

# Entanglement Entropy in Free Fermionic Hamiltonians

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# Linear Canonical Transformations I

Fermionic anti-commutation relations are defined as follows:

$$\{c_i, c_j\} = \{\tilde{c}_i, \tilde{c}_j\} = 0, \quad \{c_i, \tilde{c}_j\} = \delta_{ij}, \quad (1)$$

where in principle  $\tilde{c}$  does not need to be  $c^\dagger$  but in many applications it turns out to be.

Canonical fermionic transformations are transformations which keep the anti-commutation relations intact: they can be linear or non-linear as well. In this lecture we will entirely concentrate on the linear homogeneous ones. The most general linear homogeneous canonical transformation can be written as

$$\begin{pmatrix} \mathbf{b} \\ \tilde{\mathbf{b}} \end{pmatrix} = \mathbf{T} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}, \quad (2)$$

where  $\mathbf{T}$  satisfies the property:

$$\mathbf{T}\sigma\mathbf{T}^T = \sigma, \quad (3)$$

where we define

# Linear Canonical Transformations II

$$\sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ \cdot \\ \cdot \\ c_N \\ c_1^\dagger \\ c_1^\dagger \\ c_2^\dagger \\ \cdot \\ \cdot \\ c_N^\dagger \end{pmatrix}. \quad (4)$$

It is easy to see that the  $\mathbf{T}$  matrices have a group structure. Note that  $\tilde{\mathbf{b}}$  does not need to be the complex conjugate of  $\mathbf{b}$ . If we force  $\tilde{\mathbf{b}} = \mathbf{b}^\dagger$  then the transformation is called Bogoliubov transformation and it is unitary.

**Question 1:** Write one simple example of non-linear CT.

**Question 2:** Show that the group structure of the  $\mathbf{T}$  matrices is  $O(2N)$ .

# Useful commutation relations

Using  $[A, BC] = \{A, B\}C - B\{A, C\}$  the most basic commutation relations can be calculated as follows:

$$[c_i, c_j^\dagger c_k] = \delta_{ij} c_k, \quad [c_i^\dagger, c_j^\dagger c_k] = -\delta_{ik} c_j^\dagger, \quad (5)$$

and

$$[c_i c_j^\dagger, c_{i'} c_{j'}^\dagger] = \delta_{jj'} c_i c_{j'}^\dagger - \delta_{ij'} c_{i'} c_j^\dagger. \quad (6)$$

Now consider the following quadratic operator:

$$\mathcal{O}_{\mathbf{M}} = \frac{1}{2} (\mathbf{c}^\dagger \quad \mathbf{c}) \mathbf{M} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}, \quad (7)$$

After some algebra it is possible to prove that

$$[\mathcal{O}_{\mathbf{M}_1}, \mathcal{O}_{\mathbf{M}_2}] = \mathcal{O}_{[\mathbf{M}_1, \mathbf{M}_2]}. \quad (8)$$

Note that in the above without losing generality we can assume  $\sigma \mathbf{M}$  is an antisymmetric matrix. **Why?**

Using the standard commutation relations introduced in the previous section it is possible to show a few interesting Lie algebra structures.

**Question 3:** Show that the  $N^2$  operators  $c_i^\dagger c_j$ ,  $i, j = 1, 2, \dots, N$  form the algebra of  $U(N)$ .

For Hamiltonians with just  $c_k^\dagger c_l$  terms the particle number is a conserved quantity and so the relevant Hilbert space is the one with fixed number of fermions. In other words, the basic states in the Hilbert space are  $\{|n_1, n_2, \dots, n_N\rangle\}$ , where  $n_i = 0, 1$  and  $\sum n_i = n$ . The number of basic states are  $\frac{N!}{n!(N-n)!}$ . It is often said that the particle number conservation is a consequence of the  $U(1)$  symmetry. **Why?**

**Question 4:** Consider the  $N(2N - 1)$  operators  $c_i^\dagger c_j - \frac{1}{2}\delta_{ij}$ ,  $i, j = 1, 2, \dots, N$  and  $c_i c_j (c_i^\dagger c_j^\dagger)$ ,  $i \neq j = 1, 2, \dots, N$ . Show that they satisfy the algebra of  $SO(2N)$ .

The basic states in the Hilbert space are  $\{|n_1, n_2, \dots, n_N\rangle\}$ , where  $n_i = 0, 1$  and  $\sum n_i = n$  is odd or even. There are  $2^{N-1}$  states in each sector. This is the consequence of the parity symmetry, i.e.

$$[P, c_j c_k] = [P, c_j^\dagger c_k^\dagger] = [P, c_j^\dagger c_k] = 0, \quad (9)$$

where  $P = (-1)^{\sum_{i=1}^N c_i^\dagger c_i}$ .

**Question 5:** Consider the  $N(2N + 1)$  operators  $c_i^\dagger c_j - \frac{1}{2}\delta_{ij}$ ,  $i, j = 1, 2, \dots, N$  and  $c_i c_j (c_i^\dagger c_j^\dagger)$ ,  $i \neq j = 1, 2, \dots, N$  plus the operators  $c_i$  and  $c_i^\dagger$ ,  $i = 1, 2, \dots, N$ . Show that they satisfy the algebra of  $SO(2N + 1)$ .

# A canonical transformation

Consider the following operator

$$\mathcal{F} = e^{\frac{1}{2}(\mathbf{c}^\dagger \ \mathbf{c})\mathbf{M}\begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}}, \quad (10)$$

where without losing generality we can assume  $\sigma\mathbf{M}$  is antisymmetric matrix. Applying the Baker–Campbell– Hausdorff formula it is easy to show that

$$\mathcal{F}^{-1} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix} \mathcal{F} = \mathbf{T} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}, \quad \mathbf{T} = e^{\mathbf{M}}, \quad (11)$$

with

$$\mathbf{T} = \begin{pmatrix} \mathbf{T}_{11} & \mathbf{T}_{12} \\ \mathbf{T}_{21} & \mathbf{T}_{22} \end{pmatrix}. \quad (12)$$

It has the property:

$$\mathbf{T}\sigma\mathbf{T}^T = \sigma, \quad (13)$$

which is equivalent to say that the transformation  $\mathcal{F}$  is canonical.



