Practical Fermionic Gaussian States

Fermionic Gaussian States: practical numerical simulations

Author: Jacopo Surace

Institute: Strathclyde, ICFO

Date: March 11, 2020

Version: 1.00

Julia's code on Github

Contents

1 The canonical anticommutation relations **1**
1.1 The Hilbert space characterised by the canonical anticommutation relations . . 1
1.2 Dirac and Majorana representations 2

2 Fermionic Quadratic Hamiltonians **4**
2.1 Dirac Representation 4
2.2 Majorana Representation 4
2.3 Diagonalisation 5
2.4 Numerical diagonalisation 6

3 Fermionic Gaussian States **9**
3.1 Fermionic Gaussian states 9
3.2 Correlation Matrix 9
3.3 Covariance matrix 10
3.4 Wick's theorem 10
3.5 Diagonalisation of the correlation matrix 11
3.6 Eigenvalues of ρ and eigenvalues of Γ 13
3.7 Information measures 13

A Extended calculations **16**
A.1 Eigenvalues of Γ and H_α 16
A.2 Purity 17

B F-utilities **19**

C Useful relations **21**
C.1 Pauli Matrices 21
C.2 Operators obeying CAR 21
C.3 Jordan-Wigner Transformations 22

Chapter 1 The canonical anticommutation relations

1.1 The Hilbert space characterised by the canonical anticommutation relations

Consider a set of operators $\{a_i\}_{i=1}^N$ acting on a Hilbert space $\mathcal{H}$. We say that these operators satisfy the *canonical anticommutation relation* (CAR) when they satisfy

$$\{a_i, a_j^\dagger\} = \mathbb{I}\delta_{i,j}; \qquad \{a_i, a_j\} = 0, \tag{1.1}$$

with $\{a, b\} := ab + ba$ the notation for the anticommutator.

As shown in Nielsen (n.d.) a number of properties of the set of operators $\{a_i\}_{i=1}^N$ and of the Hilbert space $\mathcal{H}$ can be inferred just by the fact that such operators exist and obey the CAR.

The $a_i^\dagger a_i$ are a set of *commuting, hermitian, positive operators* with eigenvalues $\{0, 1\}$. We denote with $\vec{x} \in \{0, 1\}^N$ a binary string of length N with the i-th elements x_i. With $|\vec{x}\rangle$ we identify one of the 2^N states that is the simultaneous eigenstate of $a_i^\dagger a_i$ for all $i = 1, \dots, N$ with eigenvalues respectively x_i. The operator a_i acts as a *lowering operator* for $a_i^\dagger a_i$ and $a_i^\dagger$ acts as a *raising operator* for $a_i^\dagger a_i$ in the sense that

1. If $a_i^\dagger a_i|\vec{x}\rangle = |\vec{x}\rangle$, that is, it has the i-th eigenvalue equal to 1. Then the action of a_i on $|\vec{x}\rangle$ lower the corresponding eigenvalue, meaning that $a_i^\dagger a_i(a_i|\vec{x}\rangle) = 0(a_i|\vec{x}\rangle)$.
2. If $a_i^\dagger a_i|\vec{x}\rangle = 0|\vec{x}\rangle$, that is, it has the i-th eigenvalue equal to 0. Then the action of $a_i^\dagger$ on $|\vec{x}\rangle$ raise the corresponding eigenvalue, meaning that $a_i^\dagger a_i(a_i^\dagger|\vec{x}\rangle) = 1(a_i^\dagger|\vec{x}\rangle)$.

We define an *ordering* by explicitly defining $|\vec{x}\rangle := (a_1^\dagger)^{x_1}(a_2^\dagger)^{x_2} \dots (a_N^\dagger)^{x_N}|\vec{0}\rangle$, where $\vec{0}$ is the string of N zeros. The set $\{|\vec{x}\rangle\}_{\vec{x}\in\{0,1\}^N}$ form an orthonormal basis. If the dimension of the Hilbert space $\mathcal{H}$ is 2^N, then $\{|\vec{x}\rangle\}_{\vec{x}\in\{0,1\}^N}$ is an orthonormal basis of $\mathcal{H}$.

The action of the raising and lowering operators on $|\vec{x}\rangle$ is then

$$a_i|\vec{x}\rangle = \begin{cases} -(-1)^{S^i_{\vec{x}}}|\vec{x}'\rangle \text{ with } x'_i = 0 \text{ and } x'_{j\neq i} = x_{j\neq i}, & \text{if } x_i = 1 \\ 0 & \text{if } x_i = 0 \end{cases}, \tag{1.2}$$

$$a_i^\dagger|\vec{x}\rangle = \begin{cases} 0 & \text{if } x_i = 1 \\ -(-1)^{S^i_{\vec{x}}}|\vec{x}'\rangle \text{ with } x'_i = 1 \text{ and } x'_{j\neq i} = x_{j\neq i}, & \text{if } x_i = 0 \end{cases}, \tag{1.3}$$

with $S^i_{\vec{x}} = \sum_{k=1}^{i-1} x_k$.

In appendix C.2 we report some useful equalities valid for operators satisfying the CAR.

1.2 Dirac and Majorana representations

The raising and lowering operators $a_i^\dagger$,a_i are called *Dirac operators* and they represent the action of adding and removing the i-th fermionic mode.

Both a_i and its adjoint $a_i^\dagger$ are not hermitian. The hermitian combinations of the raising and lowering operators

$$x_i = \frac{a_i + a_i^\dagger}{\sqrt{2}}, \qquad p_i = \frac{a_i - a_i^\dagger}{i\sqrt{2}}, \tag{1.4}$$

are called *Majorana operators*.

The inverse transformations are:

$$a_i = \frac{x_i + i p_i}{\sqrt{2}}, \qquad a_i^\dagger = \frac{x_i - i p_i}{\sqrt{2}}. \tag{1.5}$$

In terms of Majorana operators the CARs read as

$$\{x_i, x_j\} = \{p_i, p_j\} = \delta_{i,j}, \qquad \{x_i, p_j\} = 0. \tag{1.6}$$

Remark Majorana operators labelled by i correspond Dirac operators labelled by i. Moving between Majorana and Dirac operators does not mix modes.

1.2.1 Vector notation

We can collect the Dirac operators of a system with N modes in the vector $\vec{\alpha}$ of length $2N$ defined as

$$\vec{\alpha} = \begin{pmatrix} a_0^\dagger \\ \vdots \\ a_{N-1}^\dagger \\ a_0 \\ \vdots \\ a_{N-1} \end{pmatrix}, \quad \vec{\alpha}^\dagger = \begin{pmatrix} a_0 & \dots & a_{N-1} & a_0^\dagger & \dots & a_{N-1}^\dagger \end{pmatrix}. \tag{1.7}$$

Analogously we can collect the Majorana operators in the vector $\vec{r}$ defined as

$$\vec{r} = \begin{pmatrix} x_0 \\ \vdots \\ x_{N-1} \\ p_0 \\ \vdots \\ p_{N-1} \end{pmatrix}, \tag{1.8}$$

in terms of $\vec{r}$ the CAR are conveniently written as

$$\{r_i, r_j\} = \delta_{i,j}. \tag{1.9}$$

We define the unitary matrix Ω as

$$\Omega = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbb{I} & \mathbb{I} \\ i\mathbb{I} & -i\mathbb{I} \end{pmatrix} \quad , \quad \Omega^{\dagger} = \Omega^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbb{I} & -i\mathbb{I} \\ \mathbb{I} & i\mathbb{I} \end{pmatrix} . \tag{1.10}$$

Such a matrix, applied to the vector of the Dirac operators $\vec{\alpha}$, returns the vector of Majorana operators $\vec{r} = \Omega\vec{\alpha}$.

