Practical Fermionic Gaussian States

Fermionic Gaussian States: practical numerical simulations

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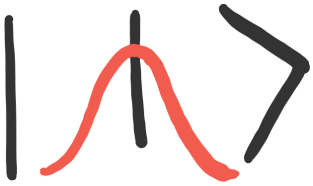
Date: April 17, 2020

Version: 1.00



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

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

with $\{a, b\} \coloneqq ab + ba$ 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 $|\vec{x}\rangle \coloneqq (a_1^\dagger)^{x_1}(a_2^\dagger)^{x_2} \dots (a_N^\dagger)^{x_N} |\vec{0}\rangle$, 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 orthonormal basis $\{|\vec{x}\rangle\}_{\vec{x}\in\{0,1\}^N}$ is called *Fock basis*. The action of the raising and lowering operators on $|\vec{x}\rangle$ is then

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

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

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

In appendix B.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)

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

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 $P = (i2)^N r_1 r_2 \dots r_{2N} = \prod_{i=1}^{N} (\mathbb{I} - 2a_i^\dagger a_i)$.

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

$$|\vec{x}\rangle\langle\vec{x}| = \left(\frac{\mathbb{I}}{2} - i(-1)^{x_1} r_1 r_2\right)\left(\frac{\mathbb{I}}{2} - i(-1)^{x_2} r_3 r_4\right) \dots \left(\frac{\mathbb{I}}{2} - i(-1)^{x_N} r_{2N-1} r_{2N}\right), \tag{1.13}$$

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

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

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

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

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

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

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

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

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

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

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

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 ($\epsilon_1 \geq \epsilon_2 \geq \cdots \geq \epsilon_N \geq 0$).

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

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

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

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

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

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

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

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

Theorem 2.1. Block diagonal form of 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 $\{\lambda_i\}_{i=1,\dots,N}$. The non-zero eigenvalues of matrix h are the imaginary numbers $\{\pm i\lambda_i\}_{i=1,\dots,N}$.

For a more general form of this theorem see appendix A.5. ♡

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

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

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

That is $\hat{H} = i\sum_{i=0}^{N-1} \lambda_i (\tilde{x}_i \tilde{p}_i - \tilde{p}_i \tilde{x}_i)$ 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

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

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

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_h(`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 ordered as 2.8. 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

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

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

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

where $Z_k = \mathrm{Tr}\left[e^{-i\epsilon_k(b_k^\dagger b_k - b_k b_k^\dagger)}\right]$.
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 $\Gamma_{i,j}^{aa^\dagger} := \langle a_i a_j^\dagger\rangle = (\mathbb{I} - \Gamma^{a^\dagger a})_{i,j}^\dagger$, 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

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

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 $\langle r_i, r_j\rangle \coloneqq i\mathrm{Tr}\left[\rho[r_i, r_j]\right]$. 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 for any f.g.s. ρ there exist a fermionic transformation U that diagonalise its parent hamiltonian . With the new Dirac operators $\vec{\beta}$ the state can be expressed as a tensor product of single mode thermal states

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

with $Z_k = \mathrm{Tr}\left[e^{-i\epsilon_k(b_k^\dagger b_k - b_k b_k^\dagger)}\right]$.

Expressed with these operators the correlation matrix is diagonal. If we consider the Fock basis $\{|\vec{k}\rangle\}_{\vec{k}\in\{0,1\}^N}$ built with the action of the operators $\vec{\beta}$ on $|0\rangle$, we have that in this basis ρ assumes a diagonal form. We call U_ρ the unitary transformation that moves from the basis $\{|\vec{x}\rangle\}_{\vec{x}\in\{0,1\}^N}$ to the one of the modes $\{|\vec{k}\rangle\}_{\vec{k}\in\{0,1\}^N}$.

It is easy to see that expressed on this basis ρ has the diagonal form

$$\rho^D = U_\rho^\dagger \rho U_\rho = \bigotimes_{i=1}^{N} \begin{pmatrix} \nu_i & 0 \\ 0 & 1-\nu_i \end{pmatrix}. \tag{3.15}$$

The same fermionic transformation U that diagonalise the parent hamiltonian brings Γ in the diagonal form

$$\Gamma^D = U^\dagger \Gamma U = \begin{pmatrix} \nu_1 & 0 & \dots & & \dots & 0 \\ 0 & \ddots & \ddots & & & \vdots \\ \vdots & \ddots & \nu_N & & & \\ & & & 1-\nu_1 & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & 0 \\ 0 & \dots & & & \dots 0 & 1-\nu_N \end{pmatrix}, \tag{3.16}$$

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

$$\gamma = O\gamma^D O^T = O\left(\bigoplus_{i=1}^{N} \begin{pmatrix} 0 & \eta_i \\ -\eta_i & 0 \end{pmatrix}\right) O^T \tag{3.17}$$

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

$$\nu_i = \frac{1}{2} - \eta_i. \tag{3.18}$$

The elements of H_D and Γ^D are related as

$$\epsilon_k = \frac{1}{2} \ln\left(\frac{1-\nu_k}{\nu_k}\right), \tag{3.19}$$

$$\nu_k = \frac{1}{1+e^{2\epsilon_k}} \tag{3.20}$$

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 A.1. In 2.8 we defined all the ϵ_k to be positive, to use the same notation, one just has to exchange b with $\tilde{b}^\dagger$ and $b^\dagger$ with $\tilde{b}$, that is exchanging occupations with vacancies for the mode with ϵ_k negative. This corresponds to switching ν_k with $1-\tilde{\nu}_k$ and $1-\nu_k$ with $\tilde{\nu}_k$.

In general the correlation matrix Γ and the parent hamiltonian H are related as Cheong and Henley (2003); Peschel (2003); Vidal et al. (2003); Zhang et al. (2020)

$$\Gamma = \frac{1}{1+e^{2H}}. \tag{3.21}$$

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 Phisicality of a state

It is known that a matrix ρ, represent a valid physical density matrix if it is a positive semi-definite hermitian matrix with trace one. The condition for a matrix Γ to represent a valid physical correlation matrix of a f.g.s. is

$$\Gamma^2 - \Gamma \leq 0, \tag{3.22}$$

or equivalently

$$\gamma\gamma^\dagger \leq -\mathbb{I}. \tag{3.23}$$

These conditions are equivalent to the request that all the eigenvalues ν_i of matrix Γ have to belong to the interval $[0, 1]$.

3.5.0.2 Ground states of fermionic quadratic hamiltonians

Suppose we have a f.q.h. H and we are interest in obtaining the correlation matrix Γ_0 associated to its ground state $|0\rangle$. In order to obtain Γ_0 we proceed by first finding the fermionic transformation U that diagonalise H. Since our algorithm associates to each free mode of the diagonalised hamiltonian a positive energy, in the diagonal basis the ground state is $|0\rangle\langle 0|$. The correlation matrix associated to the state $|0\rangle$ is the block matrix:

$$\Gamma_{|0\rangle\langle 0|} = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{I}_{N\times N} \end{pmatrix}. \tag{3.24}$$

To obtain the ground state Γ_0 we just need to move back to the original basis, thus

$$\Gamma_0 = U\Gamma_{|0\rangle\langle 0|}U^\dagger. \tag{3.25}$$

F-utilities Routine 3.2. `GS_gamma`$(H_D, U) \to \Gamma_0$

This function returns Γ_0, the ground state of the hamiltonian $H = UH_DU^\dagger$. ♠

3.5.0.3 Thermal state of fermionic quadratic hamiltonians

Suppose we have a f.q.h. H and we are interest in obtaining the correlation matrix Γ_0 associated to the thermal state $\rho_\beta = \frac{e^{-\beta H}}{\mathrm{Tr}[e^{-\beta H}]}$.

As we did for computing the ground state, we move to the diagonal basis with the fermionic transformation U. In the diagonal basis the thermal state has the correlation matrix

$$\Gamma_\beta^D = \begin{pmatrix} \frac{1}{1+e^{2\beta\epsilon_1}} & 0 & \dots & & \dots & 0 \\ 0 & \ddots & \ddots & & & \vdots \\ \vdots & \ddots & \frac{1}{1+e^{2\beta\epsilon_N}} & & & \\ & & & \frac{1}{1+e^{-2\beta\epsilon_1}} & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & 0 \\ 0 & \dots & & & \dots 0 & \frac{1}{1+e^{-2\beta\epsilon_N}} \end{pmatrix}. \tag{3.26}$$

To obtain the thermal state Γ_β we just need to move back to the original basis, thus

$$\Gamma_\beta = U\Gamma_\beta^D U^\dagger. \tag{3.27}$$

F-utilities Routine 3.3. `Thermal_fix_beta`$(H_D, U, \beta) \rightarrow \Gamma_0$

This function returns Γ_β, the termal state at inverse temperature β of the hamiltonian $H = UH_DU^\dagger$. ♠

F-utilities Routine 3.4. `Thermal_fix_energy`$(H_D, U, E) \rightarrow \Gamma_{\beta(E)}, \beta(E), \Delta(E)$

This function variationally computes and then returns $\Gamma_{\beta(E)}$, the thermal state at inverse temperature $\beta(E)$ of the hamiltonian $H = UH_DU^\dagger$, and $\beta(E)$ the temperature such that $Tr\left[\rho_{\beta(E)}H\right] = E$ and $\Delta(E)$ the difference between the required energy E and the actual energy of the state $\Gamma_{\beta(E)}$. It prints in the terminal the precision $\Delta(E)$ and $\beta(E)$. ♠

3.5.0.4 Energy of a fermionic gaussian state

Consider a f.q.h H and a f.g.s. Γ. The energy of Γ with respect to H is the expectation value $\mathrm{Tr}\left[\hat{H}\rho\right]$ of the associated $\hat{H}$ computed on the associated state ρ.

In order to compute this expectation value one just need to find the fermionic transformation U that diagonalises H and compute the energies ϵ_k the occupations $\langle b_k^\dagger, b_k\rangle$ and $\langle b_k, b_k^\dagger\rangle$. The correlation matrix Γ is not diagonal in the diagonal basis $\vec{\beta}$ of H, but we are just interested in its diagonal elements.

The energy $E_H(\Gamma)$ of Γ is thus

$$E_H(\Gamma) = \sum_k \epsilon_k(\langle b_k^\dagger b_k\rangle - \langle b_k b_k^\dagger\rangle). \tag{3.28}$$

F-utilities Routine 3.5. `Energy`$(\Gamma, H_D, U) \rightarrow E_H(\Gamma)$

This function returns $E_H(\Gamma)$ the energy of the state Γ calculated with H. Matrices H_D and U are the output of `Diag_h(H)`. ♠

3.6 Eigenvalues of ρ and eigenvalues of Γ

We have seen that the diagonal forms of the correlation matrix Γ and of the density matrix ρ of a f.g.s. can be obtained respectively with a fermionic transformation U and a unitary operation U_ρ. The Fock basis in which ρ is diagonal is the one generated by the set of operators that expresses Γ in diagonal form.

