Thesis Work: Ergotropy and Quantum Phase Transitions

January 22, 2021

Contents

Chapter 1

Introduction

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Here go motivations and outline of the work, maybe something on quantum batteries [AF13] [AKM$^+$19] [DC19], quantum machines, work extraction processes, quantum computers.
Also something on DMRG and Tensor Networks.

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We will define the ergotropy and some related quantities and study their behavior in a system that undergoes a quantum phase transition.
We will also define and measure a quantity related to ergotropy: the Max-Ergotropy.
Besides the interest of these quantities for experimental aspects related to work extraction, we will use them as quantum phase transition markers.
Entanglement plays a role, maybe focus on difference between classical and quantum work extraction.

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In the last decades, Quantum Phase Transitions (QPT) [Sac11] [Voj03] established as one of the most important research topics in theoretical and experimental [BGBE10] condensed matter physics.
QPT appear in many areas of modern research: rare-earth magnetic insulators , heavy-fermion compounds, high-temperature superconductors, two-dimensional electron gases, quantum Hall effects.
A lot of work has been done to understand what happens to the quantum wave-function that undergoes a Quantum Phase Transition.
The work of Wen et. al exploited the limitation of the symmetry breaking approach in the description of QPT [Gan07]. Topological transitions and the distinction between Long-Range and Short-Range quantum entanglement pushed in the direction of a unification between Quantum Information and Quantum Matter. [ZCZW19]
Following the incredible development of Quantum Information Theory [NC11] [Wil13],

it became clear that entanglement is a fundamental resource for the development of Quantum Technology and entanglement measures gained a renew interest.

In 2002 [OAFF02] Fazio et al. and [ON02] Nielsen et al. showed that Concurrence is sensible to QPT.

In 2008, Amico, Fazio, Osterloh and Vedral published a monumental review [AFOV08] on the topic of "Entanglement in Many-Body Systems" where they reviewed many entanglement measures and their role in QPT.

A clear and complete characterization of quantum correlations in QPT it's still an open problem [DCS18] even if by now it's clear that the various measures of entanglement are sensitive to the presence of quantum phase transitions. [WSL04]

Various entanglement measures have been studied close to a QPT: Local Convertibility [FCA+14],Quantum Discord [TRHA11], Leggett-Garg inequalities [GRMAR+16].

Here i cite various measures

Modern nanotechnology allows for testing concepts derived from classical thermodynamics in regimes where quantum effects become crucial [KFIT17] [RDT+16] [SZAW03].

Quantum Thermodynamics [GMM10] [DC19] is a relatively new field that aims to characterize the Thermodynamics aspect of Quantum Many-Body Theory and the emergence of classical Thermodynamic from Quantum Mechanics.

Following this goal, Allahverdyan et al. [ABN04] defined a quantity called ergotropy to solve the work extraction problem in the quantum regime.

Ergotropy for finite system becomes the Free Energy, the deviation of Ergotropy from is classical counterpart is proportional to quantum effects like entanglement and coherence [AGP19] [FGPP17] and this difference could be crucial in the development of quantum technologies [AF13] .

Since ergotropy is sensible to quantum correlations, we believe it would be interesting to characterize it in the proximity of a Quantum Phase Transition.

Chapter 2

Ergotropy and related measures

A very practical question we can ask ourselves is: If someone gives us a quantum mechanical system in a given state, what is the maximum amount of work we can extract from it?

This question becomes more meaningful if we restrict the ways in which we can modify the state.

A natural restriction we can set is that we want to use unitary channels only.

With this hypothesis in mind, the answer to this question exist and it is a quantity called *ergotropy* [ABN04].

2.1 Ergotropy

We will follow the derivation in [ABN04].

Consider a quantum mechanical system S described by an Hamiltonian H on which we can act on with an external potential $V(t)$.

Examples could be:

The state $\rho(t)$ of the system will thus evolve through the Hamiltonian: $H_{tot} = H + V(t)$ according to the Heisenberg equation:

$$i\hbar\dot{\rho}(t) = [H_{tot}(t), \rho(t)] \tag{2.1}$$

Defining the Unitary time-evolution operator $U(t) = \exp(iH_{tot}t/\hbar)$, we can write :

$$\rho(t) = U(t)\rho(0)U^\dagger(t) \tag{2.2}$$

Suppose now that the external potential is turned on in the time interval between $t = 0$ and $t = \tau$, the total work done on the system will be:

$$W = E(\tau) - E(0) = \text{tr}[\rho(\tau)H] - \text{tr}[\rho(0)H] \tag{2.3}$$

If we want to extract the maximum amount of work from the system we have to reach a $\rho(\tau)$ such that $E(\tau)$ has the lowest possible value.

should i give some examples?

Definition 2.1.1 (Passive State)**.** [PW78]

Given an Hilbert Space with an Hamiltonian H, a state ρ_{pas} is a passive state if:

$$\text{tr}[H\rho_{pas}] \leq \text{tr}\left[HU\rho_{pas}U^{\dagger}\right] \quad \forall U \quad \text{with} \quad UU^{\dagger} = U^{\dagger}U = I \tag{2.4}$$

That means we can't lower the energy (and eventually extract work) from a Passive State acting on it with Unitary Matrices.