1.2.2 Fermionic transformation

A transformation $\vec{r} \to \vec{s} = O\vec{r}$ is said to respect the CAR in the Majorana representation if it maps a vector of Majorana operators $\vec{r}$ to a new one $\vec{s} = O\vec{r}$. Mapping Majorana operators vectors to Majorana operators vectors corresponds to

$$\delta_{i,j} = \{s_i, s_j\} = \sum_{k,l} O_{i,k}O_{j,l}\{r_k, r_l\} = (OO^T)_{i,j}, \tag{1.11}$$

thus matrix O must be an orthogonal matrix.

We call *fermionic transformation* any transformation $\vec{\alpha} \to \vec{\beta} = U\vec{\alpha}$ that respects the CAR of the Dirac operators vectors. Matrix U has the form of $U = \Omega^{\dagger}O\Omega$ with O an orthogonal matrix. It has been shown in Bravyi (2004) that fermionic transformations are generated by f.q.h., thus have the general form $U = e^{-i\hat{H}}$, with $\hat{H}$ a generic f.q.h..

1.2.2.1 Clifford Algebra

The $\{r_i\}_{i=1,\dots,2N}$ are hermitian, traceless and generate the Clifford algebra denoted byC_{2N}. Any arbitrary operator $X \in C_{2N}$ can be represented as a polynomial of the Majorana operators as Bravyi (2004)

$$X = \alpha_0\mathbb{I} + \sum_{p=1}^{2N} \sum_{1\leq q_1<\dots<q_p\leq 2N} \alpha_{q_1,\dots,q_p} r_{q_1}\dots r_{q_p}, \tag{1.12}$$

where $\mathbb{I}$ is the identity and the coefficients α_0 and $\alpha_{q_1,\dots,q_p}$ are real. When the representation of $X \in C_{2N}$ involves only even powers of Majorana operators, we call it an *even operator*. If the representation of X involves only odd powers of Majorana operators, then X is called *odd* operator.

We define the *parity operator* as $P = (i2)^N r_1r_2\dots r_{2N} = \prod_{i=1}^{N}(\mathbb{I} - 2a_i^{\dagger}a_i)$.

Every even X operators commute with the parity operator P. The parity p_X of an operator X is defined as $PX = p_X X$ and it can assume just the two values $p \in \{-1, 1\}$.

Fermionic gaussian hamiltonians are even operators. For an N-mode fermionic system with orthonormal basis $\{|\vec{x}\rangle\}$, the matrices $|\vec{x}\rangle\langle\vec{x}|$ defined for every $\vec{x}$ have the polynomial representation

$$|\vec{x}\rangle\langle\vec{x}| = \left(\frac{\mathbb{I}}{2} - i(-1)^{x_1}r_1r_2\right)\left(\frac{\mathbb{I}}{2} - i(-1)^{x_2}r_3r_4\right)\dots\left(\frac{\mathbb{I}}{2} - i(-1)^{x_N}r_{2N-1}r_{2N}\right), \tag{1.13}$$

thus $\{|\vec{x}\rangle\langle\vec{x}|\}$ are all even operators with parity $p_{|\vec{x}\rangle\langle\vec{x}|} = -(-1)^{\sum_{i=1}^{N} x_i}$.

Mixed matrices $|\vec{x}\rangle\langle\vec{x}|$ with $\vec{x}, \neq \vec{x}'$ are odd operators if $\mathrm{mod}(d(\vec{x},\vec{x}'), 2) = 1$, where $d(\vec{x},\vec{y})$ is the hamming distance of $\vec{x}$ and $\vec{y}$, and they are even operators if $\mathrm{mod}(d(\vec{x},\vec{x}'), 2) = 0$.

Chapter 2 Fermionic Quadratic Hamiltonians

2.1 Dirac Representation

The general *fermionic quadratic hamiltonians* (f.q.h.) on a finite lattice of N sites in the Dirac operators representation can be written as

$$\hat{H} = \frac{1}{2} \sum_{i,j=1}^{N} \left(A_{i,j} a_i^\dagger a_j - \bar{A}_{i,j} a_i a_j^\dagger + B_{i,j} a_i a_j - \bar{B}_{i,j} a_i^\dagger a_j^\dagger \right), \tag{2.1}$$

where A is an *hermitian*, $A^\dagger = A$, and B is a *skew-symmetric*, $B^T = -B$, complex matrix. Defining the matrix

$$H = \begin{pmatrix} -\bar{A} & B \\ -\bar{B} & A \end{pmatrix}, \tag{2.2}$$

the compact form of equation (2.1) reads

$$\hat{H} = \frac{1}{2} \vec{\alpha}^\dagger H \vec{\alpha}. \tag{2.3}$$

We will call hamiltonians both $\hat{H}$ and H as for a fized choice of Dirac operators one completely identifies the other.

2.2 Majorana Representation

The Majorana representation of the generic f.q.h. reads as

$$\hat{H} = \frac{i}{2} \sum_{i,j=1}^{N} \left(h_{i,j}^{xx} x_i x_j + h_{i,j}^{pp} p_i p_j + h_{i,j}^{xp} x_i p_j + h_{i,j}^{px} p_i x_j \right) = \frac{i}{2} \vec{r}^\dagger h \vec{r}, \tag{2.4}$$

where

$$ih = \Omega H \Omega^\dagger = i \begin{pmatrix} \{A + B\} & \Re\{A + B\} \\ \Re\{B - A\} & \Im\{A - B\} \end{pmatrix} = i \begin{pmatrix} h^{xx} & h^{xp} \\ h^{px} & h^{pp} \end{pmatrix}. \tag{2.5}$$

Where $\Im\{\cdot\}$ and $\Re\{\cdot\}$ are respectively the imaginary and the real part of their argument. Using the properties of matrices A and B, it is easy to see that matrix h is real and skew-symmetric.

2.3 Diagonalisation

2.3.1 Hamiltonian diagonal form with Dirac operators

Given a particular f.q.h. $\hat{H}$ in the general form (2.1) it is always possible to find a new set of Dirac operators $\{b_k\}_{k=1}^N$ such that $\hat{H}$ in terms of $\{b_k\}_{k=1}^N$ reads as

$$\hat{H} = \frac{1}{2}\sum_{k=1}^{N} \epsilon_k (b_k^\dagger b_k - b_k b_k^\dagger), \tag{2.6}$$

with $\epsilon_k \in \mathbb{R}$ for all $k = 1, 2, \ldots, N$ Lieb et al. (1961).

We call hamiltonians in this form free-free fermion hamiltonians.

In compact form

$$\hat{H} = \frac{1}{2}\vec{\beta}^\dagger H_D \vec{\beta} \tag{2.7}$$

with

$$H_D = U^\dagger H U = \begin{pmatrix} -\epsilon_1 & 0 & \ldots & & \ldots & 0 \\ 0 & \ddots & \ddots & & & \vdots \\ \vdots & \ddots & -\epsilon_N & & & \\ & & & \epsilon_1 & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & 0 \\ 0 & \ldots & & & \ldots 0 & \epsilon_N \end{pmatrix}, \tag{2.8}$$

where U is the fermionic tranformation that diagonalise the hamiltonian.

We will always order the eigenvalues in descending order ($\epsilon_1 \geq \epsilon_2 \geq \cdots \geq \epsilon_N$).

2.3.2 Hamiltonian diagonal form with Majorana operators

In terms of Majorana operators the diagonal form of a generic f.q.h. reads as

$$\hat{H} = \frac{i}{2}\sum_{i=1}^{N} \lambda_i (\tilde{x}_i \tilde{p}_i - \tilde{p}_i \tilde{x}_i). \tag{2.9}$$

for a set of Majorana operators $\{\tilde{x}_i\}_i$, $\{\tilde{p}_i\}_i$. In compact form

$$\hat{H} = \frac{i}{2}\vec{s}^\dagger h_D \vec{s} \tag{2.10}$$

with

$$h_d = O^T h O = \bigoplus_{i=1}^{N} \begin{pmatrix} 0 & \lambda_i \\ -\lambda_i & 0 \end{pmatrix} \tag{2.11}$$

a block diagonal matrix and O the orthogonal transformation that diagonalise the hamiltonian in the Majorana operators representation .