In this two basis ρ and Γ assume the forms

$$\Gamma^D = \begin{pmatrix} \nu_1 & 0 & \dots & & \dots & 0 \\ 0 & \ddots & \ddots & & & \vdots \\ \vdots & \ddots & \nu_N & & & \\ & & & 1-\nu_1 & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & 0 \\ 0 & \dots & & & \dots 0 & 1-\nu_N \end{pmatrix}, \qquad \rho^D = \bigotimes_{k=1}^{N} \begin{pmatrix} \nu_k & 0 \\ 0 & 1-\nu_k \end{pmatrix} = \begin{pmatrix} \pi_{\vec{0}} & 0 & \dots \\ 0 & \ddots & \vdots \\ \vdots & \dots & \pi_{\vec{1}} \end{pmatrix}. \tag{3.29}$$

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: $\pi_{\vec{x}} = \prod_{k=1}^{N} (\vec{x}_k \nu_i + (1-\vec{x}_k)(1-\nu_k))$.

It is evocative changing the order of the Dirac operators in the representation of Γ^D

$$\vec{\beta} = \begin{pmatrix} b_0^\dagger \\ \vdots \\ b_{N-1}^\dagger \\ b_0 \\ \vdots \\ b_{N-1} \end{pmatrix} \quad \rightarrow \quad \tilde{\vec{\beta}} = \begin{pmatrix} b_0^\dagger \\ b_0 \\ b_1^\dagger \\ b_1 \\ \vdots \\ b_N^\dagger \\ b_N \end{pmatrix}, \tag{3.30}$$

this can be easily done with the fermionic transformation $\tilde{\Gamma}^D = F^\dagger_{xp\to xx} \Gamma^D F_{xp\to xx}$. With this ordering we have

$$\tilde{\Gamma}^D = \bigoplus_{k=1}^{N} \begin{pmatrix} \nu_k & 0 \\ 0 & 1-\nu_k \end{pmatrix}, \qquad \rho^D = \bigotimes_{k=1}^{N} \begin{pmatrix} \nu_k & 0 \\ 0 & 1-\nu_k \end{pmatrix}. \tag{3.31}$$

F-utilities Routine 3.6. `Eigenvalues_of_rho(`Γ`)`$\rightarrow \vec{\nu}$

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

3.7 Reduced density matrix and tensor product of fermionic gaussian states

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 $i_1,\dots,i_m$ is just the correlation matrix $\Gamma|_{\{i_1,\dots,i_m\}}$ and that the reduced state of a f.g.s. is a f.g.s. too.

F-utilities Routine 3.7. `Reduce_gamma(Γ,m,i_1)`→ $\Gamma|_{\{i_1,\dots,i_m\}}$

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

Examples: the the green the element of the matrix $M_{6\times6}$ are the one of returned by the function.

Reduce_gamma($M_{6\times6}$,2,1)→  *Reduce_gamma($M_{6\times6}$,2,3)*→ 

(3.32)♠

The correlation matrix $\Gamma_{A,B}$ of the tensor product of two f.g.s. Γ_A and Γ_B is obtained simply by collecting all the elements of Γ_A and Γ_B in a single well ordered correlation matrix $\Gamma_{A,B}$. The code for obtaining $\Gamma_{A,B}$ from Γ_A and Γ_B is

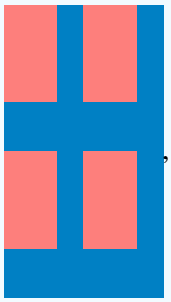
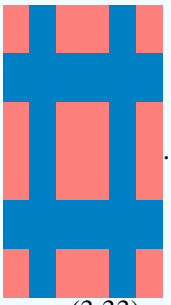
```
D_A = size(Gamma_A,1);
D_B = size(Gamma_B,1);
D   = D_A+D_B;

Gamma_AB = zeros(Complex{Float64}, D,D);
Gamma_AB = Inject_gamma(Gamma_AB,Gamma_A,1);
Gamma_AB = Inject_gamma(Gamma_AB,Gamma_B,D_A+1);
```

. This code makes use of the function `Inject_gamma`.

F-utilities Routine 3.8. `Inject_gamma(Γ, Γ_inj, i)`→ Γ_{comp}

This function takes a $2N\times2N$ matrix Γ and a $2n\times2n$ matrix Γ_{inj} with $n\le N$. It returns the $2N\times2N$ matrix Γ_{comp} as shown in the pictures.

$\Gamma =$  , $\Gamma_{inj} =$ 

`Inject_gamma`$(\Gamma, \Gamma_{inj}, 1) \rightarrow$  , `Inject_gamma`$(\Gamma, \Gamma_{inj}, 3) \rightarrow$  . (3.33)

In the last example it is clear the systems behave with periodic boundary conditions.
If Γ *is the correlation matrix of a f.g.s* ρ *and* Γ_{inj} *is the correlation matrix of a f.g.s* ρ_{inj} *then* Γ_{comp} *is the correlation matrix of the state* $Tr_{\texttt{i,...,i+n-1}}[\rho] \otimes \rho_{inj}$. ♠

It is clear that with the ordering 3.30, the tensor product of two f.g.s. corresponds to the direct sum of their correlation matrices

$$\rho_{A,B} = \rho_A \otimes \rho_B \;\rightarrow\; \tilde{\Gamma}_{A,B} = \tilde{\Gamma}_A \oplus \tilde{\Gamma}_B. \tag{3.34}$$

3.8 Correlation matrix of translational invariant state

We consider a state ρ of a system of N sites and all its reduced density matrices ρ_A, where A is any possible set of sites of the system. We denote with $A + m$ the set of sites $A + m = \{j = i + m | i \text{ i s a site of } A\}$, that is a translation of all site of A by m sites. When we will assume Periodic Boundary Conditions (PBC) we will allow for translations "over the border" of the system, in the sense that when $i + m > N$ (or $i + m < 1$) we will substitute it with $i + m \rightarrow \mod(i + m - 1, N + 1) + 1$. This is interpreted as connecting the first site with the last site of the system. Thus for PBC all translations are allowed. When we will assume Open Boundary Conditions (OBC) only translations within the system. This means that if $i \in A$ and $i + m > N$ (or $i + m < 1$), then the subset $A + m$ is not an allowed subset of sites.

Figure 3.1: System with Open Boundary Conditions. If the state is translational invariant then the reduced density matrix on sites 1 and 2 is the same as the one on sites 3 and 4, but is different from the one on sites 5 and 1

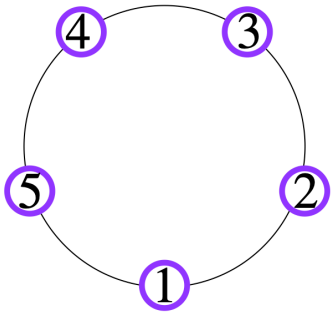


Figure 3.2: System with Periodic Boundary Conditions. If the state is translational invariant then the reduced density matrix on sites 1 and 2 or sites 3 and 4 or even sites 5 and 1 are all the same

A *translational invariant state* is a state such that for every A we have $\rho_A = \rho_{A+m}$ for every m. This property easily translate to correlation matrices of states. For the two point correlators of a translational invariant state we have that $\langle a_j^\dagger a_l\rangle = \langle a_{j+m}^\dagger a_{l+m}\rangle$ and $\langle a_j a_l\rangle = \langle a_{j+m} a_{l+m}\rangle$ for every m. The specific correlator is thus individuated just by the difference of the sites of the first and second operator $\Delta := l - j$ with $\Delta \in [-(N-1), N-1]$. Using this, we substitute $\langle a_j^\dagger a_l\rangle \to \langle a^\dagger a\rangle_\Delta$ and analogously $\langle a_j a_l\rangle \to \langle aa\rangle_\Delta$. We now focus on $\Gamma^{a^\dagger a}$, explicitly expressing it we have

$$\Gamma^{a^\dagger a} \begin{pmatrix} \langle a^\dagger a\rangle_0 & \langle a^\dagger a\rangle_1 & \langle a^\dagger a\rangle_2 & \dots & \langle a^\dagger a\rangle_{N-1} \\ \langle a^\dagger a\rangle_{-1} & \langle a^\dagger a\rangle_0 & \langle a^\dagger a\rangle_1 & \dots & \langle a^\dagger a\rangle_{N-2} \\ \langle a^\dagger a\rangle_{-2} & \langle a^\dagger a\rangle_{-1} & \langle a^\dagger a\rangle_0 & \dots & \langle a^\dagger a\rangle_{N-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \langle a^\dagger a\rangle_{-(N-1)} & \langle a^\dagger a\rangle_{-(N-2)} & \langle a^\dagger a\rangle_{-(N-3)} & \dots & \langle a^\dagger a\rangle_0 \end{pmatrix}. \tag{3.35}$$

Matrix with this structure are called *Teoplitz matrices*.

If we further require the system to have PBC, we have that the parameter Δ is restricted to the range $[0, N-1]$. Consider for example the the specific instance of the correlator $\langle a^\dagger a\rangle_{1-N} = \langle a_N^\dagger a_1\rangle$, because of the translational invariance property of the system and because of the PBC we know that $\langle a_N^\dagger a_1\rangle = \langle a_{N+1}^\dagger a_{1+1}\rangle = \langle a_1^\dagger a_2\rangle = \langle a^\dagger a\rangle_1$ (see figure 3.2).