Putting all together: we would like to find a function $V_{pas}(t)$, which is zero outside of the time interval $[0, \tau]$, such that the Hamiltonian $H_{pas} = H + V_{pas}(t)$ acting on the system trough the time-evolution operator $U_{pas}(t) = \exp(iH_{pas}t/\hbar)$ will transform the state $\rho(0)$ in the passive state ρ_{pas} that has energy:

$$E_{pas} = \text{tr}[\rho_{pas}H] = \text{tr}\left[U_{pas}(\tau)\rho(0)U_{pas}^{\dagger}(\tau)H\right] \tag{2.5}$$

And E_{pas} will be the lowest energy we can get using unitary operators.

Acting with unitary transformations only we can't change the eigenvalues of $\rho(0)$, nevertheless we can reach a passive state.

Let's first prove the following [HT13]:

Theorem 2.1.1. Given an Hilbert Space with Hamiltonian

$$H = \sum_{k\geq 1} \varepsilon_k^{(\uparrow)} \left|\varepsilon_k^{(\uparrow)}\right\rangle \left\langle\varepsilon_k^{(\uparrow)}\right| \quad \text{with} \quad \varepsilon_1^{(\uparrow)} \leq \varepsilon_2^{(\uparrow)} \leq \cdots \tag{2.6}$$

and a generic quantum state:

$$\rho = \sum_{j\geq 1} r_j^{(\downarrow)} \left|r_j^{(\downarrow)}\right\rangle \left\langle r_j^{(\downarrow)}\right| \quad \text{with} \quad r_1^{(\downarrow)} \geq r_2^{(\downarrow)} \geq \cdots \tag{2.7}$$

The state:

$$\rho_{pas} = \sum_j r_j^{(\downarrow)} \left|\varepsilon_j^{(\uparrow)}\right\rangle \left\langle\varepsilon_j^{(\uparrow)}\right| \tag{2.8}$$

is a passive state.

Proof. We represent a generic unitary matrix in the Hamiltonian basis [1]:

$$U = \sum_j U_{ij} \left|\varepsilon_i\right\rangle \left\langle\varepsilon_j\right| \tag{2.9}$$

Since U it's unitary, $|U_{ij}|^2$ is a doubly stochastic matrix (has non-negative entries and each row and column sums to 1), that means we can use the Birkhoff's Theorem [MOA11] to express it as a convex combination of permutation matrices P^n:

$$|U_{ij}|^2 = \sum_n p_n P^n \quad \text{with} \quad \sum_n p_n = 1 \tag{2.10}$$

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[1]If the basis it's not complete we can easily expand it setting the new eigenvalues to 0.

Now we apply this generic unitary transformation U to ρ_{pas} and calculate the resulting energy:

$$\text{tr}\big[U\rho_{pass}U^\dagger H\big] = \sum_{i,k}\varepsilon_i^{(\uparrow)}r_k^{(\downarrow)}\|U_{ik}\|^2 = \sum_n p_n \sum_{i,k}\varepsilon_i^{(\uparrow)}P_{ik}^n r_k^{(\downarrow)} \tag{2.11}$$

For every permutation $P(r_j^{(\downarrow)})$ of the ρ_{pass} indices it's clear that:

$$\sum_i \varepsilon_i^{(\uparrow)}[P(r_j^{(\downarrow)})]_i \geq \sum_i \varepsilon_i^{(\uparrow)}r_i^{(\downarrow)} = \text{tr}[\rho_{pas}H] \tag{2.12}$$

the permutation that gives us the lowest product is the one where the eigenvalues are arranged in the opposite direction.

We conclude that:

$$\sum_n p_n \sum_{i,k}\varepsilon_i^{(\uparrow)}P_{ik}^n r_k^{(\downarrow)} \geq \sum_n p_n \sum_i \varepsilon_i^{(\uparrow)}r_i^{(\downarrow)} = \sum_i \varepsilon_i^{(\uparrow)}r_i^{(\downarrow)} \tag{2.13}$$

Or equivalently:

$$\text{tr}[\rho_{pas}H] \leq \text{tr}\big[U\rho_{pass}U^\dagger H\big] \quad \forall U \quad \text{with} \quad UU^\dagger = U^\dagger U = I \tag{2.14}$$

$\square$

We proved that from every quantum state $\rho = \sum_{j\geq 1}r_j^{(\downarrow)}|r_j\rangle\langle r_j|$ we can form a passive state $\rho_{pas} = \sum_j r_j^{(\downarrow)}|\varepsilon_j\rangle\langle\varepsilon_j|$, it remains only to show that we can go from ρ to ρ_{pas} with an appropriate choice of the function $V(t)$.

An unitary operator that does the job is:

$$U_{pas} = \sum_j |\varepsilon_j\rangle\langle r_j| \tag{2.15}$$

Assuming that the system hamiltonian H in $H_{tot} = H + V(t)$ (2.1) does not depend on time, it is convenient to switch into the interaction picture:

$$V_I(t) = e^{iHt/\hbar}V(t)e^{-iHt/\hbar} \tag{2.16}$$

the evolution operator $U_I(t)$ obeys:

$$i\hbar\frac{dU_I(t)}{dt} = V_I(t)U_I(t) \quad \text{with} \quad U_I(0) = 1 \tag{2.17}$$

We want that at $t = \tau$:

$$U_I(\tau) = e^{iH\tau/\hbar}U_{pas} \equiv e^{-i\Lambda\tau/\hbar} \implies U_I(\tau)\rho_I(0)U_I^\dagger(\tau) = \rho_I(\tau) = (\rho_{pas})_I \tag{2.18}$$

Where the Λ matrix is obtained by diagonalization.