2.4 Numerical diagonalisation

As seen in section 2.3.1, diagonalising a general f.q.h. $\hat{H}$ reduces to diagonalising the matrix H of its compact form.

We are thus interested in finding the fermionic transformation U that maps H and the vector of Dirac operators $\vec{\alpha}$ respectively to the diagonal matrix $H_D = U^\dagger H U$ and to the vector of Dirac operators $\vec{\beta} = U\vec{\alpha}$ such that, in term of $\vec{\beta}$, the hamiltonian is in the diagonal form (2.6).

Here we focus on the numerical approach, we diagonalise the hamiltonian using standard matrix decomposition techniques. For a more physical approach we refer to Lieb et al. (1961).

First step in the diagonalisation procedure is moving to the Majorana representation of H

$$\hat{H} = \frac{1}{2}\vec{\alpha}^\dagger H \vec{\alpha} = \vec{\alpha}^\dagger \Omega^\dagger \Omega H \Omega^\dagger \Omega \vec{\alpha} = \tag{2.12}$$

$$= \frac{i}{2}\vec{r}^\dagger h \vec{r}. \tag{2.13}$$

The following theorem is a standard result in matrix theory Horn and Johnson (1985); Zumino (1962)

Theorem 2.1. Block diagonal form of real, skew-symmetric matrices

Let h be $2N \times 2N$ a real, skew-symmetric matrix. There exist a a real special orthogonal matrix O such that

$$h = O h_D O^T, \tag{2.14}$$

with h_D a block diagonal matrix of the form

$$h_D = \bigoplus_{i=1}^{N} \begin{pmatrix} 0 & \lambda_i \\ -\lambda_i & 0 \end{pmatrix} \tag{2.15}$$

for real, positive definite $\{\lambda_i\}_{i=1,\ldots,N}$. The non-zero eigenvalues of matrix h are the imaginary numbers $\{\pm i\lambda_i\}_{i=1,\ldots,N}$. ♡

Matrix h in (2.4) is real, skew-symmetric, thus, using theorem 2.14 we find the orthogonal transformation O that diagonalise the matrix

$$\hat{H} = \frac{i}{2}\vec{r}^\dagger h \vec{r} = \frac{i}{2}\vec{r}^\dagger O O^\dagger h O O^\dagger \vec{r} = \tag{2.16}$$

$$= \frac{i}{2}\vec{s}^\dagger \left(\bigoplus_{i=1}^{N} \begin{pmatrix} 0 & \lambda_i \\ -\lambda_i & 0 \end{pmatrix} \right) \vec{s} = \frac{i}{2}\vec{s}^\dagger h_D \vec{s} \tag{2.17}$$

That is $\hat{H} = \frac{i}{2}\sum_{i=0}^{N-1} \lambda_i(\tilde{x}_i\tilde{p}_i - \tilde{p}_i\tilde{x}_i)$ once defined the new collection of Majorana operators

$\vec{s} = O\vec{r}$ as

$$\vec{s} = \begin{pmatrix} \tilde{x}_0 \\ \tilde{p}_0 \\ \tilde{x}_1 \\ \tilde{p}_1 \\ \vdots \\ \tilde{x}_{N-1} \\ \tilde{p}_{N-1} \end{pmatrix}. \tag{2.18}$$

The vector of Majorana operators $\vec{s}$ has a different ordering with respect to to the vector $\vec{r}$. We call the order of the operators in $\vec{s}$ an xp ordering and the ordering of the operators in $\vec{r}$ and xx ordering. The transformation matrix $\Omega^\dagger$ maps a vector of Majorana operators in xx ordering to a vector Dirac operators, thus, before being able to move to the Dirac representation we have to reorder the element of vector $\vec{s}$. To do so we use the matrix

$$F_{xp\to xx} = \begin{array}{c} i=0 \\ i=1 \\ \vdots \\ \vdots \\ i=N \\ i=N+1 \\ \vdots \\ i=2N+1 \end{array} \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & \dots & 0 & 0 \\ 0 & \vdots & 1 & \vdots & & & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & & & 0 & \vdots \\ \vdots & 0 & 0 & 0 & & & 1 & \vdots \\ \vdots & 1 & 0 & 0 & & & 0 & \vdots \\ \vdots & 0 & \vdots & 1 & & & \vdots & \vdots \\ \vdots & \vdots & \vdots & 0 & & & \vdots & 0 \\ 0 & 0 & 0 & \vdots & \dots & \dots & 0 & 1 \end{pmatrix} \tag{2.19}$$

that applied to a vector $\vec{s}$ with the xp ordering returns a vector $\vec{\tilde{r}} = F_{xp\to xx}\vec{s}$ with xx ordering. Mapping back to the Dirac representation we obtain the diagonal form of the hamiltonian in the Dirac operators representation as

$$\hat{H} = \frac{i}{2}\left(\vec{s}F^T_{xp\to xx}\Omega\right)\left(\Omega^\dagger F_{xp\to xx} h_D F^T_{xp\to xx}\Omega\right)\left(\Omega^\dagger F_{xp\to xx}\vec{s}\right) = \tag{2.20}$$

$$= \frac{1}{2}\sum_{k=1}^{N} \epsilon_k (b_k^\dagger b_k - b_k b_k^\dagger) = \frac{1}{2}\vec{\beta}^\dagger H_D \vec{\beta}. \tag{2.21}$$

The fermionic transformation U that diagonalise the Hamiltonian H in the form (2.8) is

$$U = \Omega^\dagger \cdot O \cdot F^\dagger_{xp\to xx} \cdot \Omega. \tag{2.22}$$

We note that $\epsilon_k = \lambda_k$.

F-utilities Routine 2.1. `Diag_ferm(`H`)`$\to H_D, U$

This function diagonalise H. H_D is the diagonal form with the first half diagonal negative and the second one positive. U is the fermionic transformation such that: $H = UH_DU^\dagger$. ♠

2.4.1 Block-diagonal form of real skew-symmetric matrices

The matrix decomposition (2.14) of theorem 2.1 is numerically obtained in 3 steps

1. Compute numerically a Schur decomposition (Schur triangularisation as in Horn and Johnson (1985)) of the skew-symmetric matrix h such that: $h = \tilde{O}\tilde{h}_D\tilde{O}^T$. The matrix $\tilde{h}_D$ should be a block-diagonal matrix with each block in the anti-diagonal form
$$\begin{pmatrix} 0 & \tilde{\lambda}_i \\ -\tilde{\lambda}_i & 0 \end{pmatrix}, \tag{2.23}$$
it is not guaranteed that $\tilde{\lambda}_i$ is positive for each i. It is necessary to reorder it.
2. Build the ortogonal matrix $S = \bigoplus_{i=1}^{\lfloor N/2 \rfloor} s_i$ with
$$s_i = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2.24}$$
if $\tilde{\lambda}_i < 0$ or
$$s_i = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{2.25}$$
if $\tilde{\lambda}_i > 0$.
3. The final orthogonal transformation is $O = \tilde{O}S$ such that $h = Oh_DO^T$.

F-utilities Routine 2.2. `Diag_Real_Skew(h)` $\rightarrow h_D, O$

This function implements the algorithm for the block diagonalisation of h a generic skew-symmetric real matrix. h_D is the block-diagonal matrix of (2.14) and has the following property: it is in the block diagonal form, each 2×2 block is skew-symmetric with the upper-right element positive and real and h_D is in ascending order for the upper diagonal. O is an orthogonal matrix such that: $h = Oh_DO^T$. ♠

Chapter 3 Fermionic Gaussian States

3.1 Fermionic Gaussian states

Definition 3.1. Fermionic gaussian state

A state ρ is a fermionic gaussian state (f.g.s.) if it can be represented as

$$\rho = \frac{e^{-\hat{H}}}{Z} = \frac{e^{-\frac{1}{2}\vec{\alpha}^\dagger H\vec{\alpha}}}{Z} \tag{3.1}$$

with $Z := Tr\left[e^{-\hat{H}}\right]$ a normalisation constant and $\hat{H}$ a fermionic gaussian hamiltonian called parent hamiltonian of ρ.