With PBC, $\Gamma^{a^\dagger a}$ has the form

$$\Gamma^{a^\dagger a} = \begin{pmatrix} \langle a^\dagger a\rangle_0 & \langle a^\dagger a\rangle_1 & \langle a^\dagger a\rangle_2 & \dots & \langle a^\dagger a\rangle_{N-1} \\ \langle a^\dagger a\rangle_{N-1} & \langle a^\dagger a\rangle_0 & \langle a^\dagger a\rangle_1 & \dots & \langle a^\dagger a\rangle_{N-2} \\ \langle a^\dagger a\rangle_{N-2} & \langle a^\dagger a\rangle_{N-1} & \langle a^\dagger a\rangle_0 & \dots & \langle a^\dagger a\rangle_{N-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \langle a^\dagger a\rangle_1 & \langle a^\dagger a\rangle_2 & \langle a^\dagger a\rangle_3 & \dots & \langle a^\dagger a\rangle_0 \end{pmatrix}. \tag{3.36}$$

We see that $\Gamma^{a^\dagger a}$ is the circulant matrix (see appendix A.4) characterised by the circulant vector $\langle \vec{a^\dagger a}\rangle = \left(\langle a^\dagger a\rangle_0, \langle a^\dagger a\rangle_1, \langle a^\dagger a\rangle_2, \dots, \langle a^\dagger a\rangle_{N-1}\right)$. By the same reasoning, we see that $\Gamma^{aa^\dagger}$ is a circulant matrix characterised by the circulant vector $\langle \vec{aa^\dagger}\rangle = \left(\langle aa^\dagger\rangle_0, \langle aa^\dagger\rangle_1, \langle aa^\dagger\rangle_2, \dots, \langle aa^\dagger\rangle_{N-1}\right)$. Matrices Γ^{aa} and $\Gamma^{a^\dagger a^\dagger}$ are circulant skew-simmetric matrices, often called *skew-circulant matrices*. If N is even Γ^{aa} and $\Gamma^{a^\dagger a^\dagger}$ are specified by the circulant vectors $\langle \vec{aa}\rangle = \left(\langle aa\rangle_0, \langle aa\rangle_1, \langle aa\rangle_2, \dots, \langle aa\rangle_{\frac{N}{2}-1}, 0, -\langle aa\rangle_{\frac{N}{2}-1}, -\langle aa\rangle_{\frac{N}{2}-2}, \dots, \langle aa\rangle_1\right)$ and $\langle \vec{a^\dagger a^\dagger}\rangle = \left(\langle a^\dagger a^\dagger\rangle_0, \langle a^\dagger a^\dagger\rangle_1, \langle a^\dagger a^\dagger\rangle_2, \dots, \langle a^\dagger a^\dagger\rangle_{\frac{N}{2}-1}, 0, -\langle a^\dagger a^\dagger\rangle_{\frac{N}{2}-1}, -\langle a^\dagger a^\dagger\rangle_{\frac{N}{2}-2}, \dots, \langle a^\dagger a^\dagger\rangle_1\right)$. If N is odd Γ^{aa} and $\Gamma^{a^\dagger a^\dagger}$ are specified by the circulant vectors $\langle \vec{aa}\rangle = \left(\langle aa\rangle_0, \langle aa\rangle_1, \langle aa\rangle_2, \dots, \langle aa\rangle_{\frac{N-1}{2}}, -\langle aa\rangle_{\frac{N-1}{2}-1}, -\langle aa\rangle_{\frac{N-1}{2}-2}, \dots, \langle aa\rangle_1\right)$ and $\langle \vec{a^\dagger a^\dagger}\rangle = \left(\langle a^\dagger a^\dagger\rangle_0, \langle a^\dagger a^\dagger\rangle_1, \langle a^\dagger a^\dagger\rangle_2, \dots, \langle a^\dagger a^\dagger\rangle_{\frac{N-1}{2}}, -\langle a^\dagger a^\dagger\rangle_{\frac{N-1}{2}-1}, -\langle a^\dagger a^\dagger\rangle_{\frac{N-1}{2}-2}, \dots, \langle a^\dagger a^\dagger\rangle_1\right)$.

3.8.1 Eigenvalues using the properties of circulant-matrices

In appendix A.4 we show the general form of the eigenvalues of a circulant matrix. For Γ^{aa},$\Gamma^{a^\dagger a^\dagger}$ matrices $\Gamma^{a^\dagger a}$,$\Gamma^{aa^\dagger}$ we have that their respective eigenvalues $\lambda_k^{a^\dagger a}$,$\lambda_k^{aa^\dagger}$ are

$$\lambda_k^{a^\dagger a} = \sum_{\Delta=0}^{N-1} e^{i\frac{2\pi}{N}\Delta k}\langle a^\dagger a\rangle_\Delta \qquad \lambda_k^{aa^\dagger} = \sum_{\Delta=0}^{N-1} e^{i\frac{2\pi}{N}\Delta k}\langle aa^\dagger\rangle_\Delta. \tag{3.37}$$

For matrices Γ^{aa},$\Gamma^{a^\dagger a^\dagger}$ we have that their respective eigenvalues λ_k^{aa},$\lambda_k^{a^\dagger a^\dagger}$ are

$$\begin{aligned}
\lambda_k^{aa} &= \begin{cases} 2\sum_{\Delta=0}^{\frac{N}{2}-1} e^{i\frac{2\pi}{N}k\Delta}\langle aa\rangle_\Delta & \text{if } N \text{ even} \\ (1+e^{-i\frac{\pi}{N}})\sum_{\Delta=0}^{\frac{N}{2}-1} e^{i\frac{2\pi}{N}k\Delta}\langle aa\rangle_\Delta & \text{if } N \text{ odd} \end{cases}, \\
\lambda_k^{a^\dagger a^\dagger} &= \begin{cases} 2\sum_{\Delta=0}^{\frac{N}{2}-1} e^{i\frac{2\pi}{N}k\Delta}\langle a^\dagger a^\dagger\rangle_\Delta & \text{if } N \text{ even} \\ (1+e^{-i\frac{\pi}{N}})\sum_{\Delta=0}^{\frac{N}{2}-1} e^{i\frac{2\pi}{N}k\Delta}\langle a^\dagger a^\dagger\rangle_\Delta & \text{if } N \text{ odd} \end{cases}.
\end{aligned} \tag{3.38}$$

We notice that the eigenvalues of Γ^{aa},$\Gamma^{a^\dagger a^\dagger}$ comes in pairs $\lambda_k^{aa} = -\lambda_{k+\lceil\frac{N}{2}\rceil}^{aa}$ and $\lambda_k^{a^\dagger a^\dagger} = -\lambda_{k+\lceil\frac{N}{2}\rceil}^{a^\dagger a^\dagger}$ as expected from the property of skew-symmetric matrices (see appendix A.5).

3.8.2 Eigenvalues using the Fourier transform on a linear lattice

We introduce the Fourier transforms on a linear lattice

$$f_k = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} e^{i\frac{2\pi}{N}kj}a_j, \qquad f_k^\dagger = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} e^{-i\frac{2\pi}{N}kj}a_j^\dagger, \tag{3.39}$$

with inverse transformations

$$a_j = \frac{1}{\sqrt{N}}\sum_{k=1}^{N} e^{-i\frac{2\pi}{N}kj}f_k, \qquad a_j^\dagger = \frac{1}{\sqrt{N}}\sum_{k=1}^{N} e^{i\frac{2\pi}{N}kj}f_k^\dagger. \tag{3.40}$$

It is easy to see that the Fourier modes $\{f_k, f_k^\dagger\}_k$ obey to the CAR and are valid Dirac operators. Now we perform the substitutions 3.8.2 in the expression of $\Gamma^{a^\dagger a}$ and we further exploit the translational invariance ($\langle a^\dagger a\rangle\Delta = \frac{1}{N}\sum_{j=1}^{N}\langle a_j^\dagger a_{j+\Delta}\rangle$) to obtain

$$\langle a^\dagger a\rangle_\Delta = \frac{1}{N^2}\sum_{j}^{N}\sum_{k,k'} e^{i\frac{2\pi}{N}k'\Delta}e^{i\frac{2\pi}{N}(k-k')j}\langle f_k^\dagger f_{k'}\rangle. \tag{3.41}$$

Collecting the Kronecker delta (see appendix B.4) we can express the elements of $\Gamma^{a^\dagger a}$ as

$$\langle a^\dagger a\rangle_\Delta = \frac{1}{N}\sum_{k=1}^{N} e^{-i\frac{2\pi}{N}k\Delta}\langle f_k^\dagger f_k\rangle. \tag{3.42}$$

With the same procedure we obtain

$$\begin{aligned}
\langle a^\dagger a\rangle_\Delta &= \frac{1}{N}\sum_{k=1}^{N} e^{-i\frac{2\pi}{N}k\Delta}\langle f_k^\dagger f_k\rangle, & \langle aa^\dagger\rangle_\Delta &= \frac{1}{N}\sum_{k=1}^{N} e^{-i\frac{2\pi}{N}k\Delta}\langle f_k f_k^\dagger\rangle \\
\langle aa\rangle_\Delta &= \frac{1}{N}\sum_{k=1}^{N} e^{-i\frac{2\pi}{N}k\Delta}\langle f_k f_{N-k}\rangle, & \langle a^\dagger a^\dagger\rangle_\Delta &= \frac{1}{N}\sum_{k=1}^{N} e^{-i\frac{2\pi}{N}k\Delta}\langle f_{N-k}^\dagger f_k^\dagger\rangle.
\end{aligned} \tag{3.43}$$

with inverse transformations

$$\langle f_k^\dagger f_k\rangle = \sum_{\Delta=1}^{N} e^{i\frac{2\pi}{N}k\Delta}\langle a^\dagger a\rangle_\Delta, \qquad \langle f_k f_k^\dagger\rangle = \sum_{\Delta=1}^{N} e^{i\frac{2\pi}{N}k\Delta}\langle aa^\dagger\rangle_\Delta$$
$$\langle f_k f_{N-k}\rangle = \sum_{\Delta=1}^{N} e^{i\frac{2\pi}{N}k\Delta}\langle a^\dagger a\rangle_\Delta, \qquad \langle f_k^\dagger f_{N-k}^\dagger\rangle = \sum_{\Delta=1}^{N} e^{-i\frac{2\pi}{N}k\Delta}\langle aa^\dagger\rangle_\Delta. \tag{3.44}$$

We can easily identify

$$\lambda_k^{a^\dagger a} = \langle f_k^\dagger f_k\rangle, \qquad \lambda_k^{aa^\dagger} = \langle f_k f_k^\dagger\rangle$$
$$\lambda_k^{aa} = \langle f_k f_{N-k}\rangle, \qquad \lambda_k^{a^\dagger a^\dagger} = \langle f_k^\dagger f_{N-k}^\dagger\rangle. \tag{3.45}$$

As last, we note that the Fourier transform does not mix creation and annihilation operators and can be implement directly on the vector of Dirac operators $\vec{\alpha}$ with the fermionic transformation U_ω that has the block diagonal form

$$U_\omega = \begin{pmatrix} W & 0 \\ 0 & \bar{W} \end{pmatrix}, \tag{3.46}$$

where W is the matrix implementing the discrete Fourier transform (see appendix A.4) and it acts separately on the creation and annihilation operators sectors of $\vec{\alpha}$.