# Balian-Brezin decomposition

Using the equations of previous subsection one can now show another very useful formula

$$e^{\frac{1}{2}(\mathbf{c}^\dagger \ \mathbf{c})\mathbf{M}_1} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix} e^{\frac{1}{2}(\mathbf{c}^\dagger \ \mathbf{c})\mathbf{M}_2} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix} = e^{\frac{1}{2}(\mathbf{c}^\dagger \ \mathbf{c})\mathbf{M}} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}, \quad (14)$$

where

$$e^{\mathbf{M}} = e^{\mathbf{M}_1} e^{\mathbf{M}_2}. \quad (15)$$

Finally it is not difficult to show the following equation known as Balian-Brezin decomposition formula

$$e^{\frac{1}{2}(\mathbf{c}^\dagger \ \mathbf{c})\mathbf{M}} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix} = e^{\frac{1}{2}\mathbf{c}^\dagger \mathbf{X} \mathbf{c}^\dagger} e^{\mathbf{c}^\dagger \mathbf{Y} \mathbf{c}} e^{-\frac{1}{2}\text{Tr} \mathbf{Y}} e^{\frac{1}{2}\mathbf{c} \mathbf{Z} \mathbf{c}}, \quad (16)$$

where we have

$$\mathbf{X} = \mathbf{T}_{12}(\mathbf{T}_{22})^{-1}, \quad \mathbf{Z} = (\mathbf{T}_{22})^{-1}\mathbf{T}_{21}, \quad e^{-\mathbf{Y}} = \mathbf{T}_{22}^T \quad (17)$$

Note that  $\mathbf{X}$  and  $\mathbf{Z}$  are anti-symmetric matrices.

# Diagonalization of the free fermionic Hamiltonians I

The Hamiltonian describing a free fermionic system can be written as

$$\mathbf{H} = \sum_{ij=1}^N [c_i^\dagger A_{ij} c_j + \frac{1}{2} c_i^\dagger B_{ij} c_j^\dagger + \frac{1}{2} c_i B_{ji}^* c_j] - \frac{1}{2} \text{Tr} \mathbf{A}^*, \quad (18)$$

where  $c_i^\dagger$  and  $c_i$  are fermionic creation and annihilation operators. To have a consistent Hermitian Hamiltonian we need to consider  $\mathbf{A} = \mathbf{A}^\dagger$  and  $\mathbf{B} = -\mathbf{B}^T$ .

**Question 6:** Why we have not put linear terms in the above Hamiltonian? We first rewrite the Hamiltonian in the matrix form,

$$\mathbf{H} = \frac{1}{2} (\mathbf{c}^\dagger \quad \mathbf{c}) \mathbf{M} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}, \quad (19)$$

where

$$\mathbf{M} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^* & -\mathbf{A}^* \end{pmatrix}, \quad (20)$$

is a Hermitian matrix.

## Diagonalization of the free fermionic Hamiltonians II

There is a unitary matrix which diagonalizes the above matrix as follows:

$$\Lambda = \mathbf{U}\mathbf{M}\mathbf{U}^\dagger. \quad (21)$$

The existence of a unitary matrix which diagonalizes a Hermitian matrix is guaranteed by a theorem. It is not difficult to see that the eigenvalues of the matrix  $\mathbf{M}$  are not only real but appear also in pairs  $\pm\lambda_i$ . Using the above equation, the Hamiltonian becomes,

$$\begin{aligned} \mathbf{H}_D &= \frac{1}{2}(\mathbf{c}^\dagger \ \mathbf{c})\mathbf{U}^\dagger\mathbf{U} \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^* & -\mathbf{A}^* \end{pmatrix} \mathbf{U}^\dagger\mathbf{U} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix} \\ &= \frac{1}{2}(\boldsymbol{\eta}^\dagger \ \boldsymbol{\eta})\Lambda \begin{pmatrix} \boldsymbol{\eta} \\ \boldsymbol{\eta}^\dagger \end{pmatrix}, \end{aligned} \quad (22)$$

where we have introduced new operators  $\eta$ 's,

$$\begin{pmatrix} \boldsymbol{\eta} \\ \boldsymbol{\eta}^\dagger \end{pmatrix} = \mathbf{U} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}. \quad (23)$$

# Diagonalization of the free fermionic Hamiltonians III

It is possible to choose the matrix  $\mathbf{U}$  in a way that the new operators  $\eta_i$  and  $\eta_i^\dagger$  are also fermionic creation and annihilation operators. Such kind of maps are canonical transformations. We have

$$\mathbf{U} = \begin{pmatrix} \mathbf{g} & \mathbf{h} \\ \mathbf{h}^* & \mathbf{g}^* \end{pmatrix}, \quad (24)$$

**Question 7:** Prove the above *non-trivial* statement.

The diagonal matrix  $\Lambda$  can be written as

$$\Lambda = \begin{pmatrix} \Lambda_1 & \mathbf{0} \\ \mathbf{0} & -\Lambda_1 \end{pmatrix}. \quad (25)$$

where the elements of  $\Lambda_1$  are non-negative.

# Diagonalization of the free fermionic Hamiltonians IV

Finally, we can write the diagonalized form of the Hamiltonian as follows:

$$\mathbf{H}_D = \sum_k \lambda_k \eta_k^\dagger \eta_k - \frac{1}{2} \text{Tr} \Lambda_1. \quad (26)$$

Having the diagonalized form of the Hamiltonian one can now calculate all the  $2^n$  energies and eigenstates as follows:

$$E_{\{0,0,\dots,0\}} = -\frac{1}{2} \text{Tr} \Lambda_1, \quad |G\rangle \quad (27)$$

$$E_{\{1,0,\dots,0\}} = E_{\{0,0,\dots,0\}} + \lambda_1, \quad \eta_1^\dagger |G\rangle, \quad \dots \quad (28)$$

$$E_{\{1,1,\dots,0\}} = E_{\{0,0,\dots,0\}} + \lambda_1 + \lambda_2, \quad \eta_2^\dagger \eta_1^\dagger |G\rangle, \quad \dots \quad (29)$$

.

$$E_{\{1,1,\dots,1\}} = E_{\{0,0,\dots,0\}} + \sum_{k=1}^n \lambda_k = \frac{1}{2} \text{Tr} \Lambda_1, \quad \eta_n^\dagger \dots \eta_2^\dagger \eta_1^\dagger |G\rangle, \quad (30)$$

where  $|G\rangle$  is the vacuum defined as  $\eta_k |G\rangle = 0, \forall k$ .

# General results regarding the basic correlation functions

We start with the following definitions:

$$C_{jk} = \text{tr} \rho c_j^\dagger c_k, \quad (31)$$

$$F_{jk} = \text{tr} \rho c_j^\dagger c_k^\dagger, \quad (32)$$

where  $\rho$  is the density matrix. Then it is possible to prove that

$$\mathbf{C}^\dagger = \mathbf{C}, \quad (33)$$

$$\mathbf{F}^T = -\mathbf{F}, \quad (34)$$

Sometimes it is more convenient to work with the Majorana fermions defined as:

$$\gamma_k = c_k + c_k^\dagger, \quad (35)$$

$$\bar{\gamma}_k = i(c_k^\dagger - c_k). \quad (36)$$

With the following commutation relations:

$$\{\gamma_j, \gamma_k\} = \{\bar{\gamma}_j, \bar{\gamma}_k\} = 2\delta_{jk}, \quad \{\gamma_j, \bar{\gamma}_k\} = 0. \quad (37)$$