Every possible value of the norm of the hamiltonian is admitted, $\left\|\hat{H}\right\|_1 \in [0, +\infty]$. Both extremum values are reached with a single sided limit procedure in the definition of ρ.

All the information about the state is encoded in the $2N \times 2N$ matrix h at the exponential. ♣

Fermionic gaussian states have an immediate interpretation as thermal Gibbs state of f.q.h.. One can even rescale the parent hamiltonian as $\hat{\hat{H}} = \frac{1}{\beta}\hat{H}$ such that $\left\|\hat{\hat{H}}\right\| = 1$ and $\beta = \frac{1}{\|\hat{H}\|}$. In this way the state reads as $\rho = \frac{e^{-i\beta\hat{\hat{H}}}}{Z}$ with $\beta \in [0, +\infty]$. Since f.g.s are exponential of f.g.h. and f.g.h. are even operator, it follows that f.g.s are even operator.

3.1.1 Single mode Gaussian states

Consider the single mode parent hamiltonian $\hat{H}_1 = \epsilon(b^\dagger b - bb^\dagger)$ of the f.g.s. $\rho = \frac{1}{Z}e^{-\hat{H}_1}$. The explicit representation of ρ on the basis $\{|0\rangle, b^\dagger|0\rangle\}$ is

$$\rho = \begin{pmatrix} 1-f & 0 \\ 0 & f \end{pmatrix} \tag{3.2}$$

where $f = \langle 0|\rho|0\rangle$ and the two coherences are 0 because we cannot have the odd terms $|0\rangle\langle 1|$ and $|1\rangle\langle 0|$ in the expansion of the even operator ρ. Using the polynomial expansion (1.13) we can see that $f = \mathrm{Tr}\left[\rho b^\dagger b\right] := \langle b^\dagger b\rangle$, that is the occupation of the mode fermionic mode, thus a single mode gaussian state is completely characterised by the occupation $\langle b^\dagger b\rangle$.

3.2 Correlation Matrix

We have seen that for any f.q.h. H it is always possible to find a fermionic transformation U that diagonalise H transforming the Dirac operators vector as $\vec{\beta} = U\vec{\alpha}$. Diagonalising the parent hamiltonian of a f.g.s. ρ we obtain its decomposition in terms of single-mode thermal states

$$\rho = \frac{e^{-\frac{1}{2}\vec{\beta}^\dagger H_D\vec{\beta}}}{Z} = \frac{1}{Z}\bigotimes_{k=1}^{N} e^{-i\epsilon_k(b_k^\dagger b_k - b_k b_k^\dagger)}. \tag{3.3}$$

Each single-mode thermal state is completely characterised by its occupation number, thus ρ is completely characterised by the set of occupations $\{\langle b_i^\dagger b\rangle\}_{i=1}^N$. Expressing the occupations in term of the operators $\vec{\alpha} = U^\dagger \vec{\beta}$, we find that every f.g.s. is *completely characterised* by the collection of all the correlators $\Gamma_{i,j}^{a^\dagger a} := \langle a_i^\dagger a_j\rangle$ and $\Gamma_{i,j}^{aa} := \langle a_i a_j\rangle$. We collect these correlators in the so called *correlation matrix*

$$\Gamma := \langle \vec{\alpha}\vec{\alpha}^\dagger\rangle = \begin{pmatrix} \Gamma^{a^\dagger a} & \Gamma^{a^\dagger a^\dagger} \\ \Gamma^{aa} & \Gamma^{aa^\dagger} \end{pmatrix} \tag{3.4}$$

with $\Gamma_{i,j}^{aa} := \langle a_i a_j\rangle = -\overline{\Gamma_{i,j}^{a^\dagger a^\dagger}}$ and $\Gamma_{i,j}^{aa^\dagger} := \langle a_i a_j^\dagger\rangle = (\overline{\mathbb{I} - \Gamma^{a^\dagger a}})_{i,j}^T$, where $\overline{A}$ is the conjugate of A. The correlation matrix Γ is hermitian, Γ^{aa} and $\Gamma^{a^\dagger a^\dagger}$ are skew-symmetric, and $\Gamma^{a^\dagger a}$ and $\Gamma^{aa^\dagger}$ are hermitian.

Expressed in term of Majorana operator the correlation matrix is defined as

$$\Gamma^{maj} := \langle \vec{r}\vec{r}^\dagger\rangle = \Omega\Gamma\Omega^\dagger. \tag{3.5}$$

It interesting observing that, since a f.g.s. is completely described by its correlation matrix, with the spirit of the maximum entropy principle (see Jaynes (1957a,b)), it is possible to equivalently define fermionic gaussian states as the states that maximise the von Neumann entropy given the expectation values collected in the correlation matrix.

3.3 Covariance matrix

The *covariance matrix* of a f.g.s. is the real, skew-symmetric matrix defined as

$$\gamma := iTr\left[\rho[\vec{r}_i, \vec{r}_j]\right], \tag{3.6}$$

with $[\vec{r}_i, \vec{r}_j]$ the commutator of the two Majorana operators $\vec{r}_i$ and $\vec{r}_j$.

As for the correlation matrix, the covariance matrix of a f.g.s ρ completely describes the states. In fact γ and Γ are related by the equality

$$\gamma = -i\Omega\,(2\Gamma - \mathbb{I})\,\Omega^\dagger = -i\left(2\Gamma^{maj} - \mathbb{I}\right). \tag{3.7}$$

In this text we will use both the covariance matrix and the correlation matrix approach.

3.4 Wick's theorem

As mentioned, f.g.s. are fully characterised by their covariance matrix. This means that it must be possible to obtain the expectation value of every operator X from γ solely. To do so we just need to take the polynomial expansion (1.12) of X and apply the celebrated Wick's theorem Molinari (2017) to each monomial term. The Wick's theorem states that for a f.g.s. ρ and a monomial of Majorana operators $r_{q_1} r_{q_2} \dots r_{q_p}$ one has

$$\mathrm{Tr}\left[\rho r_{q_1} r_{q_2} \dots r_{q_p}\right] = \mathrm{Pf}(\gamma_{|q_1,q_2,\dots,q_p}) \tag{3.8}$$

where $1 \leq q_1 < q_2 < \cdots < q_p \leq 2N$, $\gamma_{|q_1,q_2,\ldots,q_p}$ is the restriction of the covariance matrix to all the two point correlators involving just the Majorana operators $\{r_{q_1}, r_{q_2}, \ldots, r_{q_p}\}$ and Pf() is called the Pfaffian. Since the Pfaffian is nonvanishing only for $2N \times 2N$ skew-symmetric matrix, it is clear that the expectation value of any odd operators is always zero.