For an example of diagonalisation of translational invariant matrices see e.g. section 5

F-utilities Routine 3.9. `Build_Fourier_matrix(`N`)`$\to U_\omega$

This function return the fermionic transformation U_ω for a system of N sites. ♠

3.9 Product Rule

It will result useful to compute the product $\rho = \rho_1\rho_2$ of the density matrices of two fermionic gaussian states. We observe that the commutator of two quadratic terms of Majorana operators $\vec{r}$ is always again a quadratic operator or zero

$$[r_i r_j, r_k r_l] = \delta_{k,i} r_l r_j + \delta_{k,j} r_i r_l - \delta_{i,l} r_k r_j - \delta_{l,j} r_i r_k. \tag{3.47}$$

This is also valid for Dirac operators. We say that the commutator of two monomial of Dirac operator of degree at most 2 is a polynomial of Dirac operators of degree at most 2. Using this observation together with the Baker-Campbell-Hausdorff formula (equation B.C.H.0 in appendix B.4), it is easy to see that ρ, the product of two f.g.s., is always a f.g.s.

$$\rho = \frac{e^{-\hat{H}}}{Z}, \tag{3.48}$$

with $\hat{H}$ given by the B.C.H.0.

It is possible to derive the covariance matrix γ of ρ directly from the covariance matrices γ_1 and γ_2 of the states ρ_1 and ρ_2. This formula appears in Fagotti and Calabrese (2010) where a more detailed description, considering even pathological cases, is given. If we assume that $\mathbb{I} - \gamma_1$ and

$\mathbb{I} - \gamma_2$ are invertible than we have

$$\gamma = \mathbb{I} - (\mathbb{I} - \gamma_2)\frac{1}{\mathbb{I} + \gamma_1\gamma_2}(\mathbb{I} - \gamma_1). \tag{3.49}$$

F-utilities Routine 3.10. `Product`$(\Gamma_1, \Gamma_2) \to \Gamma$

This function return the correlation matrix Γ *corresponding to the f.g.s* $\rho = \rho_1\rho_2$*, where* ρ_1 *and* ρ_2 *are characterised by the correlation matrices* Γ_1 *and* Γ_2*.* ♠

3.10 Information measures

3.10.1 Von Neumann Entropies

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

$$S(\rho) = -\mathrm{Tr}\left[\rho \ln(\rho)\right]. \tag{3.50}$$

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

$$S(\rho) = -\sum_{\lambda} \lambda \ln(\lambda) \tag{3.51}$$

If ρ is a f.g.s. of a system with N sites, since the VonNeumann entropy is invariant under unitary transformation of the state, substituting in (3.50) the product form (3.31) and using the fact the the VonNeumann entropy is additive for product states, the VonNeumann entropy becomes a function of the eigenvalues ν_i of the correlation matrix Γ and it is the sum of just $2N$ terms

$$S(\Gamma) \equiv S(\rho) = -\sum_{k=1}^{N} \left[\nu_k \ln(\nu_k) + (1-\nu_k)\ln(1-\nu_k)\right]. \tag{3.52}$$

F-utilities Routine 3.11. `VN_entropy`$(\Gamma) \to S$

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

3.10.2 Purity

A state is pure if its correlation matrix Γ is such that Bach et al. (1994)

$$\Gamma^2 = \Gamma, \tag{3.53}$$

or, equivalently,

$$\gamma^2 = -\mathbb{I} \tag{3.54}$$

The purity of a state ρ is defined as

$$\mathrm{Purity}(\rho) \equiv Tr\left[\rho^2\right]. \tag{3.55}$$

We have that:

$$\mathrm{Purity}(\rho) = \prod_{i=1}^{N-1} \frac{1}{2}\left(1 + \tanh(x)^2\right), \tag{3.56}$$

$$\text{Purity}(\Gamma) = \prod_{i=1}^{N-1} (2\,(\nu_i - 1)\,\nu_i + 1), \tag{3.57}$$

$$\text{Purity}(\gamma) = \prod_{i=1}^{N-1} \left(2\eta_i^2 + \frac{1}{2}\right). \tag{3.58}$$

For more details see appendix A.2.

F-utilities Routine 3.12. `Purity(Γ)`→ p

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

3.10.3 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 consider the state of a system on a chain of N sites, we divide the chain in two complementary partitions, partition A and partition B. Now suppose partition A and B are entangled and there exists a measure $\mathcal{E}(A,B)$ that quantifies the amount of entanglement between A and B. The entanglement contour $c_A(i)$ of partition A tells us how much each site i of partition A contributes to the total amount of entanglement betwen A and B. Furthermore summing $c_A(i)$ over all the sites of A one should obtain exactly $\mathcal{E}(A,B)$.
Chen and Vidal decide five reasonably properties that define when a function is a contour function. In the same paper they show that these five properties do note define a single contour function, but instead a class of functions. We will present here a specific form of entanglement contour, the one introduced by Chen and Vidal for fermionic gaussian states, for other kinds of contour function see i.e. Coser et al. (2017); Tonni et al. (2018).
First of all we restrict to pure states. For pure state it is known that a good measure of entanglement between two complementary partition A and B is the entanglement entropy, that is the VonNeumann entropy $\mathcal{E}(A,B) = S(A)$ of the reduced state on A.
We consider an Hilbert space $\mathcal{H}$ arbitrarily divided in the two complementary partitions $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, each partition with N_A and N_B sites respectively. The Schmidt decomposition of a pure state $|\psi^{A,B}\rangle$ in $\mathcal{H}$ is

$$|\psi^{A,B}\rangle = \sum_i \sqrt{p_i} |\psi_i^A\rangle \otimes |\psi_i^B\rangle, \tag{3.59}$$

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

$$\rho^A \equiv Tr_B \left[|\psi^{A,B}\rangle\langle\psi^{A,B}|\right] = \sum_i p_i |\psi_i^A\rangle\langle\psi_i^A|. \tag{3.60}$$

The entanglement entropy for this choice of partition is thus $S(A) = -\sum_i p_i ln(p_i)$.
Factorising the 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. We remind that ρ^A cannot be expressed as a product state over this factorisation of $\mathcal{H}_A$ and that the VonNeumann entropy is not addittive. Thus the VonNeumann entropy computed on each site is not a good entanglement contour function.

We know from 3.7 that ρ_A is a f.g.s., thus we can express the entanglement entropy $S(A)$ as the sum of the VonNeumman entropy of each mode in A

$$S(A) = \sum_{k=1}^{N_A} S_k = -\sum_{k=1}^{N_A} \left[\nu_k \ln(\nu_k) + (1-\nu_k)\ln(1-\nu_k)\right]. \tag{3.61}$$

Each mode k associated to the Dirac operators $\beta_k = b_k^\dagger$, $\beta_{k+N_A} = b_k$ is connected to the real space modes associated the Dirac operators $\alpha_i = a_i^\dagger$, $\alpha_{i+N_A} = a_i$ by the fermionic transformation U such that

$$\beta_k = \sum_{i=1}^{N_A} U_{k,i}\alpha_i. \tag{3.62}$$

We want to use this equation to find how much a fixed mode k contribute to a fixed site i. We call this contribution $p_i(k)$ and we define it as

$$p_i(k) := \frac{1}{2}\left[|U_{k,i}|^2 + |U_{k+N_A,i+N_A}|^2 + |U_{k,i+N_A}|^2 + |U_{k+N_A,i}|^2\right]. \tag{3.63}$$

The entanglement contour for partition A is thus defined as

$$c_A(i) := \sum_{k=1}^{N_A} p_i(k) S_k. \tag{3.64}$$

It is easy to see that each of the $p_i(k)$ is positive and that

$$\sum_{k=1}^{N_A} p_i(k) = 1, \tag{3.65}$$

as $\sum_{k=1}^{N_A} p_i(k) = \frac{1}{2}\left[\sum_{l=1}^{2N_A} U_{i,l}U^*_{l,i} + U_{i+N_A,l}U^*_{l,i+N_A}\right] = \frac{1}{2}\left((UU^\dagger)_{i,i} + (UU^\dagger)_{i+N_A,i+v}\right) = 1$, since U is unitary. Thus one has the desired property

$$\sum_{i=1}^{N_A} c_A(i) = S(A). \tag{3.66}$$

F-utilities Routine 3.13. `Contour(`Γ_A`)`$\to \vec{c}_A$

This function return the vector $\vec{c}_{Ai} = c_A(i)$ of the entanglement contour of the correlation matrix Gamma$_A$. ♠

3.11 Examples

We will use the function

F-utilities Routine 3.14. `Random_NNhamiltonianr(N)`$\to H$

Generate a random f.q.h. hamiltonian for a system of N with just nearest neighbour interactions. ♠

3.11.1 Computing the energies of H

```
using F_utilities;
using PyPlot;
using LinearAlgebra;

const Fu = F_utilities;

N = 64;

#Generate and diagonalise the hamiltonian
H = Fu.Random_NNhamiltonian(N)
H_D, U_D = Fu.Diag_h(H)

#Print the energy modes epsilon_k
figure("Energies")
plot(1:N,diag(H_D)[1:N])
xlabel(L"$k$")
ylabel(L"$\epsilon_k$")
```

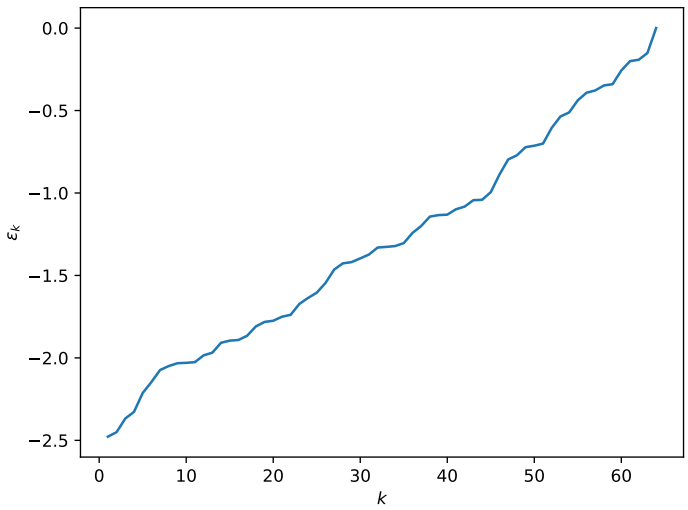


Figure 3.3: Output of examples 3.11.1.