# General results regarding the basic correlation functions II

The basic correlation functions of Majorana operators can be written as:

$$\langle \gamma_j \gamma_k \rangle = K_{jk}, \quad (38)$$

$$\langle \bar{\gamma}_j \gamma_k \rangle = iG_{jk}, \quad (39)$$

$$\langle \bar{\gamma}_j \bar{\gamma}_k \rangle = \bar{K}_{jk}. \quad (40)$$

Then we have

$$\mathbf{K} = \mathbf{F}^\dagger + \mathbf{F} + \mathbf{I} + \mathbf{C} - \mathbf{C}^T, \quad (41)$$

$$\bar{\mathbf{K}} = -\mathbf{F}^\dagger - \mathbf{F} + \mathbf{I} + \mathbf{C} - \mathbf{C}^T, \quad (42)$$

$$\mathbf{G} = -\mathbf{F}^\dagger + \mathbf{F} - \mathbf{I} + \mathbf{C} + \mathbf{C}^T. \quad (43)$$

We note that the  $\mathbf{K}$  and  $\bar{\mathbf{K}}$  matrices are Hermitian but the  $\mathbf{G}$  in general is not Hermitian except when the  $\mathbf{F}$  matrix is zero. However, the  $\mathbf{G}$  matrix is always real. One can also easily find that the diagonal elements of  $\mathbf{K}$  and  $\bar{\mathbf{K}}$  should be equal to 1. In general we have  $\mathbf{K} + \mathbf{K}^T = 2\mathbf{I}$ .

# General results regarding the basic correlation functions III

One of the key points is to define the following purely imaginary skew symmetric  $\Gamma$  correlation matrix:

$$\Gamma = \begin{pmatrix} \langle \gamma \gamma \rangle - \mathbf{I} & \langle \gamma \bar{\gamma} \rangle \\ \langle \bar{\gamma} \gamma \rangle & \langle \bar{\gamma} \bar{\gamma} \rangle - \mathbf{I} \end{pmatrix} = \begin{pmatrix} \mathbf{K} - \mathbf{I} & -i\mathbf{G}^T \\ i\mathbf{G} & \bar{\mathbf{K}} - \mathbf{I} \end{pmatrix}, \quad (44)$$

where we have  $\Gamma^* = -\Gamma$  and  $\Gamma^\dagger = \Gamma$ . When all the correlation functions are real, then we have:

$$\Gamma = \begin{pmatrix} \mathbf{0} & -i\mathbf{G}^T \\ i\mathbf{G} & \mathbf{0} \end{pmatrix}. \quad (45)$$

which means we need to deal with just one matrix  $\mathbf{G}$ . For example, when we have a Hamiltonian with real parameters the correlation functions for the ground state are all real and the above equation is true. However, when one deals with dynamical problems we do not have real correlations and one should use the equation (44). Since this matrix is purely imaginary skew symmetric matrix the eigenvalues come in pairs of opposite sign  $(\nu, -\nu)$ .



# Basic correlation functions of eigenstates

The basic correlation functions for the ground state can be found easily as follows:

$$\mathbf{C} = \mathbf{h}^\dagger \cdot \mathbf{h} \quad \mathbf{F} = \mathbf{h}^\dagger \cdot \mathbf{g} \quad (46)$$

and then we can show that

$$\mathbf{G} = (\mathbf{h}^\dagger - \mathbf{g}^\dagger)(\mathbf{h} + \mathbf{g}), \quad (47)$$

$$\mathbf{K} = (\mathbf{h}^\dagger + \mathbf{g}^\dagger)(\mathbf{h} + \mathbf{g}), \quad (48)$$

$$\bar{\mathbf{K}} = (\mathbf{h}^\dagger - \mathbf{g}^\dagger)(\mathbf{h} - \mathbf{g}). \quad (49)$$

It is also not difficult to show that we have

$$\bar{\mathbf{K}} = \mathbf{G}\mathbf{K}^{-1}\mathbf{G}^\dagger. \quad (50)$$

In addition when all the correlations are real one can prove that  $\det \mathbf{G} = \pm 1$ .

# Basic correlation functions of eigenstates

The generic excited state can be defined as:

$$|k_1, \dots, k_l\rangle = \eta_{k_1}^\dagger \dots \eta_{k_l}^\dagger |G\rangle, \quad (51)$$

Then after some algebra one can show that

$$\mathbf{C}_{\{k_1, \dots, k_l\}} = \mathbf{h}^\dagger \cdot \mathbf{h} + \mathbf{g}^T \cdot \mathbf{l}' \cdot \mathbf{g}^* - \mathbf{g}^\dagger \cdot \mathbf{l}' \cdot \mathbf{h}, \quad (52)$$

$$\mathbf{F}_{\{k_1, \dots, k_l\}} = \mathbf{h}^\dagger \cdot \mathbf{g} + \mathbf{g}^T \cdot \mathbf{l}' \cdot \mathbf{h}^* - \mathbf{h}^\dagger \cdot \mathbf{l}' \cdot \mathbf{g}, \quad (53)$$

where

$$l'_{kk'} = \begin{cases} \delta_{kk'} & : k \in \{k_1, \dots, k_l\} \\ 0 & : \text{otherwise} \end{cases} \quad (54)$$

Then one can also show that

$$\mathbf{G}_{\{k_1, \dots, k_l\}} = (\mathbf{h}^\dagger - \mathbf{g}^\dagger)(\mathbf{h} + \mathbf{g}) - 2\text{Re}[(\mathbf{h}^\dagger - \mathbf{g}^\dagger) \cdot \mathbf{l}' \cdot (\mathbf{h} + \mathbf{g})], \quad (55)$$

$$\mathbf{K}_{\{k_1, \dots, k_l\}} = (\mathbf{h}^\dagger + \mathbf{g}^\dagger)(\mathbf{h} + \mathbf{g}) - 2i\text{Im}[(\mathbf{h}^\dagger + \mathbf{g}^\dagger) \cdot \mathbf{l}' \cdot (\mathbf{h} + \mathbf{g})], \quad (56)$$

$$\bar{\mathbf{K}}_{\{k_1, \dots, k_l\}} = (\mathbf{h}^\dagger - \mathbf{g}^\dagger)(\mathbf{h} - \mathbf{g}) - 2i\text{Im}[(\mathbf{h}^\dagger - \mathbf{g}^\dagger) \cdot \mathbf{l}' \cdot (\mathbf{h} - \mathbf{g})]. \quad (57)$$

# Trace Formulas

It is easy to show that for example for Hermitian  $\mathbf{M}$  we have:

$$\text{tr} e^{\frac{1}{2}(\mathbf{c}^\dagger \ \mathbf{c})\mathbf{M}} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix} = \det(\mathbf{I} + e^{\mathbf{M}})^{\frac{1}{2}}. \quad (61)$$

One of the frequently occurring example is when  $\mathbf{B} = 0$ . Then we have the following formula:

$$\text{tr} e^{c_i^\dagger A_{ij} c_j} = \det(\mathbf{I} + e^{\mathbf{A}}). \quad (62)$$