Example 3.1 Consider a system composed by 2 fermionic modes corresponding to the Dirac operators a_1 and a_2. The Majorana operators vector is $\vec{r} = (r_1, r_2, r_3, r_4)$, thus the covariance matrix takes the form

$$\gamma = \begin{pmatrix} 0 & \langle r_1, r_2\rangle & \langle r_1, r_3\rangle & \langle r_1, r_4\rangle \\ -\langle r_1, r_2\rangle & 0 & \langle r_2, r_3\rangle & \langle r_2, r_4\rangle \\ -\langle r_1, r_3\rangle & -\langle r_2, r_3\rangle & 0 & \langle r_3, r_4\rangle \\ -\langle r_1, r_4\rangle & -\langle r_2, r_4\rangle & -\langle r_3, r_4\rangle & 0 \end{pmatrix} \tag{3.9}$$

where $\langle r_i, r_j\rangle := i\mathrm{Tr}\left[\rho[r_i, r_j]\right]$. Using Wick's theorem we have that

$$\mathrm{Tr}\left[\rho r_1 r_2 r_3 r_4\right] = \mathrm{Pf}\begin{pmatrix} 0 & \langle r_1, r_2\rangle & \langle r_1, r_3\rangle & \langle r_1, r_4\rangle \\ -\langle r_1, r_2\rangle & 0 & \langle r_2, r_3\rangle & \langle r_2, r_4\rangle \\ -\langle r_1, r_3\rangle & -\langle r_2, r_3\rangle & 0 & \langle r_3, r_4\rangle \\ -\langle r_1, r_4\rangle & -\langle r_2, r_4\rangle & -\langle r_3, r_4\rangle & 0 \end{pmatrix} = \tag{3.10}$$

$$= \langle r_1, r_2\rangle\langle r_3, r_4\rangle - \langle r_1, r_3\rangle\langle r_2, r_4\rangle + \langle r_2, r_3\rangle\langle r_1, r_4\rangle, \tag{3.11}$$

and

$$\mathrm{Tr}\left[\rho r_2 r_4\right] = \mathrm{Pf}\begin{pmatrix} 0 & \langle r_2, r_4\rangle \\ -\langle r_2, r_4\rangle & 0 \end{pmatrix} = \langle r_2, r_4\rangle, \tag{3.12}$$

and

$$\mathrm{Tr}\left[\rho r_1 r_2 r_4\right] = \mathrm{Pf}\begin{pmatrix} 0 & \langle r_1, r_2\rangle & \langle r_1, r_4\rangle \\ -\langle r_1, r_2\rangle & 0 & \langle r_2, r_4\rangle \\ -\langle r_1, r_4\rangle & -\langle r_2, r_4\rangle & 0 \end{pmatrix} = 0. \tag{3.13}$$

3.5 Diagonalisation of the correlation matrix

In section 3.2 we have seen that any f.g.s. ρ can be expressed as a tensor product of single mode thermal states

$$\rho = \frac{e^{-\frac{1}{2}\vec{\beta}^\dagger H_D \vec{\beta}}}{Z} = \frac{1}{Z}\bigotimes_{k=1}^{N} e^{-i\epsilon_k (b_k^\dagger b_k - b_k b_k^\dagger)}. \tag{3.14}$$

for a particular choice of Dirac operators b_i. Expressed in this basis the correlation matrix, as well as the density matrix of the state, are in diagonal form.

This tells us that for every correlation matrix Γ there exist a fermiomic transformation U such that Γ can be brought in the diagonal form

$$\Gamma^D = U^\dagger \Gamma U = \begin{pmatrix} \nu_1 & 0 & \dots & & \dots & 0 \\ 0 & \ddots & \ddots & & & \vdots \\ \vdots & \ddots & \nu_N & & & \\ & & & 1-\nu_1 & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & 0 \\ 0 & \dots & & & \dots 0 & 1-\nu_N \end{pmatrix}, \tag{3.15}$$

with $\nu_i \in [0,1]$ the occupation number of the i-th free mode. To numerically obtain the diagonal form of the correlation matrix we notice that the covariance matrix γ is a real, skew-symmetric matrix, thus using theorem 2.1 we know that we can find an orthogonal transformation O such that

$$\gamma = O\gamma^D O^T = O\left(\bigoplus_{i=1}^{N}\begin{pmatrix} 0 & \eta_i \\ -\eta_i & 0 \end{pmatrix}\right)O^T \tag{3.16}$$

with $\eta_i \in [-\frac{1}{2}, \frac{1}{2}]$.

Following the same procedure of section 2.4, we can write the diagonal elements of Γ^D as

$$\nu_i = \frac{1}{2} - \eta_i. \tag{3.17}$$

The elements of H_D and Γ^D are related as

$$\epsilon_k = \ln\left(\frac{1-\nu_k}{\nu_k}\right), \tag{3.18}$$

$$\nu_k = \frac{1}{1+e^{\epsilon_k}} \tag{3.19}$$

with $\nu_k \in [0,1]$ and $\epsilon_k \in [-\infty, +infty]$ where the boundary values are take with a limit. The complete calculation can be found in appendix . In general the correlation matrix Γ and the parent hamiltonian H are related as Cheong and Henley (2003); Peschel (2003a); Vidal et al. (2003); Zhang et al. (2020)

$$\Gamma = \frac{1}{1+e^H}. \tag{3.20}$$

F-utilities Routine 3.1. `Diag_Gamma(Γ)` $\to \Gamma^D, U$

This function returns Γ^D, the the diagonal form of the Dirac correlation matrix Γ and U the fermionic transformation such that $\Gamma = U\Gamma^D U\dagger$. ♠

3.5.0.1 Reduced density matrix

Trying to define a partial trace over fermionic modes subspaces one soon faces the what is often called the "partial trace ambiguity" Friis et al. (2013).

In the case of fermionic gaussian states, though, this is a much simpler task. Any reduced state formalism has to satisfy the simple criterion that the reduced density operator contains all the information about the subsystem that can be obtained from the global state when measurements are performed only on the respective subsystem alone Friis et al. (2013).

With Wick's theorem in mind it is easy to see that the correlation matrix of the reduced state on the modes $i_1, \ldots, i_m$ is just the correlation matrix $\Gamma|_{\{i_1,\ldots,i_m\}}$.

F-utilities Routine 3.2. `Reduce_Gamma(Γ,m,i_1)` $\to \Gamma|_{\{i_1,\ldots,i_m\}}$

This function takes a Dirac correlation matrix Γ, a dimensione of the partition m and the initial site of the partition i_1 and return $\Gamma|_{\{i_1,\ldots,i_m\}}$, the reduced correlation matrix on the contiguous modes $\{i_1, \ldots, i_m\}$. ♠

3.6 Eigenvalues of ρ and eigenvalues of Γ

Consider the fermionic gaussian state $\rho = \frac{e^{-\frac{1}{2}\vec{\alpha}^\dagger H \vec{\alpha}}}{Z}$ and its correlation matrix Γ. The diagonal form Γ^D of correlation matrix tells us that a basis exists in which the density matrix ρ of the state can be written as the tensor product of N density matrices, one for each site. If $\nu_{i\in[1,N]}$ are the positive eigenvalues of Γ then there exists a basis such that:

$$\rho = \bigotimes_{i=1}^{N} \begin{pmatrix} \nu_i & 0 \\ 0 & 1-\nu_i \end{pmatrix} \tag{3.21}$$

Thus the if we denote each of the 2^N eigenvalues $\pi_{\vec{x}}$ of ρ with a binary string $\vec{x} \in \{0,1\}^N$ we have that: $\pi_{\vec{x}} = \prod_{i=1}^{N} (\vec{x}_i \nu_i + (1-\vec{x}_i)(1-\nu_i))$.