To achieve the desired U_I with an interaction $V(t)$ we can define a simple function $\varphi(t)$ that respects the following conditions:

$$\varphi(0) = \dot\varphi(0) = \dot\varphi(\tau) = 0 \quad \varphi(\tau) = \tau \tag{2.19}$$

so that choosing as a potential:

$$(V_{pas}(t))_I \equiv \dot{\varphi}(t)\Lambda \tag{2.20}$$

The evolution operator will be (2.17):

$$U_I(t) = e^{-i\Lambda\varphi(t)/\hbar} \tag{2.21}$$

and because of the conditions (2.19) we imposed on φ:

$$U_I(0) = 1 \quad U_I(\tau) = e^{-i\Lambda\tau/\hbar} = e^{iH\tau/\hbar}U_{pas} \tag{2.22}$$

and $V(0) = V(\tau) = 0$.

We explained the notion of *passive state* (def. 2.1.1) and we showed that with an appropriate choice of $V(t)$ (eq. 2.20) we can transform a generic state into a passive one.

We are now ready to give a general definition of *ergotropy*:

Definition 2.1.2 (Ergotropy)**.** The ergotropy is the maximum amount of work we can extract from a state ρ using unitary operators:

$$\mathcal{W}(\rho, H) \equiv max_U[\mathrm{tr}(\rho H) - \mathrm{tr}\left(U\rho U^\dagger H\right)] = \mathrm{tr}(\rho H) - \min_U \mathrm{tr}\left(U\rho U^\dagger H\right) \tag{2.23}$$

For our problem the unitary matrices are the time-evolution operators (eq. 2.2). Using Th. 2.1.1 and the procedure of eqs. 2.15- 2.20 we can saturate the ergotropy bound:

$$\mathcal{W}(\rho, H) = \mathrm{tr}(\rho H) - \min_U \mathrm{tr}\left(U\rho U^\dagger H\right) = \mathrm{tr}(\rho H) - \mathrm{tr}(\rho_{pas}H) \tag{2.24}$$

With $\rho_{pas}(\rho, H)$ as in (eq. 2.8):

$$\rho_{pas} = \sum_j r_j^{(\downarrow)} \left|\varepsilon_j^{(\uparrow)}\right\rangle \left\langle\varepsilon_j^{(\uparrow)}\right| \tag{2.25}$$

where as usual the eigenstates with the largest eigenvalues are the least energetic ones.

difference between er-gotropy and classical ex-ctractable work?

2.2   Max-Ergotropy

Despite Ergotropy has a clear experimental meaning, its calculation is not numerically efficient. To see this let's rewrite more explicitly eq. 2.24 :

$$\mathcal{W}(\rho, H) = E(\rho) - E(\rho_{pas}) = \sum_{j,k} r_j^{(\downarrow)}\varepsilon_k^{(\uparrow)} \left(\left|\left\langle r_j^{(\downarrow)}\Big|\varepsilon_k^{(\uparrow)}\right\rangle\right|^2 - \delta_{jk}\right) \tag{2.26}$$

In the calculation of Ergotropy we need both the eigenvalues and the eigenvectors of

fix ref

ρ and H, while for other known measures like Entropy **??** or Purity **??** we only need the eigenvalues of the density matrix ρ.

To solve this issue we can define the anti-ergotropy as:

Definition 2.2.1 (Anti-Ergotropy)**.**

$$\mathcal{A}(\rho, H) \equiv E(\rho_{a-pas}) - E(\rho) = \sum_{j,k} r_j^{(\uparrow)} \varepsilon_k^{(\uparrow)} \left(\delta_{jk} - \left| \left\langle r_j^{(\uparrow)} \middle| \varepsilon_k^{(\uparrow)} \right\rangle \right|^2 \right) \qquad (2.27)$$

Where $\rho_{a-pas} = \sum_j r_j^{(\uparrow)} \left| \varepsilon_j^{(\uparrow)} \right\rangle \left\langle \varepsilon_j^{(\uparrow)} \right|$ is the most energetic state we can get acting with unitary operators on ρ, it's called an *anti-passive* state because much like def. (2.1.1):

$$E(\rho_{a-pas}) = \text{tr}[H\rho_{a-pas}] \geq \text{tr}\left[HU\rho_{a-pas}U^\dagger\right] \quad \forall U \quad \text{with} \quad UU^\dagger = U^\dagger U = I \quad (2.28)$$

And we can get rid of $E(\rho)$ defining:

Definition 2.2.2 (Max-Ergotropy)**.** The Max-Ergotropy of a state ρ given an Hamiltonian H is the (positive) difference between the Anti-Ergotropy (def. 2.2.1) and the Ergotropy (def.2.1.2) :

$$\mathcal{M}(\rho, H) \equiv \mathcal{A}(\rho, H) - \mathcal{W}(\rho, H) = E(\rho_{a-pas}) - E(\rho_{pas}) =$$
$$\sum_i (r_i^{(\uparrow)} - r_i^{(\downarrow)})\varepsilon_i^{(\uparrow)} \qquad (2.29)$$

The Max-Ergotropy of a state ρ is the maximum energy difference between any two states that are unitary connected to ρ.

Notice that the Max-Ergotropy depends only on the eigenvalues of ρ and H as we desired.

2.3 Entanglement Measures

For a pure bipartite state, the problem of quantifying entanglement is clearly solved by the Von Neumann Entropy of (either of) the reduced density.
For a generic mixed state, the problem is much more difficult and a plethora of measures exist [AFOV08].