Another useful trace formula is the following trace formula for the correlation function of  $\langle \phi_i \phi_j \rangle$ , where  $\phi_{i(j)}$  can be creation and annihilation operators, i.e.  $(\phi_1, \phi_2, \dots, \phi_N, \phi_{N+1}, \phi_{N+2}, \dots, \phi_{2N}) = (c_1, c_2, \dots, c_N, c_1^\dagger, c_2^\dagger, \dots, c_N^\dagger)$ . It is useful to see that  $\{\phi_i, \phi_j\} = \sigma_{ij}$ . Then we have

$$\text{tr}[\phi_i \phi_j e^{\frac{1}{2}(\mathbf{c}^\dagger \ \mathbf{c})\mathbf{M}} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}] = \det(\mathbf{I} + e^{\mathbf{M}})^{\frac{1}{2}} [(\mathbf{I} + e^{\mathbf{M}})^{-1} \sigma]_{ij}, \quad (63)$$

# Wick's theorem

Wick's theorem is a method to reduce expectation value of arbitrary products of creation and annihilation operators to sums of products of pairs of these operators. Although the number of states in the Hilbert space that respect the Wick's theorem is measure zero it turns out that all the eigenstates of quadratic Hamiltonians follow Wick's theorem. Consider  $|0\rangle$  as the vacuum of the annihilation operators  $c_i$ , i.e.  $c_i|0\rangle = 0$  then by direct calculation one can show that

$$\langle 0|\phi_1\dots\phi_n|0\rangle = \sum_{j=2}^n (-1)^j \langle 0|\phi_1\phi_j|0\rangle \langle 0|\phi_2\dots\phi_{j-1}\phi_{j+1}\dots\phi_n|0\rangle \quad (64)$$

where  $\phi$  can be the annihilation  $c_i^\dagger$  or creation  $c_i$  operators. In principle the Wick's theorem is valid for all the operators that can be defined using the creation and annihilation operators with a linear transformation, i.e.

$$\psi_i = \sum \alpha_{ij}\phi_j.$$

**Question 8:** Write the above  $n$ -point function as a pfaffian.

# Gaudin's theorem

There is a generalization of the Wick's theorem which is very useful in statistical physics and applies to thermal averages and it is called Gaudin formula. It is also useful to calculate the reduced density matrix. For density operator  $\rho = \frac{e^{\mathbf{K}}}{\text{Tr}e^{\mathbf{K}}}$  it can be stated as

$$\text{Tr}[\rho\phi_1\dots\phi_n] = \sum_{j=2}^n (-1)^j \text{Tr}[\rho\phi_1\phi_j] \text{Tr}[\rho\phi_2\dots\phi_{j-1}\phi_{j+1}\dots\phi_n], \quad (65)$$

where  $\mathbf{K}$  is a quadratic form of the operators  $\phi$ . Normally  $\mathbf{K}$  is a Hermitian operator, however, to prove the theorem it is not necessary.

**Question 9:** Show that we have Wick's theorem for all the eigenstates of free fermionic Hamiltonians made out of the  $\eta$  operators.

# Eigenstates in the configuration basis and the parity operator I

In this section we write the eigenstates of the quadratic Hamiltonians in the configuration basis. We first remember that for a generic quadratic free fermion Hamiltonian the *parity* is conserved which means that  $[H, P] = 0$ , where  $P = (-1)^{\hat{N}}$  and  $\hat{N} = \sum_{j=1}^N c_j^\dagger c_j$ . If the eigenstate is not degenerate then it is a superposition of states with just even or just odd number of fermions. The parity of the ground state should be found by calculating

$$\langle G|P|G\rangle = \langle G|(-1)^{\hat{N}}|G\rangle = \langle G|\prod_{j=1}^N(1 - 2c_j^\dagger c_j)|G\rangle = i^N \langle G|\prod_{j=1}^N \gamma_j \bar{\gamma}_j|G\rangle. \quad (66)$$

The above correlation can be calculated using the Wick's theorem and can be written as a pfaffian. When the parity is even in especial circumstances one can find the ground state in the configuration basis in an explicit form.

# Eigenstates in the configuration basis and the parity operator II

The idea is based on the following ansatz:

$$|G\rangle = \frac{1}{(\det[\mathbf{I} + \mathbf{R}^\dagger \mathbf{R}])^{\frac{1}{4}}} e^{\frac{1}{2} \sum_{ij} R_{ij} c_i^\dagger c_j^\dagger} |0\rangle, \quad (67)$$

where  $c_j|0\rangle = 0$ . Note that the  $\mathbf{R}$  matrix is an antisymmetric matrix. Since we should have  $\sum (g_{ij} c_j + h_{ij} c_j^\dagger) |G\rangle = 0$ , then one can easily show that

$$\mathbf{g} \cdot \mathbf{R} + \mathbf{h} = 0, \quad (68)$$

where the right hand side is the matrix zero. As far as the matrix  $\mathbf{g}$  has an inverse the above formula can be used easily to find the ground state.

**Question 10:** What should we do if the parity is odd or the matrix  $\mathbf{g}$  does not have an inverse?

**Question 11:** Generalize the above to generic excited states.

# Fermionic coherent states I

Fermionic coherent state is a very useful representation to simplify the calculations. It is defined as

$$|\xi\rangle = |\xi_1, \xi_2, \dots, \xi_N\rangle = e^{-\sum_{k=1}^N \xi_k c_k^\dagger} |0\rangle, \quad (69)$$

where  $\xi_k$ 's are Grassmann variables. It satisfies the following simple property

$$c_i |\xi\rangle = \xi_i |\xi\rangle. \quad (70)$$

The adjoint of the coherent state can be also defined as follows:

$$\langle \xi | c_i^\dagger = \langle \xi | \bar{\xi}_i. \quad (71)$$

The overlap can be calculated easily as

$$\langle \xi | \xi' \rangle = e^{\bar{\xi} \cdot \xi'}. \quad (72)$$

One can also write the following two useful relations:

$$c_i^\dagger |\xi\rangle = -\frac{\partial}{\partial \xi_i} |\xi\rangle, \quad \langle \xi | c_i = \frac{\partial}{\partial \bar{\xi}_i} \langle \xi|. \quad (73)$$



## Fermionic coherent states II

For coherent states the closure relation may be written as

$$\int \prod_i d\bar{\xi}_i d\xi_i e^{-\bar{\xi} \cdot \xi} |\xi\rangle \langle \xi| = 1. \quad (74)$$

Then one can simply expand any state in the coherent basis as follows:

$$|\psi\rangle = \int \prod_i d\bar{\xi}_i d\xi_i e^{-\bar{\xi} \cdot \xi} \psi(\bar{\xi}) |\xi\rangle, \quad (75)$$

where  $\psi(\bar{\xi}) = \langle \xi | \psi \rangle$ . The other important formula is the trace of an arbitrary operator in the coherent basis. It has the following form

$$\text{Tr} \mathbf{A} = \int \prod_i d\bar{\xi}_i d\xi_i e^{-\bar{\xi} \cdot \xi} \langle -\xi | \mathbf{A} | \xi \rangle. \quad (76)$$