F-utilities Routine 3.3. `Eigenvalues_of_rho(Γ)` $\to \vec{\nu}$

This function return the eigenvalues of the correlation matrix ρ associated to the fermionic gaussian state with Dirac correlation matrix Γ. ♠

3.7 Information measures

3.7.1 Von Neumann Entropies

The Von Neumann entropy of a quantum state described by the density matrix ρ is

$$S(\rho) = -\mathrm{Tr}\left[\rho \ln(\rho)\right]. \tag{3.22}$$

In terms of the eigenvalues λ of ρ, the Von Neumann entropy read as

$$S(\rho) = -\sum_{\lambda} \lambda \ln(\lambda) \tag{3.23}$$

If ρ is a Fermionic Gaussian state of a system with N sites , substituting in (3.22) the product form (3.21), the Von Neumann entropy becomes a function of the eigenvalues ν_i of the correlation matrix Γ and it is the sum of just $2N$ terms

$$S(\Gamma) \equiv S(\rho) = -\sum_{i=1}^{N} \left(\nu_i \ln(\nu_i) + (1-\nu_i)\ln(1-\nu_i)\right). \tag{3.24}$$

F-utilities Routine 3.4. `VN_Entropy(Γ)` $\longrightarrow S$

This function return S, the `Float64` value of the Von Neumann Entropy of the state described by the Dirac correlation matrix Γ. ♠

3.7.2 Purity

The purity of a state ρ is defined as

$$\text{Purity} \equiv Tr\left[\rho^2\right]. \tag{3.25}$$

We have that:

$$\text{Purity} = \prod_{i=1}^{N-1} \frac{1}{\text{sech}(\epsilon_i)+1}, \tag{3.26}$$

$$\text{Purity} = \prod_{i=1}^{N-1} (2\,(\nu_i - 1)\,\nu_i + 1), \tag{3.27}$$

$$\text{Purity} = \prod_{i=1}^{N-1} \left(2\eta_i^2 + \frac{1}{2}\right). \tag{3.28}$$

For more details see appendix A.2.

F-utilities Routine 3.5. `Purity(Γ)` $\longrightarrow p$

This function return p the purity of the fermionic gaussian state with Dirac correlation matrix Γ. ♠

3.7.3 Entanglement Contour

In 2014 Chen and Vidal Chen and Vidal (2014) introduced entanglement contour "a tool for identifyng which real-space degrees of freedom contribute, and how much, to the entanglement of a region A with the rest of the system B". We will present here a specific form of entanglement contour, for a more general treatment we refer to the original paper of Chen and Vidal.

We restrict to pure states.

Consider an Hilbert space $\mathcal{H}$ arbitrarily divided in two partitions $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. The Schmidt decomposition of a pure state $|\psi^{A,B}\rangle$ in $\mathcal{H}$ is

$$|\psi^{A,B}\rangle = \sum_i \sqrt{p_i}|\psi_i^A\rangle \otimes |\psi_i^B\rangle, \tag{3.29}$$

with $p_i \geq 0$, $\sum_i p_i = 1$ and

$$\rho^A \equiv Tr_B\left[|\psi^{A,B}\rangle\langle\psi^{A,B}|\right] = \sum_i p_i |\psi_i^A\rangle\langle\psi_i^A|. \tag{3.30}$$

Factorising Hilbert space $\mathcal{H}_A$ in its tensor product structure $\mathcal{H}_A = \bigotimes_{j \in A} \mathcal{H}_j$, we individuate in each local Hilbert space $\mathcal{H}_j$ a site of the partition A. Genarelly ρ^A cannot be expressed as a product state over this factorisation of $\mathcal{H}_A$.

Chen and Vidal entanglement contour c_A is a function of the sites j of partition A ($c_A : A \longrightarrow \mathbb{R}$) that attempts to express the contribution of each site to the total von Neumann entropy $S(\rho^A)$ of partition A.

The definition of entanglement contour is based on five constraints (see Chen and Vidal (2014) for the complete definition) that any possible entanglement contour function must satisfy. These constraints are not tight, thus there exist many possible functions that can be regarded as entanglement contour.

We consider an entanglement contour specifically defined for Fermionic Gaussian states (for other entanglement contours see i.e. Coser et al. (2017); Tonni et al. (2018)).

Appendix Extended calculations

A.1 Eigenvalues of Γ and H_α

We consider the state $\rho = \frac{e^{-\frac{1}{2}\vec{\alpha}^\dagger H \vec{\alpha}}}{Z}$, we diagonalise H changing the basis to $\vec{\beta} = U^\dagger \vec{\alpha}$. Thus we have

$$\rho = \frac{e^{-\frac{1}{2}\vec{\beta}^\dagger H_D \vec{\beta}}}{Z} = \frac{e^{-\frac{1}{2}\sum_{k=0}^{N-1} \epsilon_k \left(b_k^\dagger b_k - b_k b_k^\dagger\right)}}{Z}. \tag{A.1}$$

We change the basis of the correlation matrix too

$$\Gamma^b_{i,j} = \left(U^\dagger \Gamma U\right)_{i,j} = Tr\left[\rho \vec{\beta}_i \vec{\beta}_j^{\,\dagger}\right]. \tag{A.2}$$

Now we want to explicitly compute the elements of Γ^b. First of all we compute the normalisation constant

$$Z = Tr\left[e^{-\frac{1}{2}\sum_{k=0}^{N-1} \epsilon_k \left(b_k^\dagger b_k - b_k b_k^\dagger\right)}\right] = \prod_{k=1}^{N-1}\left(2\cosh\left(\frac{\epsilon_k}{2}\right)\right). \tag{A.3}$$

To compute the numerator part this equalities will result useful

- For $x \neq y$

$$\begin{aligned} Tr\left[e^{-\frac{1}{2}\sum_{k=0}^{N-1} \epsilon_k \left(b_k^\dagger b_k - b_k b_k^\dagger\right)} b_x^\dagger b_y\right] &= \sum_{v\in\{0,1\}^N} \langle v| e^{-\frac{1}{2}\sum_{k=0}^{N-1} \epsilon_k \left(b_k^\dagger b_k - b_k b_k^\dagger\right)} b_x^\dagger b_y |v\rangle = \\ &= \sum_{v\in\{0,1\}^N} \langle v| e^{-\frac{1}{2}\sum_{k=0}^{N-1} \epsilon_k \left(b_k^\dagger b_k - b_k b_k^\dagger\right)} |\tilde{v}\rangle = \\ &= \sum_{v\in\{0,1\}^N} e^{-\frac{1}{2}\sum_{k=0}^{N-1}(-1)^{v_k+1}\epsilon_k} \langle v|\tilde{v}\rangle = 0 \end{aligned} \tag{A.4}$$

$$Tr\left[e^{-\frac{1}{2}\sum_{k=0}^{N-1} \epsilon_k \left(b_k^\dagger b_k - b_k b_k^\dagger\right)} b_x b_y^\dagger\right] = 0 \tag{A.5}$$

-

- $\forall x, y$

$$Tr\left[e^{-\frac{1}{2}\sum_{k=0}^{N-1} \epsilon_k \left(b_k^\dagger b_k - b_k b_k^\dagger\right)} b_x b_y\right] = 0 \tag{A.6}$$

$$Tr\left[e^{-\frac{1}{2}\sum_{k=0}^{N-1} \epsilon_k \left(b_k^\dagger b_k - b_k b_k^\dagger\right)} b_x^\dagger b_y^\dagger\right] = 0 \tag{A.7}$$

Thus the numerator can be explicitly written as

$$Tr\left[e^{-\frac{1}{2}\sum_{k=0}^{N-1} \epsilon_k \left(b_k^\dagger b_k - b_k b_k^\dagger\right)} \vec{\alpha}_i \vec{\alpha}_j^{\,\dagger}\right] = \tag{A.8}$$

$$= \sum_{l=1}^{2N}\sum_{m=1}^{2N} U_{i,l}U^{\dagger}_{m,j} Tr\left[e^{-\frac{1}{2}\sum_{k=0}^{N-1}\epsilon_k\left(b^{\dagger}_k b_k - b_k b^{\dagger}_k\right)}\vec{\beta}_l\vec{\beta}_m^{\dagger}\right] =$$

$$= \sum_{l=1}^{N} U_{i,l}U^{\dagger}_{l,j} Tr\left[e^{-\frac{1}{2}\sum_{k=0}^{N-1}\epsilon_k\left(b^{\dagger}_k b_k - b_k b^{\dagger}_k\right)} b^{\dagger}_l b_l\right] + \sum_{l=1}^{N} U_{i,l+N}U^{\dagger}_{l+N,j} Tr\left[e^{-\frac{1}{2}\sum_{k=0}^{N-1}\epsilon_k\left(b^{\dagger}_k b_k - b_k b^{\dagger}_k\right)} b_l b^{\dagger}_l\right] =$$

$$= \sum_{l=1}^{N} U_{i,l}U^{\dagger}_{l,j} e^{-\frac{\epsilon_l}{2}} \prod_{k\neq l} 2\cosh(\frac{\epsilon_k}{2}) + \sum_{l=1}^{N} U_{i,l+N}U^{\dagger}_{l+N,j} e^{\frac{\epsilon_l}{2}} \prod_{k\neq l} 2\cosh(\frac{\epsilon_k}{2})$$