2.3.1 Entanglement Entropies

Definition 2.3.1 (Von Neumann Entropy)**.** The Von Neumann Entropy of a density matrix ρ is:

$$S(\rho) = -\text{tr}\left(\rho \log \rho\right) \qquad (2.30)$$
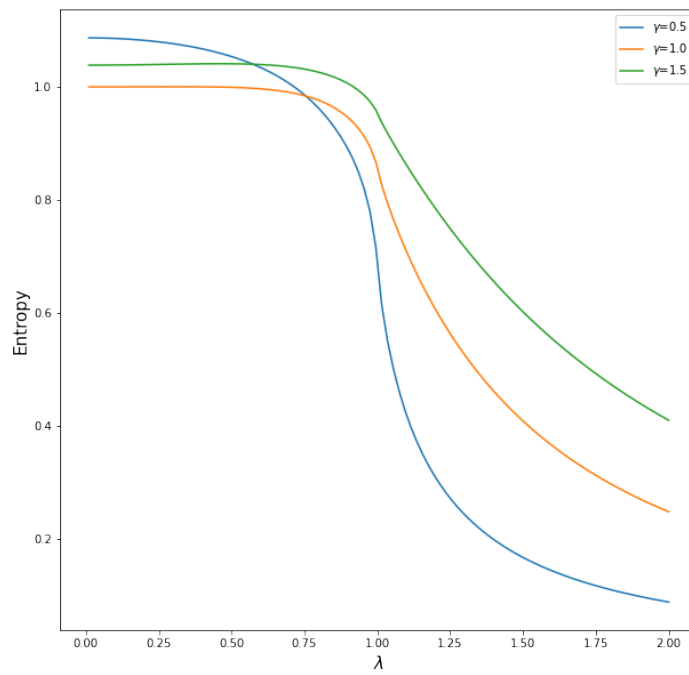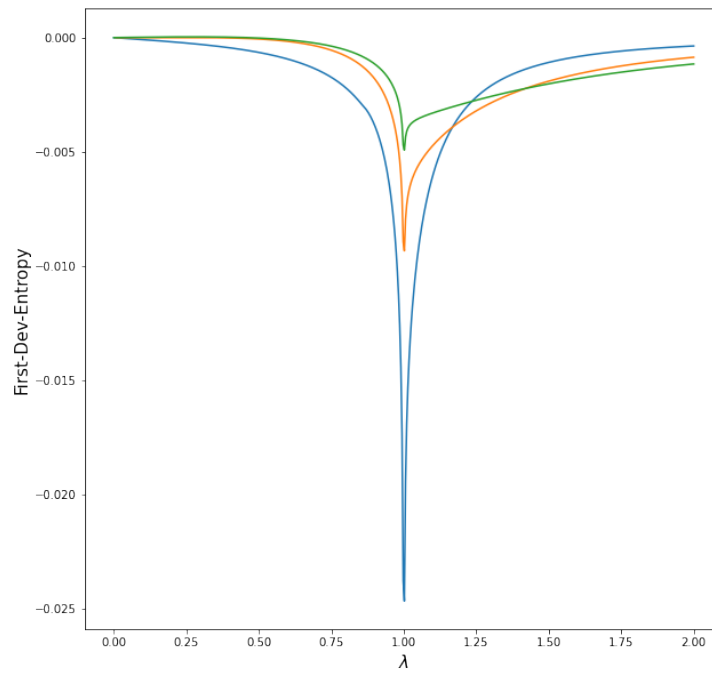
Figure 2.1: Analitical 2 site Von Neumann Entropy

Figure 2.2: Analitical 2 site first-dev Von Neumann entropy

Definition 2.3.2 (Rényi entropy)**.** The Rényi entropy of a density matrix ρ is:

2.3.2 Concurrence

Definition 2.3.3 (Concurrence)**.** The concurrence is defined only for a mixed state ρ of two qubits (in our case the sites i and j) as :

$$C(i,j) = \max\left\{0, r_1(i,j) - r_2(i,j) - r_3(i,j) - r_4(i,j)\right\} \tag{2.31}$$

where $r_\alpha(i,j)$ are the square roots of the eigenvalues of the product matrix $R = \rho(i,j)\tilde{\rho}(i,j)$ and $\tilde{\rho}$ is obtained by a spin-flipping operation:

$$\tilde{\rho} \equiv \sigma^y \otimes \sigma^y \rho^* \sigma^y \otimes \sigma^y \tag{2.32}$$

[OAFF02] Fazio et al. and [ON02] Nielsen et al. studied the behavior of the concurrence $C(i,j)$ for an XY Model in the proximity of a quantum phase transition
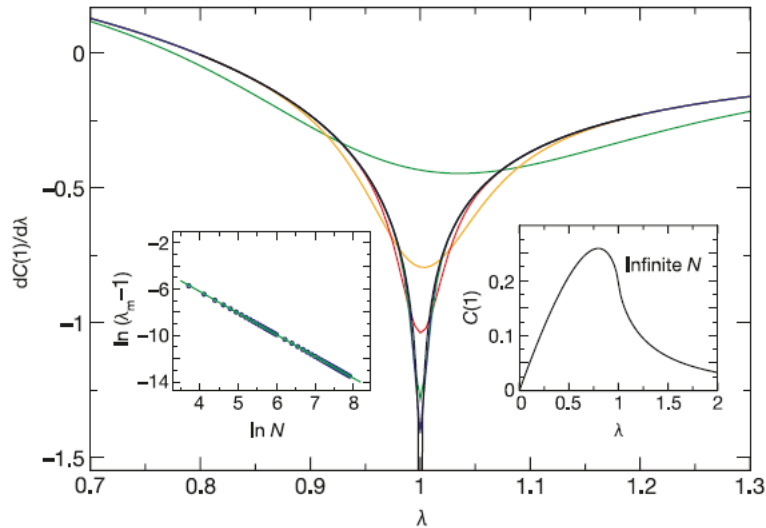
Finite size study of Ergo?