The matrix element of a normal-ordered operator  $A(c_i^\dagger, c_i)$  between two coherent states is very simple:

$$\langle \xi | A(\{c_i^\dagger\}, \{c_i\}) | \xi' \rangle = e^{\bar{\xi} \cdot \xi'} A(\{\bar{\xi}_i\}, \{\xi'_i\}). \quad (77)$$

# Fermionic coherent states III

One of the most interesting equations is the following expectation value

$$\langle \xi | e^{c^\dagger A c} | \xi' \rangle = e^{\bar{\xi} \cdot e^A \cdot \xi'} \quad (78)$$

**Question 11:** Prove the above equation.

There is another interesting formula regarding the Grassmann integration of the coherent states with respect to some variables. It can be written as follows

$$\int d\xi_j |\xi_1, \xi_2, \dots, \xi_N\rangle = -|\xi_1, \xi_2, \dots, 1_j, \dots, \xi_N\rangle \quad (79)$$

It means that taking a Grassmann integration over a variable at site  $j$  is like putting a fermion in that site. The above formula can be easily generalized for arbitrary sites.

# End of The First Lecture

## EE in Free Fermionic Hamiltonians: Lecture II

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Topics

# Reduced density matrix I: wave function method: I

We start by writing the density matrix of the vacuum state (even parity)

$$\rho = |C|^2 e^{\frac{1}{2} \sum_{i,j} R_{ij} c_i^\dagger c_j^\dagger} |0\rangle \langle 0| e^{\frac{1}{2} \sum_{i,j} -R_{ij}^* c_i c_j}, \quad (80)$$

where  $C = \frac{1}{\sqrt[4]{\det[I+R^\dagger R]}}$ . One can write the density operator in the coherent basis as follows:

$$\rho(\boldsymbol{\xi}, \boldsymbol{\xi}') = \langle \boldsymbol{\xi} | \rho | \boldsymbol{\xi}' \rangle = |C|^2 e^{\frac{1}{2} \sum_{i,j} R_{ij} \bar{\xi}_i \bar{\xi}_j} e^{-\frac{1}{2} \sum_{i,j} R_{ij}^* \xi'_i \xi'_j}. \quad (81)$$

To calculate the reduced density matrix, we first divide the system into two parts (sets)  $\mathbb{1}$  and  $\mathbb{2}$ , where the full system is given by  $\mathbb{1} + \mathbb{2}$ . To find the RDM for subsystem  $\mathbb{1}$  we need to trace out the subsystem  $\mathbb{2}$ , i.e.

$\rho_{\mathbb{1}} = \text{tr}_{\mathbb{2}} \rho$ . One can write

$$\rho_{\mathbb{1}}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \int \prod_{l \in \mathbb{2}} d\bar{\xi}_l d\xi_l e^{-\sum_{n \in \mathbb{2}} \bar{\xi}_n \xi_n} \langle \xi_1, \dots, \xi_k, -\xi_{k+1}, \dots, -\xi_L | \rho | \xi'_1, \dots, \xi'_k, \xi_{k+1}, \dots, \xi_L \rangle, \quad (82)$$

where indices  $\{1, \dots, k\} \in \mathbb{1}$  and  $\{k+1, \dots, L\} \in \mathbb{2}$ .

# Reduced density matrix I: wave function method: II

After a bit of calculations we get for the reduced density matrix

$$\rho_1(\xi, \xi') = \frac{\sqrt{\det[\mathbb{I} + R_{22}^\dagger R_{22}]}}{\sqrt{\det[\mathbb{I} + R^\dagger R]}} e^{\frac{1}{2}(\bar{\xi} \quad \xi') \Omega \begin{pmatrix} \xi \\ \xi' \end{pmatrix}} \quad (83)$$

where  $\Omega$  matrix is given by

$$\Omega = \begin{pmatrix} R_{11} + R_{12} [R_{22} - (R_{22}^*)^{-1}]^{-1} R_{12}^T & -R_{12} R_{22}^{-1} (R_{22}^{-1} - R_{22}^*)^{-1} R_{12}^\dagger \\ R_{12}^* (R_{22}^{-1} - R_{22}^*)^{-1} R_{22}^{-1} R_{12}^T & -R_{11}^* + R_{12}^* (R_{22}^{-1} - R_{22}^*)^{-1} R_{12}^\dagger \end{pmatrix}.$$

where we divided R matrix into four submatrices  $R_{11}$ ,  $R_{12}$ ,  $R_{21} = -R_{12}^T$  and  $R_{22}$ .

**Question 12:** What should we do if the parity of the ground state is odd?

# Reduced density matrix I: wave function method: III

One can use the above equation to write the operator form of the reduced density matrix. We first need to write

$$\langle \xi | \rho | \xi' \rangle = |C|^2 e^{\sum_{i,j} \frac{1}{2} x_{ij} \bar{\xi}_i \bar{\xi}_j} e^{\sum_{i,j} y_{ij} \bar{\xi}_i \xi'_j} e^{\sum_{i,j} -\frac{1}{2} x_{ij}^* \xi'_i \xi'_j}; \quad (84)$$

with

$$\mathcal{X} = R_{11} - R_{12} \mathcal{Q} R_{22}^* R_{12}^T \quad \text{and} \quad 2\mathcal{Y} = R_{12} \mathcal{Q} R_{12}^\dagger + R_{12}^* \mathcal{Q}^* R_{12}^T, \quad (85)$$

where  $\mathcal{Q} = (I + R_{22}^\dagger R_{22})^{-1}$  and  $|C|^2 = \frac{\sqrt{\det[I + R_{22}^\dagger R_{22}]}}{\sqrt{\det[I + R^\dagger R]}}$ . Next, we can write the reduced density matrix as:

$$\rho_1 = |C|^2 e^{\frac{1}{2} \begin{pmatrix} c^\dagger & c \end{pmatrix} \mathcal{M}_1 \begin{pmatrix} c \\ c^\dagger \end{pmatrix}} e^{\frac{1}{2} \begin{pmatrix} c^\dagger & c \end{pmatrix} \mathcal{M}_2 \begin{pmatrix} c \\ c^\dagger \end{pmatrix}} e^{\frac{1}{2} \begin{pmatrix} c^\dagger & c \end{pmatrix} \mathcal{M}_3 \begin{pmatrix} c \\ c^\dagger \end{pmatrix}} e^{\frac{1}{2} \text{tr} \ln(\mathcal{Y})}, \quad (86)$$

# Reduced density matrix I: wave function method: IV

where  $\mathcal{M}_1$ ,  $\mathcal{M}_2$  and  $\mathcal{M}_3$  are given by

$$\mathcal{M}_1 = \begin{pmatrix} 0 & \mathbf{x} \\ 0 & 0 \end{pmatrix}, \quad \mathcal{M}_2 = \begin{pmatrix} \ln(\mathcal{Y}) & 0 \\ 0 & -\ln(\mathcal{Y}) \end{pmatrix}, \quad \mathcal{M}_3 = \begin{pmatrix} 0 & 0 \\ -\mathbf{x}^* & 0 \end{pmatrix}. \quad (87)$$

These three matrices can be infused together to one matrix  $\mathcal{M}$ . Finally we have a compact operator form for the reduced density matrix as:

$$\rho_1 = |C'|^2 \mathbf{e}^{\frac{1}{2} \begin{pmatrix} c^\dagger & c \end{pmatrix} \mathcal{M} \begin{pmatrix} c \\ c^\dagger \end{pmatrix}}, \quad \text{where } e^{\mathcal{M}} = e^{\mathcal{M}_1} e^{\mathcal{M}_2} e^{\mathcal{M}_3}, \quad (88)$$

where  $|C'|^2 = |C|^2 e^{\frac{1}{2} \text{tr} \ln \mathcal{Y}}$ .