3.11.2 Computing the entanglement contour of a partition of a ground state

```
using F_utilities;
using PyPlot;
using LinearAlgebra;
```

```
const Fu = F_utilities;

N = 64;
H = Fu.Random_NNhamiltonian(N);
H_D, U_D = Fu.Diag_h(H);

Gamma = Fu.GS_Gamma(H_D, U_D);
println("The energy of the ground state is: ", Fu.Energy_fermions(
    Gamma,H_D, U_D));

N_A = 32;
#I consider the reduced state over the sites 17,2,...,48
Gamma_A = Fu.Reduce_gamma(Gamma,N_A,17);
#I compute the entangement entropy
S_A = Fu.VN_entropy(Gamma_A);
#I compute the contour of partition A
c_A = Fu.Contour(Gamma_A);

lbl_title = string(L"$S(A) = $", S_A);
lbl_legend = string(L"$\sum_{i=1}^{N_A} c_A(i) = $", sum(c_A));
figure("Contour of A")
title(lbl_title)
plot(1:N_A, c_A, marker="o", label=lbl_legend);
xlabel("i")
ylabel(L"$c_A(i)$")
legend();
```

Output:

```
The energy of the ground state is:  -83.1750144099933
```

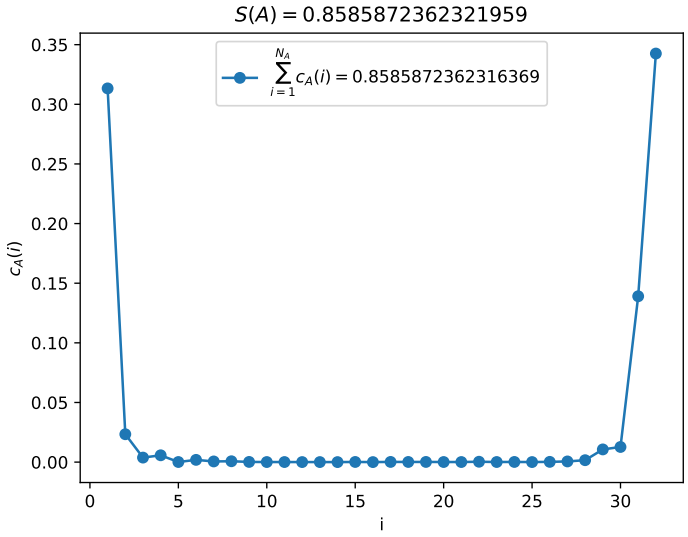


Figure 3.4: Output of examples 3.11.2, note how for a nearest neighbour hamiltonian, the contour is higher on the boundary of the partition.

Chapter 4 Time evolution

4.1 Real Time Evolution

In the previous sections we talked about hamiltonians and states. It is now the time to put this two ingredient together and finally talk about the unitary evolution of fermionic gaussian states. We start by say that *the space of fermionic gaussian states is closed under evolution induced by fermionic quadratic hamiltonians*. The best way for seeing this is using the Majorana operators representation. We consider a general f.q.h. $\hat{H}$ and a generic f.g.s. $\rho = \frac{e^{-\hat{H}_\rho}}{Z}$ with both $\hat{H}$ a and $\hat{H}_\rho$ of the form 2.4. Using standard notation we call $\rho(t)$ the state ρ at time t defined as

$$\rho(t) := e^{-it\hat{H}}\rho e^{it\hat{H}} = \frac{e^{-it\hat{H}}e^{-\hat{H}_\rho}e^{it\hat{H}}}{Z}. \tag{4.1}$$

As already observed in section 3.9, the commutator of two quadratic monomial of Dirac operators is a polynomial at most quadratic in Dirac operators. Using this observation together with the Baker-Campbell-Hausdorff formula (equation B.C.H.0 in appendix B.4), it is easy to see that $\rho(t)$ has the form

$$\rho(t) = \frac{e^{-\hat{H}_{\rho(t)}}}{Z}, \tag{4.2}$$

with $\hat{H}_{\rho(t)}$ a fermionic quadratic hamiltonian. Thus $\rho(t)$ is again a gaussian state and we proved that the space of gaussian states is closed under evolution induced by fermionic quadratic hamiltonians.

We will now compute an explicit formula for the time evolution of the correlation matrix $\Gamma(t)$ of the f.g.s. state $\rho(t)$. The first step is computing the time evolution of the creation and annihilation operators in the Heisenberg picture. We denote with $\vec{\beta}$ the vector of Dirac operators that diagonalise H. The annihilation and creation operators b_k and $b_k^\dagger$ evolved at time t are (see appendix **??**)

$$b_k(t) = e^{-i\hat{H}t}b_k e^{i\hat{H}t} = e^{-i2\epsilon_k t}b_k, \tag{4.3}$$

$$b_k^\dagger(t) = e^{-i\hat{H}t}b_k^\dagger e^{i\hat{H}t} = e^{i2\epsilon_k t}b_k^\dagger. \tag{4.4}$$

In compact form this can be written as

$$\vec{\beta}(t) = e^{i2H_D t}\vec{\beta}. \tag{4.5}$$

It is easy now to compute the time evolution of the correlators $\langle\vec{\beta}\vec{\beta}^\dagger\rangle$

$$\langle\vec{\beta}(t)\vec{\beta}^\dagger(t)\rangle = \langle e^{i2H_D t}\vec{\beta}\vec{\beta}^\dagger e^{-i2H_D t}\rangle. \tag{4.6}$$

Thus, if U is the fermionic transformation such that $\vec{\beta} = U\vec{\alpha}$, the fermionic transformation implementing the time evolution of $\vec{\alpha}$ is $U^\dagger e^{i2H_D t}U = e^{i2Ht}$. We finally obtain that the correlation

matrix Γ evolves with H as

$$\Gamma(t) = e^{i2Ht}\Gamma e^{-i2Ht}. \tag{4.7}$$

F-utilities Routine 4.1. `Evolve(Γ, H_D, U, t)`→ $\Gamma(t)$

This function return the correlation matrix Γ evolved at time t with H. Matrices H_D and U are the output of `Diag_h(H)`. ♠

4.2 Imaginary-time evolution

In order to find the ground state of a non-degenerate Hamiltonian H one can use the following equality

$$|GS\rangle = \lim_{\tau\to\infty} \frac{e^{-H\tau}|\psi\rangle}{||e^{-H\tau}|\psi\rangle||} \tag{4.8}$$

starting from a generic state $|\psi\rangle$ with $\langle GS|\psi\rangle \neq 0$.

To see this, let's consider the orthononormal basis $\{|E_i\rangle\}_i$ generated by the collection of the eigenvectors of H, with eigenvalues $\{E_i\}_i$ such that $E_0 \lneq E_1 \leq E_2 \leq \cdots \leq E_{dim(\mathcal{H})}$, where $\mathcal{H}$ is the Hilbert space on which H act.

Expanding $|\psi\rangle$ on this basis one obtains $|\psi\rangle = \sum_i c_i|E_i\rangle$, with $c_0 \neq 0$ from the fact that $\langle GS|\psi\rangle \neq 0$. One can thus see that eq (4.8) is just a projection to the ground state:

$$\lim_{\tau\to\infty} \frac{e^{-H\tau}|\psi\rangle}{||e^{-H\tau}|\psi\rangle||} = \lim_{\tau\to\infty} \sum_i \frac{e^{-E_i\tau}c_i}{\sqrt{\sum_i e^{-2E_i\tau}|c_i|^2}}|E_i\rangle = \tag{4.9}$$

$$= \lim_{\tau\to\infty} \sum_i \frac{e^{-\frac{E_i}{E_0}\tau}c_i}{\sqrt{\sum_i e^{-2\frac{E_i}{E_0}\tau}|c_i|^2}}|E_i\rangle = |E_0\rangle, \tag{4.10}$$

and thus that $\lim_{\tau\to\infty} \frac{e^{-H\tau}}{||e^{-H\tau}||}$ is the projector on the ground state:

$$\lim_{\tau\to\infty} \frac{e^{-H\tau}}{||e^{-H\tau}||} = \lim_{t\to\infty} \frac{\sum_i e^{-E_i\tau}|E_i\rangle\langle E_i|}{\sqrt{\sum_i e^{-2E_i\tau}}} = \tag{4.11}$$

$$= \lim_{\tau\to\infty} \frac{\sum_i e^{-\frac{E_i}{E_0}\tau}|E_i\rangle\langle E_i|}{\sqrt{\sum_i e^{-2\frac{E_i}{E_0}\tau}}} = |E_0\rangle\langle E_0|. \tag{4.12}$$

Applying the same method to the density matrix one can obtain the ground state ρ_{GS} of a non degenerate Hamiltonian H from a general density matrix ρ such that $Tr[\rho\rho_{GS}] \neq 0$ as

$$\rho_{GS} = \lim_{\tau\to\infty} \frac{e^{-H\tau}\rho e^{-H\tau}}{Tr\left[\rho e^{-2H\tau}\right]}. \tag{4.13}$$

We refer to the method for obtaining the ground state using (4.8) as performing an *imaginary time evolution*.

This is the case because, if for the time evolution operator $U(t) = e^{-iHt}$ for the Hamiltonian H, we select $t = -i\tau$ we obtain the operator $e^{-H\tau}$ that is the one of eq (4.8). One can thus write in a non-formal way $|GS\rangle = \lim_{t\to -i\infty} \frac{|\psi(t)\rangle}{||\psi(t)\rangle||}$.

It's important to keep in mind that the operator $e^{-H\tau}$ is not unitary and for this reason it doesn't

preserve the norm of the state and one has to renormalise it.

We know already how to compute the ground state of any f.q.h., but it could result useful to be able to simulate an imaginary time evolution with f.g.s. in the case one is interested in benchmarking more complex algorithms.

4.3 Numerical Imaginary time evolution

In the numerical approach to imaginary time evolution one faces some difficulties.

Almost in all cases one is forced to evolve the state step by step renormalising every time, performing a discrete imaginary time evolution.

This procedure doesn't allow to reach infinite time in a finite amount of time steps, thus one has to find a criterion to stop the evolution when the convergence is accurate up to some confidence parameter. To check if the reached state is the expected state is tricky and theoretically impossible in most of the cases since one does not always have the exact value of the energy of the ground state.

A method for checking the convergence is to check the energy difference between two steps of the discrete imaginary time evolution. Once the difference in energy between two steps is lower than an acceptable value ϵ, one decides that the algorithm converged.

It is not always the case though. It is also possible that the approximate imaginary time evolution stops at some plateau and thus trick the algorithm in believing in a false convergence to the ground state.

4.3.1 Imaginary time evolution of the correlation matrix

The imaginary time evolution of the correlation matrix is defined as

$$\Gamma_{i,j}(\tau) = Tr\left[\rho(\tau)\vec{\alpha}_i\vec{\alpha}_j^\dagger\right] = \tag{4.14}$$

$$= \frac{Tr\left[e^{-\hat{H}\tau}\rho e^{-\hat{H}\tau}\vec{\alpha}_i\vec{\alpha}_j^\dagger\right]}{Tr\left[e^{-\hat{H}\tau}\rho e^{-\hat{H}\tau}\right]}. \tag{4.15}$$

Obtaining an explicit form for $\Gamma(\tau)$ just in term of H and $\Gamma(0)$ is not easy. One can compute the imaginary time evolution in Heisenberg picture with $e^{-\hat{H}\tau}$ of the operator $\vec{\alpha}_i\vec{\alpha}_j^\dagger$. Using *BCH2* (i.e. $e^A B e^A = \sum_{n=0}^{\infty}\frac{1}{n!}\underbrace{\{A,\ldots\{A}_{n},B\underbrace{\}\ldots\}}_{n}$) and moving in the diagonal basis with Dirac operators $\vec{\beta}$ one can write the Hamiltonian as $\hat{H} = \sum_k \epsilon(k)\left(b_k^\dagger b_k - b_k b_k^\dagger\right)$.