I can divide by Z and obtain

$$\begin{aligned}\Gamma_{i,j} &= \sum_{l=1}^{N} U_{i,l}U^{\dagger}_{l,j} \frac{e^{-\frac{\epsilon_l}{2}}}{e^{\frac{\epsilon_l}{2}} + e^{-\frac{\epsilon_l}{2}}} + \sum_{l=1}^{N} U_{i,l+N}U^{\dagger}_{l+N,j} \frac{e^{\frac{\epsilon_l}{2}}}{e^{\frac{\epsilon_l}{2}} + e^{-\frac{\epsilon_l}{2}}} \\ &= \sum_{l=1}^{N} U_{i,l}U^{\dagger}_{l,j} \frac{1}{1+e^{\epsilon_l}} + \sum_{l=1}^{N} U_{i,l+N}U^{\dagger}_{l+N,j} \frac{1}{1+e^{-\epsilon_l}} = \\ &= \sum_{l=1}^{2N} U_{i,l}U^{\dagger}_{l,j} \frac{1}{1+e^{\epsilon_l}} = U\Gamma^{D}U^{\dagger}.\end{aligned} \tag{A.9}$$

So the same transformation U that moves to the free Hamiltonian H_D is also the transformation that diagonalise the correlation matrix. The eigenvalues ν_i of the correlation matrix Γ are related to the eigenvalues of the parent hamiltonian H by

$$\nu_i = \frac{1}{1+e^{\epsilon_i}}, \tag{A.10}$$

$$\epsilon_i = ln\left(\frac{1-\nu_i}{\nu_i}\right), \tag{A.11}$$

since $\nu_i \in [0,1]$ the eigenvalues $\epsilon_i \in [-\infty, +\infty]$.

A.2 Purity

From the previous subsection we have:

$$Z^2 = \prod_{k=1}^{N-1}\left(2\cosh\left(\frac{\epsilon_k}{2}\right)\right)^2 \tag{A.12}$$

and

$$Tr\left[e^{-\sum_{k=0}^{N-1}\epsilon_k\left(b^{\dagger}_k b_k - b_k b^{\dagger}_k\right)}\right] = \prod_{k=1}^{N-1}\left(2\cosh\left(\epsilon_k\right)\right). \tag{A.13}$$

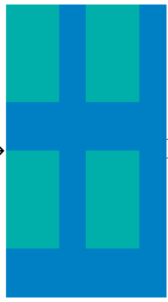
Thus the purity is:

$$\text{Purity} = \prod_{k=1}^{N-1} \frac{1}{\operatorname{sech}(\epsilon_k) + 1} \tag{A.14}$$

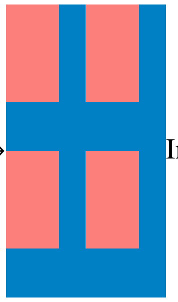
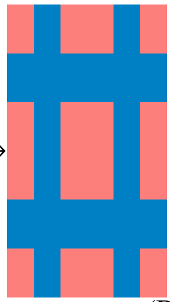
Appendix F-utilities

1. `Print_matrix(title, M)`: Print a graphical representation of matrix `M` in a figure called title.
2. `Build_Omega(N)`$\longrightarrow \Omega$: This function return the $2N \times 2N$ matrix Ω (1.10).
3. `Build_FxxTxp(N)`$\longrightarrow F_{xx\to xp}$: This function return the $2N \times 2N$ matrix $F_{xx\to xp}$ (2.19).
4. `Build_FxpTxx(N)`$\longrightarrow F_{xp\to xx}$: This function return the $2N \times 2N$ matrix $F^T_{xx\to xp}$.
5. `Diag_Real_Skew(h)`$\longrightarrow h_D, O$: This function implements the algorithm for the block diagonalisation of h a generic skew-symmetric real matrix. h_D is the block-diagonal matrix of (2.14) and has the following property: it is in the block diagonal form, each 2×2 block is skew-symmetric with the upper-right element positive and real and h_D is in ascending order for the upper diagonal. O is an orthogonal matrix such that: $h = Oh_DO^T$.
6. `Diag_ferm(M)`$\longrightarrow M_f, U_f$:This function implement the fermionic algorithm of section **??** with $M = H_a$. M_f is the matrix we called H_D and it is in diagonal form with the first half diagonal negative and the second one positive. U_f is the orthogonal matrix that we called U and it is a unitary matrix such that: $M = U_f M_f U_f^\dagger$.
7. `Diag_Gamma(M)`$\longrightarrow M_f, U$ This function returns M_f, the the diagonal form (**??**) of the Dirac correlation matrix M and U the fermionic transformation such that $M = UM_fU\dagger$.
8. `Purity(M)`$\longrightarrow p$: This function takes as input the correlation matrix Γ and return a Float p from 0 to 1 that is the purity.
9. `Evolve_gamma(M,D,U,t)`$\longrightarrow M_t$: This function evolve for a time `t` (last argument) the correlation matrix Γ (first argument), `D` is the Dirac Hamiltonian diagonalised, U is the unitary transformation that change basis from the diagonal one to the original one. e.g. If I want to evolve the correlation matrix M with H_a for a time t I would write `M_t=Evolve_gamma(M,Diag_ferm(`H_a`),`t`)`.
10. `Evolve_gamma_imag(M,D,U,t)`$\longrightarrow M_t$: This function evolve for a time `t` (last argument) the pure state correlation matrix Γ (first argument) with the evolution **??**, `D` is the Dirac Hamiltonian diagonalised, U is the unitary transformation that change basis from the diagonal one to the original one .N.B. `M` must be a pure state (Purity$(M) = 1$), `Evolve_gamma_imag(M,D,U,t)` is a pure state.
11. `Energy_fermion(M,D,U)`$\longrightarrow e$: This function return the energy of the correlation matrix M with respect of the Hamiltonian in the diagonal form M where U is the change of basis from the diagonal one to the space one. e.g. If I want to compute the energy of the correlation matrix Γ with respect to the generic quadratic Hamiltonian represented by H I would write `Energy_fermion(`Γ`,Diag_ferm(`H`))`.
12. `Reduce_gamma(M,N_partition,first_index)` $\longrightarrow M_r$: This function return the corre-

lation matrix of a subsystem with `N_partition` size starting from the site at `first_index`. e.g. `Reduce_gamma()` return the green the element of the matrix $M_{6\times6}$

Reduce_gamma($M_{6\times6}$,2,1)$\longrightarrow$  Reduce_gamma($M_{6\times6}$,2,3)$\longrightarrow$  (B.1)

13. `Inject_gamma(gamma, injection, first_index)`$\longrightarrow$ M_T:This function overwrite the subsystem of gamma starting at `first_index` with the system with correlation matrix injection. The system of injection has to be smaller then the one of gamma. The returned system has same dimension of gamma. e.g. `Inject_gamma()` return the red and blue matrix where the elements in red are the one of the matrix injection.

Inject_gamma($M_{6\times6}$,2,1)$\longrightarrow$  Inject_gamma($M_{6\times6}$,2,3)$\longrightarrow$  (B.2)

14. `Eigenvalues_of_rho(M)`$\longrightarrow$ $\vec{e}$: This function take as input a correlation matrix Γ and return the vector with all its eigenvalues. N.B. The number of eigenvalues grows exponentially with the size of Γ.
15. `VN_Entropy(Γ)` $\longrightarrow$ S This function return S, the `Float64` value of the Von Neumann Entropy of the state described by the Dirac correlation matrix Γ.