**Question 13:** Simplify the above equation for the real matrix  $R$ ?



## Reduced density matrix II: correlation function method I

Here we will present an alternative form for the reduced density matrix of the eigenstates of the free fermions which uses the Gaudin theorem. Compare to the formulas of the previous section it has its own (dis)advantages. All the calculations are much easier in the Majorana representation. Consider the following generic Hermitian quadratic operator:

$$\mathcal{O} = \sum_{ij=1}^N [c_i^\dagger P_{ij} c_j + \frac{1}{2} c_i^\dagger Q_{ij} c_j^\dagger + \frac{1}{2} c_i Q_{ji}^* c_j] - \frac{1}{2} \text{Tr} \mathbf{P}^*, \quad (89)$$

where  $\mathbf{P}$  and  $\mathbf{Q}$  are Hermitian and antisymmetric matrices respectively. One can write the above operator in the Majorana representation as follows:

$$\mathcal{O} = \frac{1}{4} (\gamma \ \bar{\gamma}) \mathbf{W} \begin{pmatrix} \gamma \\ \bar{\gamma} \end{pmatrix}, \quad (90)$$

$$\mathbf{W} = \begin{pmatrix} \mathbf{P}_a + \mathbf{Q}_s & i(\mathbf{Q}_a + \mathbf{P}_s) \\ i(\mathbf{Q}_a - \mathbf{P}_s) & \mathbf{P}_a - \mathbf{Q}_s \end{pmatrix}, \quad (91)$$

## Reduced density matrix II: correlation function method II

where  $\mathbf{P}_{s(a)} = \frac{\mathbf{P} \pm \mathbf{P}^T}{2}$  and  $\mathbf{Q}_{s(a)} = \frac{\mathbf{Q} \pm \mathbf{Q}}{2}$ . The  $\mathbf{W}$  matrix is purely imaginary antisymmetric matrix (consequently Hermitian) so in principle it can be *block-diagonalized* using an orthogonal matrix  $\mathbf{V}$  then the  $\mathbf{W}$  matrix can be *block-diagonalized* as follows: First we write


$$\frac{1}{4} \mathbf{V} \cdot \mathbf{W} \cdot \mathbf{V}^T = \frac{i}{4} \begin{pmatrix} 0 & \mathbf{D}_1 \\ -\mathbf{D}_1 & 0 \end{pmatrix}, \quad (92)$$

where  $\mathbf{D}_1$  is a diagonal matrix with the modes as entries. Then it is also easy to go back to the normal fermionic representation as follows:

$$\begin{pmatrix} \delta \\ \delta^\dagger \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \cdot \mathbf{V} \begin{pmatrix} \gamma \\ \bar{\gamma} \end{pmatrix}. \quad (93)$$

Finally, we can write the diagonalized form of the operator as follows:

$$\mathcal{O} = \sum_k d_k \delta_k^\dagger \delta_k - \frac{1}{2} \text{Tr} \mathbf{D}_1. \quad (94)$$

The results of this section are an alternative to the results of the section corresponding to the diagonalization of free Hamiltonians too. 

## Reduced density matrix II: correlation function method III

Consider a state which follows Wick's theorem. Then because of Gaudin's theorem one can make the following ansatz for the reduced density matrix of the domain  $D$ :

$$\rho_D = \frac{1}{Z_D} e^{\mathcal{O}}, \quad (95)$$

where we assumed  $\mathcal{O}$  is in the form (91) and  $Z_D = \prod_k 2 \cosh \frac{d_k}{2}$  is the normalization constant. By definition if  $\rho_D$  is the reduced density matrix the correlation functions inside the domain should match to those that one calculates using the state of the full system. First we write the reduced density matrix as follows:

$$\rho_D = \prod_k \frac{e^{-\frac{d_k}{2}} + 2 \sinh \frac{d_k}{2} \delta_k^\dagger \delta_k}{2 \cosh \frac{d_k}{2}}. \quad (96)$$

Then it is easy to show that

$$\langle \delta_k^\dagger \delta_{k'} \rangle = \frac{\delta_{kk'}}{1 + e^{-\frac{d_k}{2}}}, \quad \langle \delta_k \delta_{k'} \rangle = 0. \quad (97)$$

$$\Gamma = \tanh \frac{\mathbf{W}}{2}. \quad (98)$$

At this stage we can also write the equation (97) with respect to the eigenvalues of the  $\Gamma$  matrix, i.e.  $\nu$ 's as follows:

$$\rho_D = \prod_k \left( \frac{1 - \nu_k}{2} + \nu_k \delta_k^\dagger \delta_k \right) = \prod_k \left( \frac{1 + \nu_k}{2} \delta_k^\dagger \delta_k + \frac{1 - \nu_k}{2} \delta_k \delta_k^\dagger \right) \quad (99)$$

Finally the reduced density matrix can be also written as:

$$\rho_D = \left[ \det \frac{I - \Gamma}{2} \right]^{\frac{1}{2}} e^{\frac{1}{4}(\gamma \bar{\gamma}) \cdot \ln \frac{I + \Gamma}{I - \Gamma}} \cdot \begin{pmatrix} \gamma \\ \bar{\gamma} \end{pmatrix}, \quad (100)$$

One can also come back and write the argument of the exponential in the original fermion representation as follows:

$$\rho_D = \left[ \det \frac{I - \Gamma}{2} \right]^{\frac{1}{2}} e^{\frac{1}{2}(\mathbf{c}^\dagger \ \mathbf{c}) \ln \frac{I + \tilde{\Gamma}}{I - \tilde{\Gamma}}} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}, \quad (101)$$

where we have

$$\tilde{\Gamma} = \frac{1}{\sqrt{2}} \begin{pmatrix} I & iI \\ I & -iI \end{pmatrix} \cdot \Gamma \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ -iI & iI \end{pmatrix}. \quad (102)$$