Thus one has

$$e^{-\hat{H}\tau}\vec{\beta}_l\vec{\beta}_j^\dagger e^{-\hat{H}\tau} = \sum_{n=0}^{\infty}\frac{-\tau^n}{n!}\underbrace{\{\hat{H},\ldots\{\hat{H}}_{n},\vec{\beta}_l\vec{\beta}_j^\dagger\underbrace{\}\ldots\}}_{n}. \tag{4.16}$$

Since $b_l^\dagger b_j \hat{H} = (\hat{H} + 2\Delta_{l,j}) b_l^\dagger b_j$, we cannot simplify this expression as in the case of real time evolution.

To obtain a numerical algorithm for the imaginary time evolution one has to realise that, for each value of τ, $\Gamma(\tau)$ is just the correlation matrix of the f.g.s.

$$\rho(\tau) = \frac{e^{-\hat{H}\tau}\rho e^{-\hat{H}\tau}}{\mathrm{Tr}\left[e^{-\hat{H}\tau}\rho e^{-\hat{H}\tau}\right]}. \tag{4.17}$$

The correlation matrix $\Gamma(\tau)$ can be easily obtained by the product rule (see section 3.9) of the initial f.g.s. ρ and the thermal state $\rho_{\beta=\tau} = \frac{e^{-H\tau}}{\mathrm{Tr}\left[e^{-\hat{H}\tau}\right]}$.

F-utilities Routine 4.2. `Evolve_imag(Γ, H_D, U, τ)`$\to \Gamma(\tau)$

This function return the correlation matrix Γ evolved at imaginary time τ with H. Matrices H_D and U are the output of `Diag_h(H)`. ♠

Chapter 5 Hopping model

We consider the translational invariant hopping hamiltonian for a system of N sites

$$\hat{H} = \sum_{i=1}^{N-1} [a_i^\dagger a_{i+1} - a_i a_{i+1}^\dagger] + \delta [a_N^\dagger a_1 - a_N a_1^\dagger], \tag{5.1}$$

with $\delta = 1$ for periodic boundary conditions and $\delta = 0$ for open boundary conditions.

The compact form (2.2) of $\hat{H}$ is specified by the two circulant matrices (see A.4)

$$A = \begin{pmatrix} 0 & \frac{1}{2} & 0 & \dots & 0 & \delta\frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \dots & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & \dots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \delta\frac{1}{2} & 0 & 0 & \dots & \frac{1}{2} & 0 \end{pmatrix} \qquad B = \begin{pmatrix} 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{pmatrix} \tag{5.2}$$

As seen in section **??** and appendix A.4) we know that H is diagonalised with a Fourier transformation. Indeed, if we express the hopping hamiltonian (5.1) in term of the Fourier modes (3.8.2) we obtain

$$\hat{H} = \sum_{k=1}^{N} \phi_k (f_k^\dagger f_k - f_k f_k^\dagger), \tag{5.3}$$

where

$$\phi_k = \cos(\frac{2\pi}{N} k). \tag{5.4}$$

The fermionic transformation that diagonalise the Hamiltonian is U_ω as definied in (3.46).

5.1 Numerical diagonalisation

In the following code we show how to initialise and diagonalise the hopping hamiltonian using functions of `F-utilities`.

```
using F_utilities;
using PyPlot;
using LinearAlgebra;

const Fu = F_utilities;



N =127;

H  = Fu.Build_hopping_hamiltonian(N,true);
```

```
U_omega = Fu.Build_Fourier_matrix(N);
D_omega = U_omega'*H*U_omega;
D,U = Fu.Diag_h(H);


figure("Energies")
plot(diag(real.(D_omega))[(N+1):(2*N)],label="Method Fourier");
plot(real.(diag(D))[(N+1):(2*N)], label="Method Diag_h");
xlabel(L"$k$");
ylabel(L"$\epsilon_k$");
legend();

Gamma_omega = Fu.GS_gamma(D_omega,U_omega);
Gamma = Fu.GS_gamma(D,U);
println("")
println("Energy GS Method Fourier: ",Fu.Energy(Gamma_omega,(D_omega,
    U_omega)))
println("En GS Method Diag_h: ",Fu.Energy(Gamma,(D,U)))

Fu.Print_complex_matrix("Differenza Gamma", Gamma-Gamma_omega)
```

Output:

```
Energy GS Method Fourier:  -80.85277253991693
En GS Method Diag_h:  -80.85277253997737
```

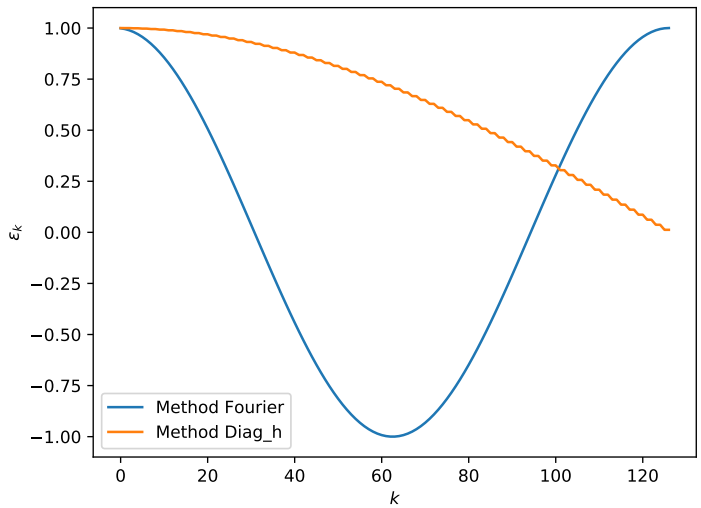


Figure 5.1: In this example we diagonalised the hamiltonian with two different methods. Using the Fourier transform method we obtain the energies specified in (5.4). These energies are both positive and negative. Using the `Diag_h` method of `F_utilities` we obtain just positive energies. The difference in the diagonal energies comes from the fact that `Diag_h` for every eigenmode with negative energy substitute creation and annihilation operators in order to redefine the energy as positive, and then reorder the modes in order to have the energies in descending order. If we diagonalise with the Fourier transform than the ground state is obtained filling all the modes with negative energy. If we diagonalise with `Diag_h` then the ground state corresponds to the empty state.

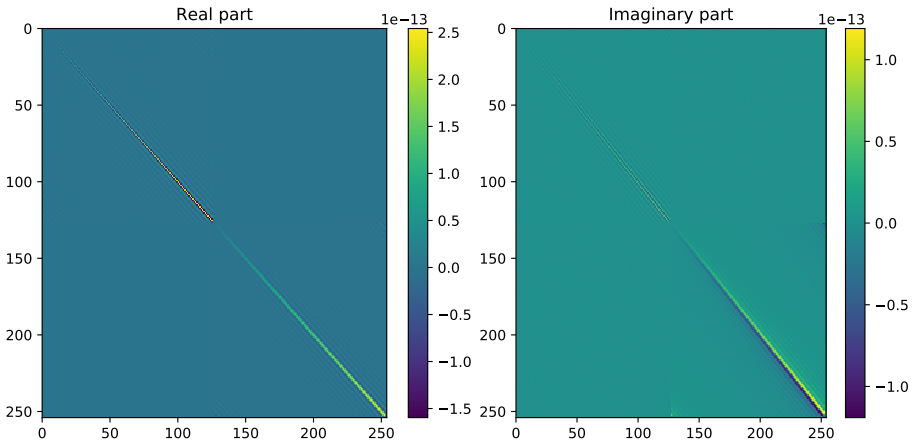


Figure 5.2: Here we plot the real and imaginary part of the differences correlation matrices of the ground state computed with the two methods. On the real space basis of $a, a^\dagger$ the ground state must be the same.

F-utilities Routine 5.1. `Build_hopping_hamiltonian(`N`, PBC=true)`$\to H$

This functions return the hamiltonian H if dimension $2N \times 2N$ for the hopping model. If `PBC=false` it return the hopping hamiltonian with open boundary conditions

For the numerical diagonalisation of the hamiltonian we used two methods, the analytical one using the Fourier modes, and the numerical one introduced in the previous section.

These methods return the hopping hamiltonian in the diagonal forms

$$\hat{H}_\omega = \sum_{k=1}^{N} \phi_k (f_k^\dagger f_k - f_k f_k^\dagger), \qquad \hat{H} = \sum_{k=1}^{N} \epsilon_k (b_k^\dagger b_k - b_k b_k^\dagger), \tag{5.5}$$

where the difference in the energies are due to the fact that `Diag_h` consider all the energies ϵ_k positive, thus defines $b_k = f_k^\dagger$ and $b_k^\dagger = f_k$ for each k such that $\phi_k < 0$, and then reorder the modes such that to modes with smaller k correspond biggest energies.

5.2 Time evolution

For the hopping model we analytically obtained the fermionic transformation U_ω that diagonalise the Hamiltonian. This allows us to give an analytical expression for the time evolution of the correlation matrix.

Expressing the correlation matrix Γ in term of the operators $\vec{\phi}$ and computing the time evolution

with the diagonal hamiltonian 5.3 we obtain

$$\langle a_l^\dagger a_m\rangle(t) = \frac{1}{N}\sum_{k,k'} e^{i2(\phi_k-\phi_{k'})t} e^{i\frac{2\pi}{N}(k(l-x)-k'(m-y))} a_x^\dagger a_y \tag{5.6}$$

$$\langle a_l a_m\rangle(t) = \frac{1}{N}\sum_{k,k'} e^{-i2(\phi_k+\phi_{k'})t} e^{-i\frac{2\pi}{N}(k(l-x)+k'(m-y))} a_x a_y. \tag{5.7}$$

Because of the block diagonal structure of U_ω there is not mixing of the two types of correlators during the evolution of the correlation matrix.