Figure 2.3: First derivative of the concurrence $\partial_\lambda C$ in a Ising Model the curves correspond to different lattice sizes: $N = 11, 41, 101, 251, 401, \infty$. In the right inset is showed the concurrence for an infinite system. From [OAFF02]
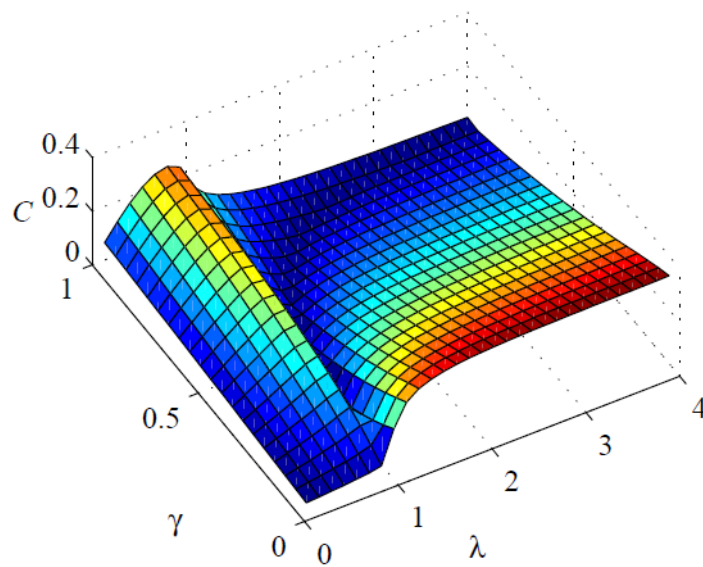
Redo fig. 2.4

Figure 2.4: Analytical calculation, concurrence for the XY-model.where $\lambda = 1/\lambda$ From [ON02]

Chapter 3

Quantum Phase Transitions

The freezing of water or the magnetization of iron are some of the most famous phase transitions.

If we study the properties of a system for different values of the thermodynamic variables we can draw a phase diagram [Hua] (fig. 3.1).
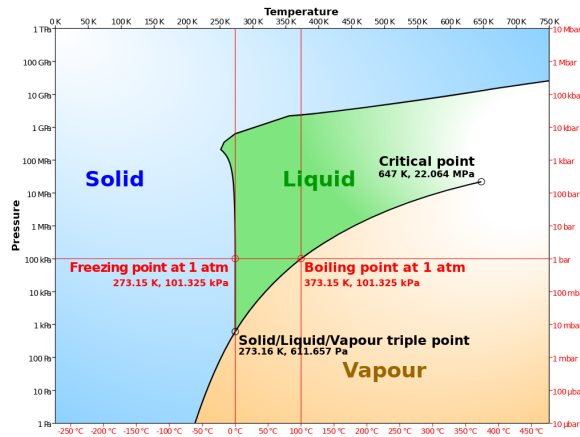

Figure 3.1: Phase diagram of water, the solid lines represent the phase boundary. Note that the system can pass from liquid to vapour without experiencing a phase transition.

The region of thermodynamic states where the macroscopic properties of the system are uniform it's called *phase*.

Depending on the properties we are interested in, we can define for example the "solid phase" for water or the "ferromagnetic phase" for iron.

A *phase transition* occurs when the system phase changes "abruptly". The points where this phenomenon happens are called *phase boundary*.

This "abrupt" change corresponds mathematically to a non-analytic behavior of some thermodynamic function [Gol92].

For classical thermodynamic systems, the standard function used to detect phase transitions is the free-energy.

A phase transition that occurs at $T = 0$ is called a *Quantum phase transition*. [Sac11].

In a classical system at $T = 0$ every particle is freezed in a completely motionless state

: even theoretically a phase transition is impossible. On the other hand, in Quantum Mechanics, the Heisenberg uncertainty principle generates some fluctuations in the quantum state; at sufficiently low temperatures, these fluctuations become relevant and can drive a phase transition.

Practically speaking, the quantum phase boundary correspond to non-analitical points in the ground-state energy of an infinite lattice system.
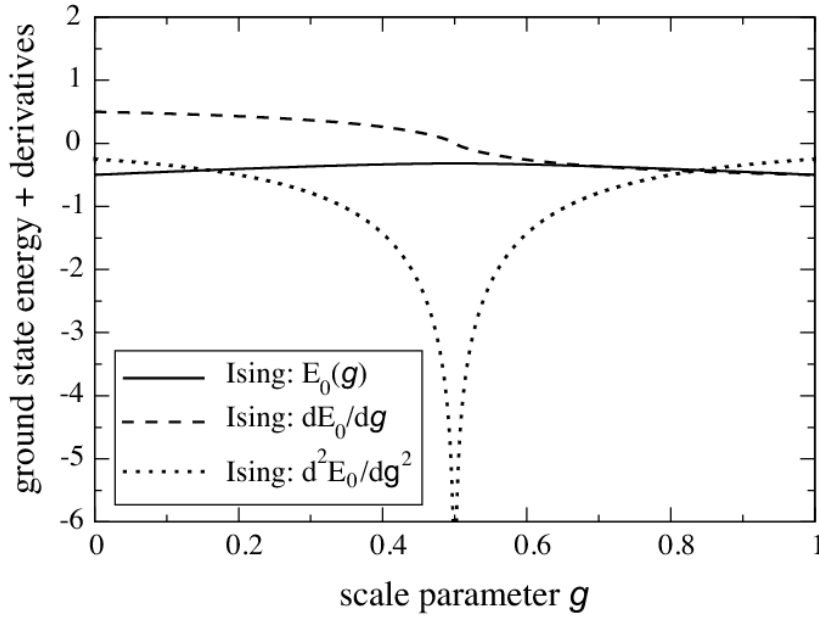