When all the couplings are real like when we are dealing with the eigenstate of a Hamiltonian with real couplings the reduced density matrix can be written as:

$$\rho_D = \det \left[ \frac{1}{2} (I - \mathbf{G}) \right] e^{\mathcal{H}}, \quad (103)$$

$$\mathcal{H} = \frac{1}{2} (\mathbf{c}^\dagger \ \mathbf{c}) \begin{pmatrix} \mathbf{M} & \mathbf{N} \\ -\mathbf{N} & -\mathbf{M} \end{pmatrix} \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix} + \frac{1}{2} \text{Tr} \ln (\mathbf{F}_s), \quad (104)$$

where  $\mathcal{H}$  is the entanglement Hamiltonian and

$$\begin{pmatrix} \mathbf{M} & \mathbf{N} \\ -\mathbf{N} & -\mathbf{M} \end{pmatrix} = \ln \begin{pmatrix} \mathbf{F}_s - \mathbf{F}_a \mathbf{F}_s^{-1} \mathbf{F}_a & \mathbf{F}_a \mathbf{F}_s^{-1} \\ -\mathbf{F}_s^{-1} \mathbf{F}_a & \mathbf{F}_s^{-1} \end{pmatrix}, \quad (105)$$

where  $\mathbf{F}_a = \frac{\mathbf{F} - \mathbf{F}^T}{2}$  and  $\mathbf{F}_s = \frac{\mathbf{F} + \mathbf{F}^T}{2}$  and as before  $\mathbf{F} = \frac{\mathbf{I} + \mathbf{G}}{\mathbf{I} - \mathbf{G}}$ . When the  $\mathbf{G}$  matrix is real and symmetric one can write everything with respect to the  $\mathbf{C}$  matrix as follows:

$$\rho_D = \det[\mathbf{I} - \mathbf{C}] e^{c_i^\dagger (\ln \mathbf{F})_{ij} c_j}, \quad (106)$$

where  $\mathbf{F} = \frac{\mathbf{C}}{\mathbf{I} - \mathbf{C}}$ .

# Reduced density matrix II: correlation function method: Grassmann representation I

The reduced density matrix in the Grassmann representation can be written as follows: We first decompose the reduced density matrix to three exponentials by using Balian-Brezin decomposition and then write every single term in the Grassmann form and then sum up all the arguments of the exponentials. To follow this procedure we first write

$$\Theta = \frac{I + \tilde{\Gamma}}{I - \tilde{\Gamma}} = \begin{pmatrix} \Theta_{11} & \Theta_{12} \\ \Theta_{12}^\dagger & \Theta_{22} \end{pmatrix} = \begin{pmatrix} I & \Theta_{12}\Theta_{22}^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} \Theta_{11} - \Theta_{12}\Theta_{22}^{-1}\Theta_{12}^\dagger & 0 \\ 0 & \Theta_{22} \end{pmatrix} \begin{pmatrix} I & 0 \\ \Theta_{22}^{-1}\Theta_{12}^\dagger & I \end{pmatrix} \quad (107)$$

Then we have

$$\rho_D = \left[ \det \frac{I - \Gamma}{2} \right]^{\frac{1}{2}} e^{\frac{1}{2} \mathbf{c}^\dagger \mathbf{X} \mathbf{c}^\dagger} e^{\mathbf{c}^\dagger \mathbf{Y} \mathbf{c}} e^{-\frac{1}{2} \text{Tr} \mathbf{Y}} e^{\frac{1}{2} \mathbf{c} \mathbf{Z} \mathbf{c}}, \quad (108)$$

where

$$\mathbf{X} = \Theta_{12}\Theta_{22}^{-1}, \quad \mathbf{Z} = \Theta_{22}^{-1}\Theta_{12}^\dagger, \quad e^{-\mathbf{Y}} = \Theta_{22}^T. \quad (109)$$

## Reduced density matrix II: correlation function method: Grassmann representation II

The matrices  $\mathbf{X}$  and  $\mathbf{Z}$  are antisymmetric and  $\mathbf{Y}$  is Hermitian. Since the reduced density matrix should be Hermitian we can also assume that  $\mathbf{Z} = -\mathbf{X}^*$ . Finally the Grassmann representation is as follows:

$$\langle \xi' | \rho_D | \xi \rangle = \left[ \det \frac{I - \Gamma}{2} \right]^{\frac{1}{2}} e^{\frac{1}{2} \bar{\xi}' \mathbf{X} \bar{\xi}' + \bar{\xi}' e^{\mathbf{Y}} \xi - \frac{1}{2} \text{Tr} \mathbf{Y} + \frac{1}{2} \xi \mathbf{Z} \xi}, \quad (110)$$

After a bit of reorganization we have:

$$\langle \xi' | \rho_D | \xi \rangle = \left[ \det \frac{I - \Gamma}{2} \right]^{\frac{1}{2}} e^{-\frac{1}{2} \text{Tr} \mathbf{Y}} e^{\frac{1}{2} (\bar{\xi}' \quad \xi) \mathbf{N} \begin{pmatrix} \bar{\xi}' \\ \xi \end{pmatrix}}, \quad (111)$$

$$\mathbf{N} = \begin{pmatrix} \mathbf{X} & e^{\mathbf{Y}} \\ -e^{\mathbf{Y}^T} & \mathbf{Z} \end{pmatrix}. \quad (112)$$

When all the parameters are real then we can write  $\mathbf{X} = -\mathbf{Z} = \mathbf{F}_a$  and  $e^{\mathbf{Y}} = \mathbf{F}_s$ . Then we have

$$\langle \xi' | \rho_D | \xi \rangle = \left[ \det \frac{I - \mathbf{G}}{2} \right] e^{\frac{1}{2} (\bar{\xi}' - \xi) \mathbf{F} (\bar{\xi}' + \xi)}. \quad (113)$$



# Rényi Entanglement Entropy I: wave function method

The Rényi entanglement entropy is defined as follows:

$$S_\alpha = \frac{1}{1-\alpha} \ln \text{tr} \rho_{\mathbb{1}}^\alpha. \quad (114)$$

Using the equation (89) and (61) one can easily write

$$S_\alpha = \frac{1}{1-\alpha} |C'|^{2\alpha} \det[\mathbb{1} + e^{\alpha \mathcal{M}}]^{1/2}. \quad (115)$$

# Rényi Entanglement Entropy II: correlation function method I

The  $\text{tr}\rho^\alpha$  can be calculated easily by using the trace formulas of lecture I. Then we have

$$\text{tr}\rho^\alpha = \left( \det\left[\left(\frac{I-\Gamma}{2}\right)^\alpha + \left(\frac{I+\Gamma}{2}\right)^\alpha\right] \right)^{\frac{1}{2}} \quad (116)$$

Finally we have:

$$S_\alpha = \frac{1}{1-\alpha} \sum_\nu \ln\left[\left(\frac{1-\nu}{2}\right)^\alpha + \left(\frac{1+\nu}{2}\right)^\alpha\right], \quad (117)$$

where the sum is over all the positive eigenvalues of the purely imaginary skew-symmetric matrix  $\Gamma$ . When  $\alpha = 1$  we have von Neumann entanglement entropy with the following formula:

$$S_{vN} = - \sum_\nu \left(\frac{1-\nu}{2}\right) \ln\left[\frac{1-\nu}{2}\right] + \left(\frac{1+\nu}{2}\right) \ln\left[\frac{1+\nu}{2}\right]. \quad (118)$$