5.2.1 Time evolution of translational invariant states

Let us consider a translational invariant state Γ. In section 3.8 we expressed Γ in term of the Fourier modes $f_k^\dagger, f_k$. Using the diagonal form (5.5) of the Hopping Hamiltonian to compute the time evolution of the correlators of Γ expressed as in (3.43) we have that Γ evolves as

$$\begin{aligned}
\langle a^\dagger a\rangle_\Delta(t) &= \frac{1}{N}\sum_{k=1}^{N} e^{-i\frac{2\pi}{N}k\Delta}\langle f_k^\dagger f_k\rangle, & \langle aa^\dagger\rangle_\Delta(t) &= \frac{1}{N}\sum_{k=1}^{N} e^{-i\frac{2\pi}{N}k\Delta}\langle f_k f_k^\dagger\rangle \\
\langle aa\rangle_\Delta(t) &= \frac{1}{N}\sum_{k=1}^{N} e^{i4\phi(k)t} e^{-i\frac{2\pi}{N}k\Delta}\langle f_k f_{N-k}\rangle, & \langle a^\dagger a^\dagger\rangle_\Delta(t) &= \frac{1}{N}\sum_{k=1}^{N} e^{-i4\phi(k)t} e^{-i\frac{2\pi}{N}k\Delta}\langle f_{N-k}^\dagger f_k^\dagger\rangle.
\end{aligned} \tag{5.8}$$

```
using F_utilities;
using PyPlot;
using LinearAlgebra;

const Fu = F_utilities;



N=50;
N_steps = 100;
delta_steps = 0.1;

#Build the circulant vector for the adaa part of the Gamma with
    exponential decaying correlations
adaa = zeros(Complex{Float64},N);#
for i=1:div(N,2)
   adaa[i] = exp(-i*0.15)*(rand()+im*rand())
end
adaa[((div(N,2))+1):N]= reverse(adaa[1:div(N,2)]);
#Build the translational invariant adaa part of the Gamma
Gamma_adaa = Fu.Circulant(adaa);
Gamma_adaa = (Gamma_adaa+Gamma_adaa')/2.
```

```
#Build the circulant vector for the aa part of the Gamma
aa = zeros(Complex{Float64},N);
aa[2] = rand()+im*rand();
aa[3] = rand()+im*rand();
#Build the translational invariant aa part of the Gamma
Gamma_aa = Fu.Circulant(aa)
Gamma_aa = (Gamma_aa-transpose(Gamma_aa))/2.;

#Build the translational invariant Gamma
Gamma= zeros(Complex{Float64}, 2N,2N);
Gamma[(1:N),(1:N)]   = Gamma_adaa;
Gamma[(1:N).+N,(1:N).+N] = (I-Gamma_adaa)';
Gamma[(1:N).+N,(1:N)] = Gamma_aa;
Gamma[(1:N),(1:N).+N] = -conj(Gamma_aa);
Fu.Print_complex_matrix("Gamma",Gamma)

H  = Fu.Build_hopping_hamiltonian(N,true);
D,U = Diag_h(H);



Gamma_evolved = copy(Gamma);
adaa     = zeros(Complex{Float64}, N_steps)
aa       = similar(adaa);

#Start the time evolution cycle
#at each cycle it saves the value of two correalotors
adaa[1]  = Gamma_evolved[1,2];
aa[1]    = Gamma_evolved[N+1,2];
for t=2:N_steps
   global Gamma_evolved = Fu.Evolve(Gamma_evolved,(D,U),delta_steps);
   adaa[t]  = Gamma_evolved[1,2];
   aa[t]    = Gamma_evolved[N+1,2];
end

figure("Evolutions")
plot(real.(adaa), color="black", label=L"$\mathfrak{R}(\langle a_1^{\
    dagger}a_2 \rangle)(t)$");
```

```
plot(imag.(adaa), color="black",linestyle="--", label=L"$\mathfrak{I
    }(\langle a_1^{\dagger} a_2 \rangle)(t)$");
plot(real.(aa), color="purple", label=L"$\mathfrak{R}(\langle a_1a_2 \
    rangle|(t))$");
plot(imag.(aa), color="purple", linestyle="--", label=L"$\mathfrak{I
    }(\langle a_1 a_2 \rangle)(t)$");
legend()
xlabel("timestep")
```

Output:

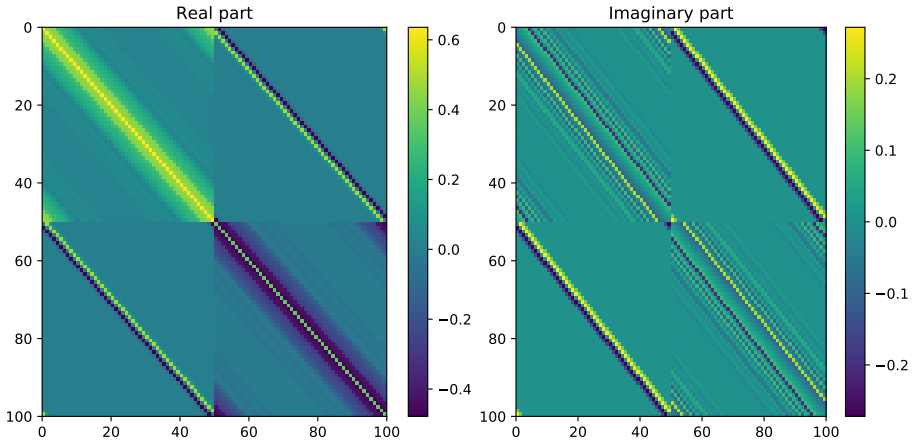


Figure 5.3: This is the correlation matrix Γ of a translational invariant state with exponentially decaying correlations

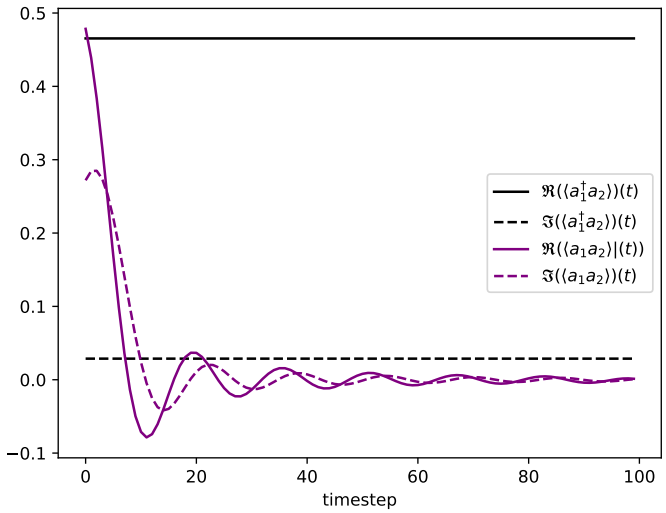


Figure 5.4: The time evolution induced by the Hopping hamiltonian of the real and imaginary part of $\langle a_1^\dagger a_2\rangle$ and $\langle a_1 a_2\rangle$ of the translational invariant state specified in the code.

Chapter 6 Transverse Field Ising Model

The hamiltonian of the Transverse Field Ising model (TFI) is written as

$$\hat{H} = -\sum_{n=1}^{N-1} \sigma_n^x \sigma_{n+1}^x - \delta \sigma_N^x \sigma_1^x - \cot(\theta) \sum_{n=1}^{N} \sigma_n^z, \tag{6.1}$$

where N is the number of sites, σ_i^α with $\alpha = x, y, z$ are the Pauli matrices at the i-th site and $\cot(\theta)$ is the magnetic field, with $0 < \theta < \frac{\pi}{2}$.

The parameter δ encodes the boundary conditions: here we consider $\delta = 1$ or $\delta = 0$, corresponding, respectively, to periodic boundary conditions and open boundary conditions.

The model is called *transverse* field Ising model because the field interacts with the spins with σ_i^z, while the spins interact between each others with $\sigma_i^x \sigma_{i+1}^x$.

The TFI hamiltonian can be exactly diagonalised using Jordan-Wigner transformation (see appendix A.6) mapping spin operators to spinless fermions Cabrera and Jullien (1987); Calabrese et al. (2012); Henkel (1999); Lieb et al. (1961); Mattis (1976); Pfeuty (1970); Schultz et al. (1964); Suzuki et al. (2013).

Appendix Extended calculations

A.1 Eigenvalues of Γ and H_α

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

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

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

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

To compute the numerator part this equalities will result useful

- For $x \neq y$

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

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

- $\forall x, y$

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

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

Thus the numerator can be explicitly written as

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

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

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

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

I can divide by Z and obtain

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

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

$$\nu_i = \frac{1}{1+e^{2\epsilon_i}}, \tag{A.10}$$

$$\epsilon_i = \frac{1}{2} ln\left(\frac{1-\nu_i}{\nu_i}\right), \tag{A.11}$$

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

A.2 Purity

From the previous subsection we have:

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

and

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

Thus the purity is:

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

A.3 Real Time Evolution

We want to compute the time evolution in the Heisenberg picture of the annihilation operator b_k induced by the hamiltonian $\hat{H} = \sum_{l=1}^{N} \epsilon_l (b_l^\dagger b_l - b_l b_l^\dagger)$. First we simplify the expression exploiting the commuting terms

$$b_k(t) = e^{i\hat{H}t} b_k e^{-i\hat{H}t} = e^{it\sum_{l=1}^{N} \epsilon_l (b_l^\dagger b_l - b_l b_l^\dagger)} b_k e^{it\sum_{l=1}^{N} \epsilon_l (b_k^\dagger b_l - b_l b_l^\dagger)} = \tag{A.15}$$

$$= e^{it\epsilon_k (b_k^\dagger b_k - b_k b_k^\dagger)} b_k e^{it\epsilon_k (b_k^\dagger b_k - b_k b_k^\dagger)}. \tag{A.16}$$

Secondly applying B.C.H.1 (see B.C.H.1 in B.4) we obtain that

$$b_k(t) = \sum_{n=0}^{\infty} \frac{(ie_k t)^n}{n!} \underbrace{[b_k^\dagger b_k - b_k b_k^\dagger, \dots [v_k^\dagger b_k - b_k b_k^\dagger}_{n}, b_k \underbrace{] \dots]}_{n}, \tag{A.17}$$

and using the fact that

$$[b_k^\dagger b_k - b_k b_k^\dagger, b_k] = -2b_k, \tag{A.18}$$

we obtain

$$b_k(t) = \sum_{n=0}^{\infty} \frac{(2ie_k t)^n}{n!} b_k = e^{-i2e_k t} b_k. \tag{A.19}$$

A.4 Circulant Matrices

An $N \times N$ circulant matrix C is a matric of the form

$$C = \begin{pmatrix} c_0 & c_1 & c_2 & \dots & c_{N-1} \\ c_{N-1} & c_0 & c_1 & \dots & c_{N-2} \\ c_{N-2} & c_{N-1} & c_0 & \dots & c_{N-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_1 & c_2 & c_3 & \dots & c_0 \end{pmatrix}. \tag{A.20}$$

A circulant matrix is completely specified by the *circulant vector* $\vec{c}$, that is its first row.

$$\vec{c} = (c_0, c_1, c_2, \dots, c_{N-1}). \tag{A.21}$$

All the other rows of the matrix are cyclic permutations of $\vec{c}$ with offset increasing by one going down with the rows.