Figure 3.2: From [MSS10]: Ground state energy and derivatives of an Ising Model with a transition at $g = 0.5$

3.1   XY model

The XY model in a transverse magnetic field it's one of the few integrable models to exhibits non trivial phases [Fra17], in 1D it is described by the Hamiltonian:

$$H_{XY} = -\frac{1}{2} \sum_{l=1}^{N} \left(\frac{1+\gamma}{2} \sigma_l^x \sigma_{l+1}^x + \frac{1-\gamma}{2} \sigma_l^y \sigma_{l+1}^y + \lambda \sigma_l^z \right) \tag{3.1}$$

On the l site lives a Spin-1/2 variable described by the 3 Pauli Matrices $\sigma_l^x, \sigma_l^y, \sigma_l^z$, N is the total number of sites.

The Hamiltonian has 2 parameters: $\lambda \in \mathbb{R}$ is the strength of the external magnetic field and $\gamma \in \mathbb{R}$ it's used to quantify the amount of anisotropy in the spin-spin interaction. For $\gamma = 1$ we have the well-known 1D Transverse-Field Ising Model (TFIM) while at $\gamma = 0$ the Hamiltonian is the 1D XX model.

This model was solved for the first time by Lieb Schultz and Mattis [LSM61] for $\lambda = 0$, Katsura [Kat62] solved it for $\lambda \neq 0$ and later Barouch and McCoy calculated the

correlation functions on the ground state [BMD70] [BM71b] [BM71a].

A rotation by $\pi/2$ along the z-axis interchanges the x and y spin interactions and is equivalent to $\gamma \to -\gamma$, while a reflection of the spin across the x-y plane is compensated by $h \to -h$: thus we will concentrate only on the first quadrant of the phase diagram $(\gamma \geq 0, \lambda \geq 0)$.
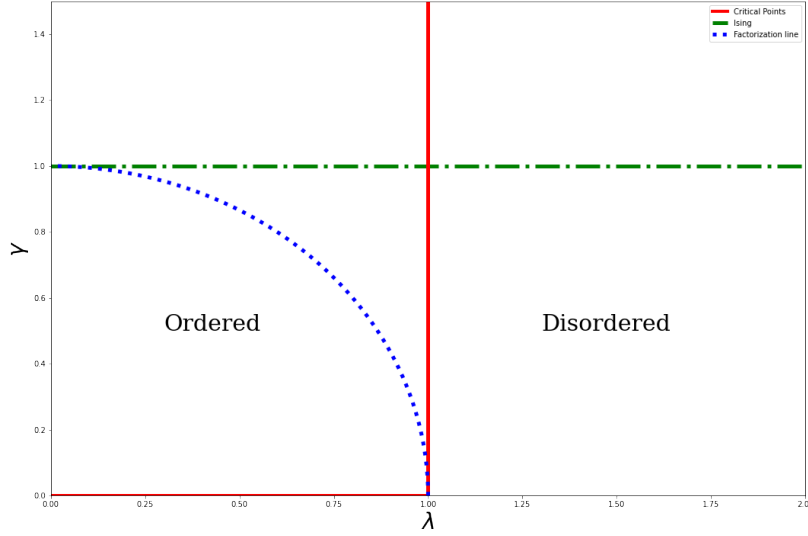

Figure 3.3: Zero temperature phase diagram of the XY-Model. The phase boundary corresponds to the red line. For $\gamma^2 + h^2 = 1$ the the ground state becomes a product state (blue dashed line).

For $\gamma > 0$ we see that the critical line at $\lambda = 1$ identifies two phases: the "ordered" or *ferromagnetic* phase and the "disordered" or *paramagnetic* phase.

For $\lambda < 1$ the interaction term (eq. 3.2) dominates.

$$H_{int} = -\frac{1}{2} \sum_{l=1}^{N} \left(\frac{1+\gamma}{2}\sigma_l^x\sigma_{l+1}^x + \frac{1-\gamma}{2}\sigma_l^y\sigma_{l+1}^y \right) \tag{3.2}$$

The ground states are a combination of two states completely aligned in opposite directions (ferromagnetic states):

$$|\psi_g\rangle = \alpha \,|\rightarrow\rightarrow \, ... \, \rightarrow\rangle + \beta \,|\leftarrow\leftarrow \, ... \, \leftarrow\rangle \tag{3.3}$$

The ferromagnetic states are aligned in the x-direction if $\gamma > 0$ and in the y-direction if $\gamma < 0$.

In real systems with a large number of spins, $|\psi_g\rangle$ is never found in this quantum superposition: decoherence makes the system choose one of the two ordered states.

