_{n \rightarrow 1} \right] dt \sim -0.0857148. \quad (\text{B34})$$

$$e. \quad -z \ln z$$

$$f. \quad \zeta'(-1) - \zeta'(-1, z)$$

$$\sum_{k=-\frac{n-1}{2}, \dots, \frac{n-1}{2}} \ln G(1 + k/n) = \begin{cases} \sum_{k=0}^{n-1} \ln G(1 + k/n) - \sum_{k=1}^{(n-1)/2} \ln \Gamma(1 - k/n) & (n : \text{ odd}) \\ \sum_{k=0}^{n-1} \ln G(1 + 1/(2n) + k/n) - \sum_{k=0}^{n/2-1} \ln \Gamma(1 - 1/(2n) - k/n) & (n : \text{ even}) \end{cases} \quad (\text{B35})$$

Notice that

$$\sum_{k=0}^{n-1} \zeta(s, z + k/n) = n^s \zeta(s, nz), \quad (\text{B36})$$

$$\zeta(s, -q) = (-q)^{-s} + \zeta(s, 1 - q), \quad (\text{B37})$$

$$\zeta'(s, q) = -sq^{-s-1} \quad (\text{B38})$$

we have for odd n

$$\sum_{k=-\frac{n-1}{2}, \dots, \frac{n-1}{2}} \ln G(1 + k/n) = \sum_{k=0}^{n-1} \ln G(1 + k/n) - \sum_{k=1}^{(n-1)/2} \ln \Gamma(1 - k/n) \quad (\text{B39})$$

$$= \sum_{k=0}^{n-1} (k/n) \ln \Gamma(k/n) + n \zeta'(-1) - \sum_{k=0}^{n-1} \zeta'(-1, k/n) - \sum_{k=1}^{(n-1)/2} \ln \Gamma(1 - k/n). \quad (\text{B40})$$

$$\left. \frac{d}{ds} \left[\sum_{k=0}^{n-1} \zeta(s, k/n) \right] \right|_{s \rightarrow -1} = \left. \frac{d}{ds} \left[n^s \zeta(s) \right] \right|_{s \rightarrow -1} \quad (\text{B41})$$

$$= \left[n^s (\zeta(s) \ln n + \zeta'(s)) \right] \Big|_{s \rightarrow -1} \quad (\text{B42})$$

$$= \frac{1 - \ln n - 12 \ln A}{12n} \quad (\text{B43})$$

$$= \frac{1/12 - \ln A}{n} - \frac{\ln n}{12n}. \quad (\text{B44})$$

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¹ P. Deift, A. Its, and I. Krasovsky, Communications on Pure and Applied Mathematics **66**, 1360 (2012), arXiv:1207.4990.

² V. S. Adamchik, arXiv preprint math/0308086, 18 (2003), arXiv:0308086 [math].