# Rényi Entanglement Entropy II: correlation function method II

When all the couplings are real we can again write everything with respect to the matrix  $\mathbf{G}$  as follows:

$$S_\alpha = \frac{1}{1-\alpha} \text{tr} \ln \left( \frac{I - \sqrt{\mathbf{G}^T \mathbf{G}}}{2} \right)^\alpha + \left( \frac{I + \sqrt{\mathbf{G}^T \mathbf{G}}}{2} \right)^\alpha \mathbb{1} \right) \quad (119)$$

Finally when the matrix  $\mathbf{G}$  is symmetric we can write

$$S_\alpha = \frac{1}{1-\alpha} \text{tr} \ln \left[ \left( I - \mathbf{C} \right)^\alpha + \mathbf{C}^\alpha \right]. \quad (120)$$

The above formulas can be used to calculate bipartite entanglement entropy of the ground state and excited states of the quadratic Hamiltonians. They are valid in any dimension. When the  $\mathbf{G}$  or  $\mathbf{C}$  matrix is a Toeplitz matrix one can do analytical calculations. Otherwise the only way to proceed is numerical calculations.

# Elements of the reduced density matrix in the configurational basis and formation probabilities I

In this part we explain a method to calculate all the elements of the reduced density matrix in the configurational basis. Consider an element of the configurational basis  $|C\rangle$  where  $C$  is a configuration of fermions made of bunch of zeros and ones. Then this configuration can be written in the Grassmann representation as follows:

$$|C\rangle = \int d\xi_k d\xi_j \dots |0, 0, \xi_j, 0, \dots, \xi_k, \dots, 0\rangle = |0, 0, \dots, 1_j, 0, \dots, 1_k, 0, \dots, 0\rangle \quad (121)$$

It means that taking a Grassmann-Berezin integration over a variable at site  $j$  is like putting a fermion in that site. Using the above equation it is easy to calculate

$$\langle C' | \rho_A | C \rangle = \left[ \det \frac{I - \Gamma}{2} \right]^{\frac{1}{2}} e^{-\frac{1}{2} \text{Tr} \mathbf{Y}} \text{pf}[\tilde{\mathbf{N}}], \quad (122)$$

where  $\tilde{\mathbf{N}}$  is the submatrix of the matrix  $\mathbf{N}$ , where the rows and columns corresponding to the sites without fermions have been removed. The Grassmann integration over the rest of the variables gives the Pfaffian.

# Elements of the reduced density matrix in the configurational basis and formation probabilities II

The corresponding submatrices for the diagonal elements are the principal submatrices which their pfaffians give the probabilities. These probabilities are often called formation probabilities. They are all positive. When all the couplings are real we can again write the probabilities with respect to the matrix  $\mathbf{G}$  as follows:

$$p_C = \det\left[\frac{I - \mathbf{G}}{2}\right] \det[\tilde{\mathbf{F}}], \quad (123)$$

where  $\det[\tilde{\mathbf{F}}]$  is the principal minor corresponding to the configuration  $C$ .

# Periodic one dimensional free fermions I

In this section we study the simplest example of free fermion Hamiltonian which is the one dimensional system with periodic boundary conditions. We write the Hamiltonian as follows:

$$H = \sum_{r=-R}^R \sum_{j \in \Lambda} a_r c_j^\dagger c_{j+r} + \frac{b_r}{2} (c_j^\dagger c_{j+r}^\dagger - c_j c_{j+r}) + \text{const.} \quad (124)$$

Using the Majorana operators one can also write,

$$H = \frac{i}{2} \sum_{r=-R}^R \sum_{j \in \Lambda} t_r \bar{\gamma}_j \gamma_{j+r}; \quad (125)$$

where we defined as before the Majorana operators  $\gamma_k = c_k + c_k^\dagger$  and  $\bar{\gamma}_j = i(c_j^\dagger - c_j)$  and  $t_r = -(a_r + b_r)$  and  $t_{-r} = -(a_r - b_r)$ . It is very useful to put the coupling constants as the coefficients of the following holomorphic function  $f(z) = \sum_r t_r z^r$ .

# Periodic one dimensional free fermions II

Then the Hamiltonian can be diagonalized by going to the Fourier space and then Bogoliubov transformation as follows:

$$H = \sum_q |f(q)| \eta_q^\dagger \eta_q + \text{const}, \quad (126)$$

where  $\eta_q = \frac{1}{2}(1 + \frac{f(q)}{|f(q)|})c_q^\dagger + \frac{1}{2}(1 - \frac{f(q)}{|f(q)|})c_{-q}$  with  $f(q) := f(e^{iq})$  and  $q = \frac{2\pi j}{L}$  with  $j = 1, 2, \dots, L$ . Using the dispersion relation  $\epsilon(q) = |f(q)|$  one can distinguish different phases easily as follows: The critical point happens when there is a  $q$  where the gap closes. In other words, when the dispersion relation is zero. This happens just when  $f(z)$  has zero on the unit circle. The number of possible zero's  $n$  can fix the central charge of the corresponding system because one can always linearize the dispersion relation around the zero and have one Majorana field theory with central charge  $c = \frac{1}{2}$  corresponding to that zero. Clearly when there are  $n$  zeros on the unit circle we have  $c = \frac{n}{2}$ .

# Periodic one dimensional free fermions III

One can also define the correlation matrix of the eigenstate of the Hamiltonian (125) like before as  $iG_{jk} = \langle \bar{\gamma}_j \gamma_k \rangle$ , where  $\langle \rangle$  is the expectation value in the ground state. Note that here we have  $\delta_{jk} = \langle \gamma_j \gamma_k \rangle = -\langle \bar{\gamma}_j \bar{\gamma}_k \rangle$  which means that  $\mathbf{K} = \bar{\mathbf{K}} = \mathbf{I}$ . Using the Wick's theorem which is valid for the eigenstates of the above Hamiltonian one can write all the other correlation functions with respect to these three basic correlation functions. Finally after a bit of calculation one can write the following explicit formula for the correlation matrix of the ground state:

$$G_{jk} = \int_0^{2\pi} \frac{dq}{2\pi} \frac{f(q)}{|f(q)|} e^{iq(j-k)}. \quad (127)$$

The above correlation matrix has a Toeplitz structure which makes it a suitable candidate for analytical calculations. It is possible to show that when the gap closes the above correlation function decays like a power-law for large  $|j - k|$  and when there is a gap the above correlation function decays like an exponential.



**Question 14:** Take a simple example of the above Hamiltonian and calculate the EE. Does your example follow an area-law or a logarithmic law?

**Question 15:** Take the Hamiltonian of question 14 and write the reduced density matrix for  $L = 4$  explicitly in the onfiguration basis.

# The End