



Practical Fermionic Gaussian States

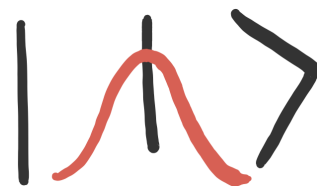
Fermionic Gaussian States: practical numerical simulations

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Julia's code on Github

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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

$$\{a_i, a_j^\dagger\} = \mathbb{I}\delta_{i,j}; \quad \{a_i, a_j\} = 0, \quad (1.1)$$

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

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

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

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

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

$$x_i = \frac{a_i + a_i^\dagger}{\sqrt{2}}, \quad p_i = \frac{a_i - a_i^\dagger}{i\sqrt{2}}, \quad (1.4)$$

are called *Majorana operators*.

The inverse transformations are:

$$a_i = \frac{x_i + ip_i}{\sqrt{2}}, \quad a_i^\dagger = \frac{x_i - ip_i}{\sqrt{2}}. \quad (1.5)$$

In terms of Majorana operators the CARs read as

$$\{x_i, x_j\} = \{p_i, p_j\} = \delta_{i,j}, \quad \{x_i, p_j\} = 0. \quad (1.6)$$

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

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

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

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

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

$$\{r_i, r_j\} = \delta_{i,j}. \quad (1.9)$$



We define the unitary matrix Ω as

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

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

Remark The $\{r_i\}_{i=1,\dots,2N}$ are hermitian, traceless and form a Clifford algebra C_{2N} characterised by the MCAR (1.9).

1.2.2 Fermionic transformation

A transformation O is said to respect the CAR in the Majorana representation if maps a vector of Majorana operators \vec{r} to a new one $\vec{s} = O\vec{r}$. That is for all $i, j = 1, 2, \dots, N$ it must hold

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

that corresponds to the request for O to be an orthogonal matrix.

A transformation U of a vector of Dirac operators $\vec{\alpha}$ to a new one $\vec{\beta} = U\vec{\alpha}$ that respects the CAR, we call it a *fermionic transformation*, has the form of $U = \Omega^\dagger O \Omega$ with O an orthogonal matrix.

Chapter 2 Fermionic Quadratic Hamiltonians

2.1 Dirac Representation

The general *fermionic quadratic hamiltonians* on a finite lattice of N sites in the Dirac operators representation can be written as

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

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

Defining the matrix

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

the compact form of equation (2.1) reads

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

2.2 Majorana Representation

The Majorana representation of the generic fermionic quadratic hamiltonian reads as

$$\hat{H} = \frac{i}{2} \vec{r}^\dagger h \vec{r}, \quad (2.4)$$

where

$$ih = \Omega H \Omega^\dagger = i \begin{pmatrix} \{A + B\} & \Re\{A + B\} \\ \Re\{B - A\} & \Im\{A - B\} \end{pmatrix}. \quad (2.5)$$

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 fermionic quadratic hamiltonian \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

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

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

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

In compact form

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

with

$$H_D = U^\dagger H U = \begin{pmatrix} -\epsilon_1 & 0 & \dots & \dots & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & -\epsilon_N & & \\ & & & \epsilon_1 & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & 0 \\ 0 & \dots & & \dots & 0 & \epsilon_N \end{pmatrix}, \quad (2.8)$$

where U is the fermionic transformation that diagonalise the hamiltonian.

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

2.3.2 Hamiltonian diagonal form with Majorana operators

In terms of Majorana operators the diagonal form of a generic fermionic quadratic hamiltonian reads as

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

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

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

with

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

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 fermionic quadratic hamiltonian \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

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

$$= \frac{i}{2} \vec{r}^\dagger h \vec{r}. \quad (2.13)$$

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 real special orthogonal matrix O such that

$$h = O h_D O^T, \quad (2.14)$$

with h_D a block diagonal matrix of the form

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

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

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

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

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

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

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

The vector of Majorana operators \vec{s} has a different ordering with respect 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 Ω^\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

$$F_{xp \rightarrow xx} = \begin{matrix} i = 0 \\ i = 1 \\ \vdots \\ \vdots \\ i = N \\ i = N + 1 \\ \vdots \\ i = 2N + 1 \end{matrix} \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & \dots & 0 & 0 \\ 0 & \vdots & 1 & \vdots & & & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & & & 0 & \vdots \\ \vdots & \vdots & 0 & 0 & 0 & & 1 & \vdots \\ \vdots & 1 & 0 & 0 & & & 0 & \vdots \\ \vdots & 0 & \vdots & 1 & & & \vdots & \vdots \\ \vdots & \vdots & \vdots & 0 & & & \vdots & 0 \\ 0 & 0 & 0 & \vdots & \dots & \dots & 0 & 1 \end{pmatrix} \quad (2.19)$$