For $\lambda >> 1$ there is only one ground state: $|\uparrow\uparrow \, ... \, \uparrow\rangle$; due to this missing degeneracy, the system makes a transition from a gapless to a gapped ground-state (fig. **??**.
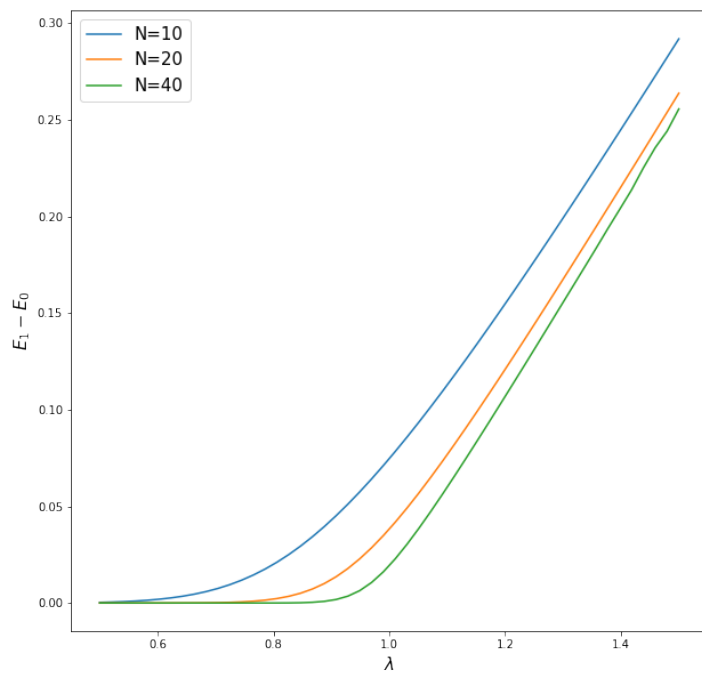
Figure 3.4

Chapter 4

Analitical Calculations for the XY model

In this Chapter we will find an analytical expression for the quantities we described in chap. 2 in a 1D space (chain) with an XY Hamiltonian :

$$H_{XY} = -\frac{1}{2} \sum_l \left(\frac{1+\gamma}{2} \sigma_l^x \sigma_{l+1}^x + \frac{1-\gamma}{2} \sigma_l^y \sigma_{l+1}^y + \lambda \sigma_l^z \right) \tag{4.1}$$

With $\gamma, \lambda \in [0, \infty]$.

We will calculate the reduced density matrix on L sites for the ground state of the XY model.

To get the reduced density matrix we will follow the road map described in [LRV03]:

1. Transform the Hamiltonian using Majorana operators

2. Write the correlation matrix for the new operators on the ground state of the whole chain

3. Restrict the correlation matrix to the subsystem of interest

4. Expand the reduced density matrix in the Pauli basis

5. Find the density matrix expectation values on the ground state using Wick's theorem

The non-local transformation:

$$\check{a}_{2l-1} \equiv \left(\prod_{m<l} \sigma_m^z \right) \sigma_l^x; \quad \check{a}_{2l} \equiv \left(\prod_{m<l} \sigma_m^z \right) \sigma_l^y \tag{4.2}$$

$$\check{a}_m^\dagger = \check{a}_m, \quad \{\check{a}_m, \check{a}_n\} = 2\delta_{mn} \tag{4.3}$$

defines 2N Majorana operators (2 for every site: "even" and "odd") and maps the Hamiltonian 4.1 to :

$$H = \frac{i}{2} \sum_{l=-\frac{N-1}{2}}^{\frac{N-1}{2}} \check{a}_{2l}\check{a}_{2l+1} + \lambda\check{a}_{2l-1}\check{a}_{2l} \tag{4.4}$$

From here we can derive the correlation matrix for the Majorana operators on the ground state of the whole chain (the details of the calculation are shown in A):

$$\langle \breve{a}_m \breve{a}_n \rangle = \delta_{mn} + i \left(\Gamma^A \right)_{mn}, \tag{4.5}$$

$$\Gamma^A = \begin{bmatrix} \Pi_0 & \Pi_1 & \cdots & \Pi_{N-1} \\ -\Pi_1^T & \Pi_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ -\Pi_{N-1}^T & \cdots & \cdots & \Pi_0 \end{bmatrix} \tag{4.6}$$

$$\Pi_l = \begin{bmatrix} 0 & g_l \\ -g_{-l} & 0 \end{bmatrix} \qquad g_l = \frac{1}{2\pi} \int_0^{2\pi} d\phi \, e^{-il\phi} \frac{\lambda - \cos\phi + i\gamma\sin\phi}{|\lambda - \cos\phi + i\gamma\sin\phi|} \tag{4.7}$$

Now if we expand the L sites density matrix in the Pauli basis:

$$\rho_L = 2^{-L} \sum_{\mu_1,\cdots,\mu_L = 0,x,y,z} \rho_{\mu_1\cdots\mu_L} \sigma_1^{\mu_1} \cdots \sigma_L^{\mu_L} \tag{4.8}$$

We need only to calculate the expectation values on the ground state:

$$\rho_{\mu_1\cdots\mu_L} = \langle \sigma_1^{\mu_1} \cdots \sigma_L^{\mu_L} \rangle \tag{4.9}$$

And this can be done using: the majorana basis (4.2), Wick's theorem and the L sites-restricted correlation matrix Γ_L^A

$$\Gamma_L^A = \begin{bmatrix} \Pi_0 & \Pi_1 & \cdots & \Pi_{L-1} \\ -\Pi_1^T & \Pi_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ -\Pi_{L-1}^T & \cdots & \cdots & \Pi_0 \end{bmatrix} \tag{4.10}$$