Since each descending diagonal from left to right is constant, circulant matrices are a special case of Toeplitz matrices.

Because of their special structure, circulant matrices are diagonalised by taking their Fourier transform.

Given a vector $\vec{v}$ of length N its Fourier transform is expressed as $\vec{w} = W\vec{v}$, with W defined as

$$W = \frac{1}{\sqrt{N}} \begin{pmatrix} \omega & \omega^2 & \omega^3 & \cdots & \omega^{N-1} & 1 \\ \omega^2 & \omega^4 & \omega^6 & \cdots & \omega^{2(N-1)} & 1 \\ \omega^3 & \omega^6 & \omega^9 & \cdots & \omega^{3(N-1)} & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & 1 \\ \omega^{N-1} & \omega^{2(N-1)} & \omega^{3(N-1)} & \cdots & \omega^{(N-1)(N-1)} & 1 \\ 1 & 1 & 1 & 1 & \cdots & 1 \end{pmatrix}, \tag{A.22}$$

with $\omega = e^{-i\frac{2\pi}{N}}$.

The columns of W are the normalised eigenvectors $|\lambda_i\rangle$ of every circulant matrix of dimension $N \times N$.

The corresponding eigenvalues depend on the specific circulant vector $\vec{c}$ specifying the circulant matrix and are given by

$$\lambda_j = c_0\omega^j + c_1\omega^j + c_2\omega^{j2} + \cdots + c_{N-2}\omega^{j(N-2)} + c_{N-1}\omega^{j(N-1)}. \tag{A.23}$$

A.5 Block diagonal form of skew-symmetric matrices

Let h be a $N \times N$ skew-symmetric matrix of rank $2m$, where $N \geq 2m$.

Then there exist a $N \times N$ unitary matrix U such that Horn and Johnson (1985)

$$U^T hU = \begin{pmatrix} 0 & \lambda_1 \\ -\lambda_1 & 0 \end{pmatrix} \oplus \begin{pmatrix} 0 & \lambda_2 \\ -\lambda_2 & 0 \end{pmatrix} \oplus \cdots \oplus \begin{pmatrix} 0 & \lambda_m \\ -\lambda_m & 0 \end{pmatrix} \oplus \hat{0}_{N-2m}, \tag{A.24}$$

where $\hat{0}_{N-2m}$ is a $(N-2m)\times(N-2m)$ matrix with all elements equal to zero and where the real and positive-definite $\{\lambda_i\}_{i=1,m}$ are the singular values of h.

Since a skew-symmetric matrix h is similar to its own transposeh^T, then h and h^T must have the same eigenvalues. Thus, the eigenvalues of a skew-symmetric matrix of even dimension will always come in pairs $\pm\tilde{\lambda}$ (for the case of odd dimension there will be an unpaired eigenvalue equal to 0).

A.6 Jordan-Wigner transformation

The Jordan-Wigner transformation, introduced in the original paper Jordan and Wigner (1928), is a transformation that maps spin-$\frac{1}{2}$ systems to fermionic systems.

Suppose we have a system of N spins-$\frac{1}{2}$ with the usual Pauli matrices σ_j^x, σ_j^y and σ_j^z acting on the j-th spin of the system The Jordan-Wigner transformation defines the operator a_j as

$$a_j = -\left(\otimes_{k=1}^{j-1}\sigma_k^z\right) \otimes \sigma_j^- \left(\otimes_{k=j+1}^{N}\mathbb{I}_k\right), \tag{A.25}$$

where $\sigma_j^{\pm} = \frac{\sigma_j^x \pm i\sigma_j^y}{2}$ and $\mathbb{I}_j$ is the identity acting on the j-th spin. Taking the adjoint obtains

$$a_j^\dagger = -\left(\otimes_{k=1}^{j-1}\sigma_k^z\right) \otimes \sigma_j^+ \left(\otimes_{k=j+1}^{N}\mathbb{I}_k\right). \tag{A.26}$$

Computing the anticommutator of these two operators we notice that they obey the CAR, thus using this transformation for every site j we are able to build a legitimate set of Dirac fermionic operators starting from a set of Pauli matrices.

Knowing the expression for the creation and annihilation operators, we can easily find the mapping of the single site occupation operator in term of Pauli operators:

$$a_j^\dagger a_j = -\left(\otimes_{k=1}^{j-1}\sigma_k^z\right)\otimes\frac{\sigma_j^z+\mathbb{I}_j}{2}\left(\otimes_{k=j+1}^{N}\mathbb{I}_k\right). \tag{A.27}$$

Finally there are two important remarks. We notice that the mapping from spins to fermions is not local, in the sense that equation A.25 maps a string of Pauli operators acting non trivially on j spins to a Dirac operator local only on site j.

We even notice that in the definition of the annihilation operator A.25 it is encoded some information on the geometrical structure of the spin system, in particular it is encoded the distance of site j from the border.

When using the Jordan-Wigner transformation one has to be careful about these two observations.

In the main text we are interested in mapping the transverse field Ising hamiltonian to a fermionic system, thus we need the inverse Jordan-Wigner transformation. We have that the Pauli operator σ_j^z is easily mapped to fermionic annihilation and creation operators as

$$\sigma_j^z = a_j^\dagger a_j - a_j a_j^\dagger. \tag{A.28}$$

We see that for this transformation local spin operators are mapped to local fermionic operators. We know nonetheless that the Jordan-Wigner transformation does not preserve locality in general, indeed we have that the Pauli operators σ_j^x and σ_j^y maps to fermionic operators as

$$\begin{aligned}\sigma_j^x &= -\left(\otimes_{k=1}^{j-1}\sigma_k^z\right)\otimes(a_j+a_j^\dagger)\left(\otimes_{k=j+1}^{N}\mathbb{I}_k\right)\\ \sigma_j^y &= i\left(\otimes_{k=1}^{j-1}\sigma_k^z\right)\otimes(a_j-a_j^\dagger)\left(\otimes_{k=j+1}^{N}\mathbb{I}_k\right),\end{aligned} \tag{A.29}$$

where for each σ_k^z one should use the substitution (A.28).

Fortunately, if we consider the product of Pauli operators, as for example are the spin-spin interactions in the TFI model we have

$$\begin{aligned}\sigma_j^x\sigma_{j+1}^x &= (a_j^\dagger - a_j)(a_{j+1}+a_{j+1}^\dagger),\\ \sigma_j^y\sigma_{j+1}^y &= -(a_j^\dagger + a_j)(a_{j+1}^\dagger - a_{j+1}),\\ \sigma_j^x\sigma_{j+1}^y &= i(a_j^\dagger - a_j)(a_{j+1}^\dagger + a_{j+1}),\\ \sigma_j^y\sigma_{j+1}^x &= i(a_j^\dagger + a_j)(a_{j+1}^\dagger + a_{j+1}),\end{aligned} \tag{A.30}$$

nearest neighbour interactions are mapped to nearest neighbour interactions.

It easy to see that an interaction of this kind between two arbitrary spins at site j and k will map to a string of Dirac operators acting non trivially on all sites between j and k.

We have seen that the Jordan-Wigner transformation defines an isomorphism from a system of

n fermions to a system of n spins. One should ask why we cannot completely identify spin systems with fermionic systems or vice versa. To answer to this question we remind that, as specified above, the Jordan-Wigner mapping does not preserve the locality. One of the consequence of this fact is that the procedure of partial tracing does not generally commute with the Jordan-Wigner mapping Friis (2016); Friis et al. (2013). Consider for example a state of N fermions ρ_{AB} defined on a system divided in two complementary partitions A and B. We map ρ_{AB} with a Jordan-Wigner transformation to a a state $\tilde{\rho}_{AB}$ of N spins. Now we consider the marginals ρ_A and $\tilde{\rho}_A$ on partition A of the states ρ_{AB} and $\tilde{\rho}_{AB}$. If, using a Jordan-Wigner transformation, we map the state ρ_A to the spin state $\tilde{\tilde{\rho}}_A$, we will generally have that $\tilde{\rho}_A \neq \tilde{\tilde{\rho}}_A$. We show a schematic picture of this in figure A.6.

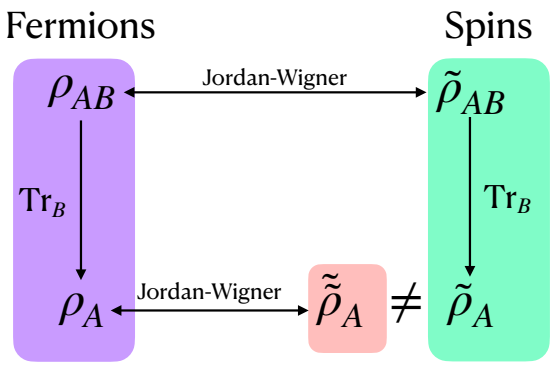


Figure A.1: The mapping of the reduced state is different from the reduced state of the mapping Friis (2016)

Due to antisymmetrisation the fermionic Fock space is not naturally equipped with a tensor product structure with respect to the individual mode subspaces. Spins instead yes. Partial trace is well defined for fermions. Partial trace is well defined for spins. This is the limitation of the mapping. One has to take care when considering entanglement in fermionic systems.**??**

Appendix Useful relations

B.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. $\sigma^-\sigma^+ = \frac{\mathbb{I} - \sigma^z}{2}$

B.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. $xp = -\frac{i}{2}\left(a^\dagger a - aa^\dagger\right) = -i\left(a^\dagger a - \frac{1}{2}\right)$

B.3 Jordan-Wigner Transformations

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

B.3.2 spins → 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. $\sigma_j^y \sigma_{j+1}^x = i(a_j^\dagger + a_j)(a_{j+1}^\dagger + a_{j+1})$

B.4 Formulas

1. B.C.H. 1: $e^A e^B = e^Z$ with $Z = A + B + \frac{1}{2}[A,B] + \frac{1}{12}[A,[A,B]] + \frac{1}{12}[B,[A,B]] +$ . . . higher commutators of A and B
2. B.C.H 2: $e^A B e^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!} \underbrace{[A,\ldots[A}_{n}, B \underbrace{]\ldots]}_{n}$ where $[A,B] = AB - BA$.
3. B.C.H 3: $e^A B e^A = \sum_{n=0}^{\infty} \frac{1}{n!} \underbrace{\{A,\ldots\{A}_{n}, B \underbrace{\}\ldots\}}_{n}$ where $\{A,B\} = AB + BA$.
4. Kronecker Delta: $\delta_{n,m} = \frac{1}{N} \sum_{k=1}^{N} e^{i\frac{2\pi}{N}k(n-m)}$.

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