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

$$\hat{H} = \frac{i}{2} \left(\vec{s} F_{xp \rightarrow xx}^T \Omega \right) \left(\Omega^\dagger F_{xp \rightarrow xx} h_D F_{xp \rightarrow xx}^T \Omega \right) \left(\Omega^\dagger F_{xp \rightarrow xx} \vec{s} \right) = \quad (2.20)$$

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

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

$$U = \Omega^\dagger \cdot O \cdot F_{xp \rightarrow xx}^\dagger \cdot \Omega. \quad (2.22)$$

We note that $\epsilon_k = \lambda_k$.

F-utilities Routine 2.1. `Diag_ferm(H) \rightarrow 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: $H = U H_D U^\dagger$.

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

$$\begin{pmatrix} 0 & \tilde{\lambda}_i \\ -\tilde{\lambda}_i & 0 \end{pmatrix}, \quad (2.23)$$

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

$$s_i = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (2.24)$$

if $\tilde{\lambda}_i < 0$ or

$$s_i = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (2.25)$$

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) → hD, 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



Appendix Extended calculations

A.1 Eigenvalues of Γ and H_α

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

$$\rho = \frac{e^{-\frac{1}{2}\vec{\beta}^\dagger M_D \vec{\beta}}}{Z} = \frac{e^{-\frac{1}{2}\sum_{k=0}^{N-1} \epsilon_k (b_k^\dagger b_k - b_k b_k^\dagger)}}{Z}. \quad (\text{A.1})$$

We change the basis of the correlation matrix too

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

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

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

To compute the numerator part this equalities will result useful

- For $x \neq y$

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

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

•

- $\forall x, y$

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

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

Thus the numerator can be explicitly written as

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

$$\begin{aligned}
&= \sum_{l=1}^{2N} \sum_{m=1}^{2N} U_{i,l} U_{m,j}^\dagger \text{Tr} \left[e^{-\frac{1}{2} \sum_{k=0}^{N-1} \epsilon_k (b_k^\dagger b_k - b_k b_k^\dagger)} \vec{\beta}_l \vec{\beta}_m^\dagger \right] = \\
&= \sum_{l=1}^N U_{i,l} U_{l,j}^\dagger \text{Tr} \left[e^{-\frac{1}{2} \sum_{k=0}^{N-1} \epsilon_k (b_k^\dagger b_k - b_k b_k^\dagger)} b_l^\dagger b_l \right] + \sum_{l=1}^N U_{i,l+N} U_{l+N,j}^\dagger \text{Tr} \left[e^{-\frac{1}{2} \sum_{k=0}^{N-1} \epsilon_k (b_k^\dagger b_k - b_k b_k^\dagger)} b_l b_l^\dagger \right] = \\
&= \sum_{l=1}^N U_{i,l} U_{l,j}^\dagger e^{-\frac{\epsilon_l}{2}} \prod_{k \neq l} 2 \cosh\left(\frac{\epsilon_k}{2}\right) + \sum_{l=1}^N U_{i,l+N} U_{l+N,j}^\dagger e^{\frac{\epsilon_l}{2}} \prod_{k \neq l} 2 \cosh\left(\frac{\epsilon_k}{2}\right)
\end{aligned}$$

I can divide by Z and obtain

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

So the same transformation U that moves to the free Hamiltonian M_D is also the transformation that diagonalise the correlation matrix. The eigenvalues v_i of the correlation matrix Γ are related to the eigenvalues of the Hamiltonian M_ρ by

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

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

since $v_i \in [0, 1]$ 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

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

Thus the purity is:



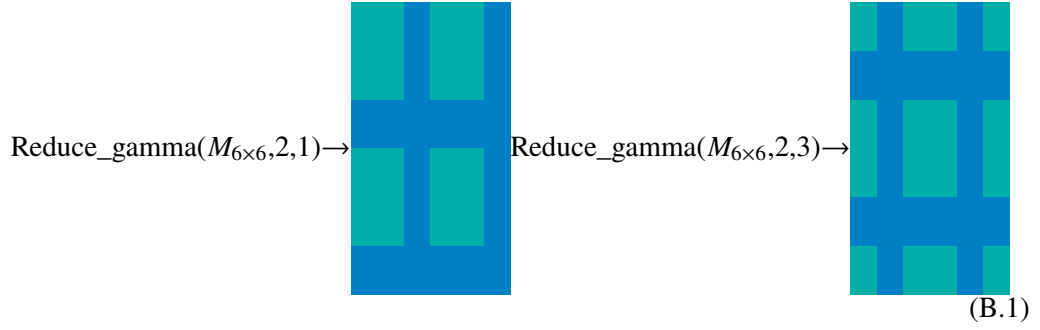
$$\text{Purity} = \prod_{k=1}^{N-1} \frac{1}{\text{sech}(\epsilon_k) + 1} \quad (\text{A.14})$$