Appendix Useful relations

C.1 Pauli Matrices

1. $\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $\sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$, $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $|+\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, $|-\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$, $|+\rangle_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$, $|-\rangle_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$, $|0_-\rangle_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, $|1_+\rangle_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
2. $\sigma^z \sigma^- = -\sigma^-$
3. $\sigma^z \sigma^+ = \sigma^+$
4. $\sigma^- \sigma^z = \sigma^-$
5. $\sigma^+ \sigma^z = -\sigma^+$
6. $\sigma^+ \sigma^- = \frac{\sigma^z + \mathbb{I}}{2}$
7. $\sigma^- \sigma^+ = \frac{\mathbb{I} - \sigma^z}{2}$

C.2 Operators obeying CAR

1. $\{a_i, a_j^\dagger\} = \mathbb{I}\delta_{i,j} \qquad \{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0$
2. $a_i a_j = -a_j a_i; \qquad a_i^\dagger a_j^\dagger = -a_j^\dagger a_i^\dagger$
3. $a_i^2 = \left(a_j^\dagger\right)^2 = 0$
4. $a_i a_j^\dagger = \delta_{i,j} - a_j^\dagger a_i$
5. $a_i a_j = \frac{a_i a_j - a_j a_i}{2}$
6. $a_i a_j^\dagger = \frac{a_i a_j^\dagger - a_j^\dagger a_i}{2} + \frac{\delta_{i,j}}{2}$
7. $a_i^\dagger a_j = \frac{a_i^\dagger a_j - a_j a_i^\dagger}{2} + \frac{\delta_{i,j}}{2}$

Commutators

1. $[a_i^\dagger, a_j] = \delta_{i,j} - 2a_j a_i^\dagger = a_i^\dagger a_j - \delta_{i.j}$
2. $[a_i, a_j^\dagger] = \delta_{i,j} - 2a_j^\dagger a_i = a_i a_j^\dagger - \delta_{i,j}$
3. $[a_i, a_j] = 2a_i a_j$
4. $[a_i^\dagger, a_j^\dagger] = 2a_i^\dagger a_j^\dagger$

Majorana operators

1. $x_i^2 = p_i^2 = \frac{1}{2}$
2. $a^\dagger a = \frac{i}{2}(xp - px) + \frac{1}{2} = ixp + \frac{1}{2}$
3. $aa^\dagger = \frac{i}{2}(px - xp) + \frac{1}{2} = ipx + \frac{1}{2}$
4. $xp = -\frac{i}{2}\left(a^\dagger a - aa^\dagger\right) = -i\left(a^\dagger a - \frac{1}{2}\right)$

C.3 Jordan-Wigner Transformations

C.3.1 spinless fermions $\longrightarrow$ spins

1. $a_j = -\bigotimes_{k=1}^{j-1} \sigma_k^z \otimes \sigma_j^- \bigotimes_{k=j+1}^{N} \mathbb{I}_k$
2. $a_j^\dagger = -\bigotimes_{k=1}^{j-1} \sigma_k^z \otimes \sigma_j^+ \bigotimes_{k=j+1}^{N} \mathbb{I}_k$
3. $a_j^\dagger a_j = \bigotimes_{k=1}^{j-1} \otimes \frac{\sigma_j^z + \mathbb{I}_j}{2} \bigotimes_{k=j+1}^{N} \mathbb{I}_k$

C.3.2 spins $\longrightarrow$ spinless fermions

1. $\sigma_j^z = a_j^\dagger a_j - a_j a_j^\dagger$
2. $\sigma_j^x = -\bigotimes_{k=1}^{j-1} \sigma_j^z \otimes (a_j + a_j^\dagger) \bigotimes_{k=j+1}^{N} \mathbb{I}_j$
3. $\sigma_j^x = i \bigotimes_{k=1}^{j-1} \sigma_j^z \otimes (a_j^\dagger - a_j) \bigotimes_{k=j+1}^{N} \mathbb{I}_j$
4. $\sigma_j^x \sigma_{j+1}^x = (a_j^\dagger - a_j)(a_{j+1} + a_{j+1}^\dagger)$
5. $\sigma_j^y \sigma_{j+1}^y = -(a_j^\dagger + a_j)(a_{j+1}^\dagger - a_{j+1})$
6. $\sigma_j^x \sigma_{j+1}^y = i(a_j^\dagger - a_j)(a_{j+1}^\dagger + a_{j+1})$
7. $\sigma_j^y \sigma_{j+1}^x = i(a_j^\dagger + a_j)(a_{j+1}^\dagger + a_{j+1})$

Bibliography

Bravyi, Sergey, "Lagrangian Representation for Fermionic Linear Optics," 2004.

Chen, Yangang and Guifre Vidal, "Entanglement Contour," *Journal of Statistical Mechanics: Theory and Experiment*, October 2014, *2014* (10), P10011.

Cheong, Siew-Ann and Christopher L. Henley, "Many-Body Density Matrices for Free Fermions," *arXiv:cond-mat/0206196*, November 2003.

Coser, Andrea, Cristiano De Nobili, and Erik Tonni, "A Contour for the Entanglement Entropies in Harmonic Lattices," *J. Phys. A: Math. Theor.*, July 2017, *50* (31), 314001.

Friis, Nicolai, Antony R Lee, and David Edward Bruschi, "Fermionic-Mode Entanglement in Quantum Information," *Physical Review A*, February 2013, *87* (2), 022338.

Horn, Roger A. and Charles R. Johnson, "Matrix Analysis by Roger A. Horn," /core/books/matrix-analysis/9CF2CB491C9E97948B15FAD835EF9A8B December 1985.

Jaynes, E. T., "Information Theory and Statistical Mechanics," *Physical Review*, May 1957, *106* (4), 620–630.

Jaynes, Edwin T, "Information Theory and Statistical Mechanics. II," *Physical Review*, 1957, *108* (2), 171–190.

Lieb, Elliott, Theodore Schultz, and Daniel Mattis, "Two Soluble Models of an Antiferromagnetic Chain," *Annals of Physics*, December 1961, *16* (3), 407–466.

Molinari, Luca Guido, "Notes on Wick's Theorem in Many-Body Theory," *arXiv:1710.09248 [cond-mat, physics:math-ph]*, October 2017.

Nielsen, Michael A, "The Fermionic Canonical Commutation Relations and the Jordan-Wigner Transform," p. 8.

Peschel, Ingo, "Calculation of Reduced Density Matrices from Correlation Functions," *J. Phys. A: Math. Gen.*, March 2003, *36* (14), L205–L208.

—, "Calculation of Reduced Density Matrices from Correlation Functions," *J. Phys. A: Math. Gen.*, March 2003, *36* (14), L205–L208.

Tonni, Erik, Javier Rodríguez-Laguna, and Germán Sierra, "Entanglement Hamiltonian and Entanglement Contour in Inhomogeneous 1D Critical Systems," *J. Stat. Mech.: Theory Exp.*, April 2018, *2018* (4), 043105.

Vidal, G., J. I. Latorre, E. Rico, and A. Kitaev, "Entanglement in Quantum Critical Phenomena," *Phys. Rev. Lett.*, June 2003, *90* (22), 227902.

Zhang, Jiaju, Pasquale Calabrese, Marcello Dalmonte, and M. A. Rajabpour, "Lattice Bisognano-Wichmann Modular Hamiltonian in Critical Quantum Spin Chains," *arXiv:2003.00315 [cond-mat]*, February 2020.

Zumino, Bruno, "Normal Forms of Complex Matrices," *Journal of Mathematical Physics*, September 1962, *3* (5), 1055–1057.