Appendix F-utilities

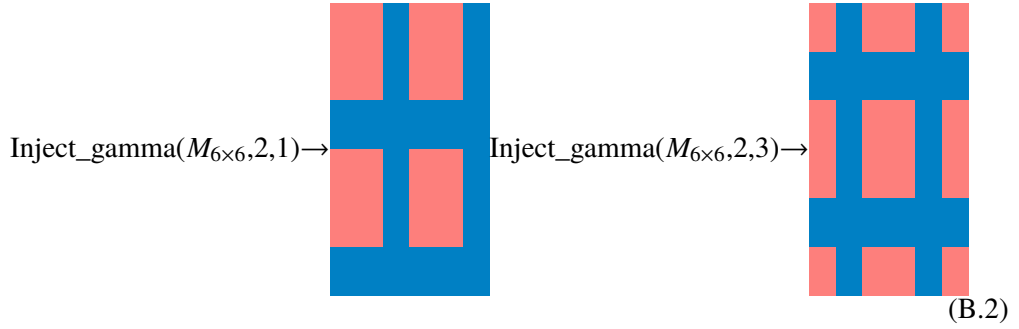
1. `Print_matrix(title, M)`: Print a graphical representation of matrix M in a figure called `title`.
2. `Build_Omega(N) → Ω`: This function return the $2N \times 2N$ matrix Ω (1.10).
3. `Build_FxxTxx(N) → Fxx→xp`: This function return the $2N \times 2N$ matrix $F_{xx \rightarrow xp}$ (2.19).
4. `Build_FxpTxx(N) → Fxp→xx`: This function return the $2N \times 2N$ matrix $F_{xp \rightarrow xx}^T$.
5. `Diag_Real_Skew(h) → hD, 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: $h = O h_D O^T$.
6. `Diag_ferm(M) → Mf, Uf`: 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) → Mf, U` This function returns M_f , the the diagonal form (??) of the Dirac correlation matrix M and U the fermionic transformation such that $M = U M_f U^\dagger$.
8. `Purity(M) → 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) → Mt`: 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 $M_t = \text{Evolve_gamma}(M, \text{Diag_ferm}(H_a), t)$.
10. `Evolve_gamma_imag(M, D, U, t) → Mt`: 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 ($\text{Purity}(M) = 1$), $\text{Evolve_gamma_imag}(M, D, U, t)$ is a pure state.
11. `Energy_fermion(M, D, U) → 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 $\text{Energy_fermion}(\Gamma, \text{Diag_ferm}(H))$.
12. `Reduce_gamma(M, N_partition, first_index) → Mr`: This function return the corre-

lation matrix of a subsystem with $N_{\text{partition}}$ size starting from the site at first_index .

e.g. `Reduce_gamma()` return the green the element of the matrix $M_{6 \times 6}$



13. `Inject_gamma(gamma, injection, first_index) $\rightarrow M_T$` : 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.



14. `Eigenvalues_of_rho(M) $\rightarrow \vec{e}$` : 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) $\rightarrow S$` 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. $\{a_i, a_j^\dagger\} = \mathbb{I} \delta_{i,j} \quad \{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0$
2. $a_i a_j = -a_j a_i; \quad a_i^\dagger a_j^\dagger = -a_j^\dagger a_i^\dagger$
3. $a_i^2 = (a_j^\dagger)^2 = 0$
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. $xp = -\frac{i}{2} (a^\dagger a - aa^\dagger) = -i \left(a^\dagger a - \frac{1}{2} \right)$

C.3 Jordan-Wigner Transformations

C.3.1 spinless fermions \rightarrow 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. $a_j^\dagger a_j = \bigotimes_{k=1}^{j-1} \sigma_k^z \otimes \frac{\sigma_j^z + \mathbb{I}_j}{2} \bigotimes_{k=j+1}^N \mathbb{I}_k$

C.3.2 spins \rightarrow spinless fermions

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

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