We'll need the inverse transformations of 4.2

$$\sigma_l^z = -i\breve{a}_{2l-1}\breve{a}_{2l} \tag{4.11}$$

$$\sigma_l^x = \left(\prod_{m<l} \sigma_m^z \right) \breve{a}_{2l-1} = \left(\prod_{m<l} -i\breve{a}_{2m-1}\breve{a}_{2m} \right) \breve{a}_{2l-1} \tag{4.12}$$

$$\sigma_l^y = \left(\prod_{m<l} -i\breve{a}_{2m-1}\breve{a}_{2m} \right) \breve{a}_{2l} \tag{4.13}$$

4.1   One site

4.1.1   Eigenvalues

$$\langle \breve{a}_m \breve{a}_n \rangle = \delta_{mn} + i\Gamma_1^A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + i \begin{bmatrix} 0 & g_0 \\ -g_0 & 0 \end{bmatrix} \tag{4.14}$$

Γ_1^A is in the block diagonal form, so The density matrix ρ_1 has eigenvalues:

$$p_1 = (1 + g_0)/2 \quad p_2 = (1 - g_0)/2 \tag{4.15}$$

$$p_1 = (1 + \langle \sigma_1^z \rangle)/2 \quad p_2 = (1 - \langle \sigma_1^z \rangle)/2 \tag{4.16}$$

4.1.2 Reduced Density Matrix

We want to calculate (4.8-4.9):

$$\rho_1 = \frac{1}{2} \sum_{\mu_1 = 0, x, y, z} \rho_{\mu_1} \sigma_1^{\mu_1} \tag{4.17}$$

where:

$$\rho_{\mu_1} = \langle \sigma_1^{\mu_1} \rangle \quad \mu_1 = 0, x, y, z \tag{4.18}$$

are the expectation values on the ground state.

First we express the pauli matrices in the Majorana basis using the inverse transformation of 4.2:

$$\sigma_1^x = \check{a}_1 \quad \sigma_1^y = \check{a}_2 \quad \sigma_1^z = -i\check{a}_1\check{a}_2 \tag{4.19}$$

And now looking at the L=1 correlation matrix 4.10 Γ_1^A:

$$\Gamma_1^A = \Pi_0 = \begin{bmatrix} 0 & g_0 \\ -g_0 & 0 \end{bmatrix} \tag{4.20}$$

we are able to write all the possible expectation values of the Majorana operators (4.5):

$$\langle \check{a}_m \check{a}_n \rangle = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + i \begin{bmatrix} 0 & g_0 \\ -g_0 & 0 \end{bmatrix} \quad m, n = 1, 2 \tag{4.21}$$

We obtain:

$$\rho_1 = \frac{1}{2}\rho_0 \sigma_1^0 + \frac{1}{2}\rho_z \sigma_1^z = \frac{1}{2}\sigma_1^0 + \frac{1}{2}g_0 \sigma_1^z \tag{4.22}$$

So:

$$\rho_1 = \frac{1}{2} \begin{bmatrix} 1 + g_0 & 0 \\ 0 & 1 - g_0 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 + \langle \sigma_1^z \rangle & 0 \\ 0 & 1 - \langle \sigma_1^z \rangle \end{bmatrix} \tag{4.23}$$

with:

$$g_0 = \langle \sigma_1^z \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\phi \frac{\lambda - \cos\phi + i\gamma\sin\phi}{|\lambda - \cos\phi + i\gamma\sin\phi|} \tag{4.24}$$

We plot $(1 + g_0)/2$ in fig. **??**

4.1.3   Ergotropy

$$\rho_1 = \frac{1}{2}\begin{bmatrix} 1 + \langle \sigma_1^z \rangle & 0 \\ 0 & 1 - \langle \sigma_1^z \rangle \end{bmatrix} \tag{4.25}$$

$$H_1 = -\frac{\lambda}{2}\sigma^z = \frac{1}{2}\begin{bmatrix} -\lambda & 0 \\ 0 & \lambda \end{bmatrix} \tag{4.26}$$

$$\mathcal{W}_1(\rho, H) = \text{tr}(\rho_1 H_1) - \text{tr}(\rho_{pas1} H_1) = 0 \tag{4.27}$$

Because ρ_1 is already a passive state.

4.1.4   Max-Ergotropy

The density matrix ρ_1 has eigenvalues 4.15:

$$p_1 = (1 + g_0)/2 \quad p_2 = (1 - g_0)/2 \tag{4.28}$$

With $g_0 = \langle \sigma_1^z \rangle$ (fig. 4.1) :

$$g_0 = \frac{1}{2\pi}\int_0^{2\pi} d\phi \frac{\lambda - \cos\phi + i\gamma\sin\phi}{|\lambda - \cos\phi + i\gamma\sin\phi|} \tag{4.29}$$

- Purity:

$$\mathfrak{P}_1 = \sum_i (p_i)^2 = \frac{1 + g_0^2}{2} = \frac{1 + \langle \sigma_1^z \rangle^2}{2} \tag{4.30}$$

- Max-Ergo:

$$\mathcal{M}_1 = 2\sum_{i=1}^{D/2}\left(p_i^{(\downarrow)} - p_{D-i+1}^{(\downarrow)}\right)\left|\epsilon_i^{(\uparrow)}\right| = 2(p_1^{(\downarrow)} - p_2^{(\downarrow)})\left|\varepsilon_1^{(\uparrow)}\right| = 2g_0\left|\frac{\lambda}{2}\right| = g_0|\lambda| = \langle \sigma_1^z \rangle|\lambda| \tag{4.31}$$

- Rescaled-Max-Ergotropy

$$\mathfrak{M}_1 = g_0 = \langle \sigma_1^z \rangle \tag{4.32}$$

The second derivative with respect to λ of the Max-Ergotropy is very sensible to the phase transition (fig. 4.2)

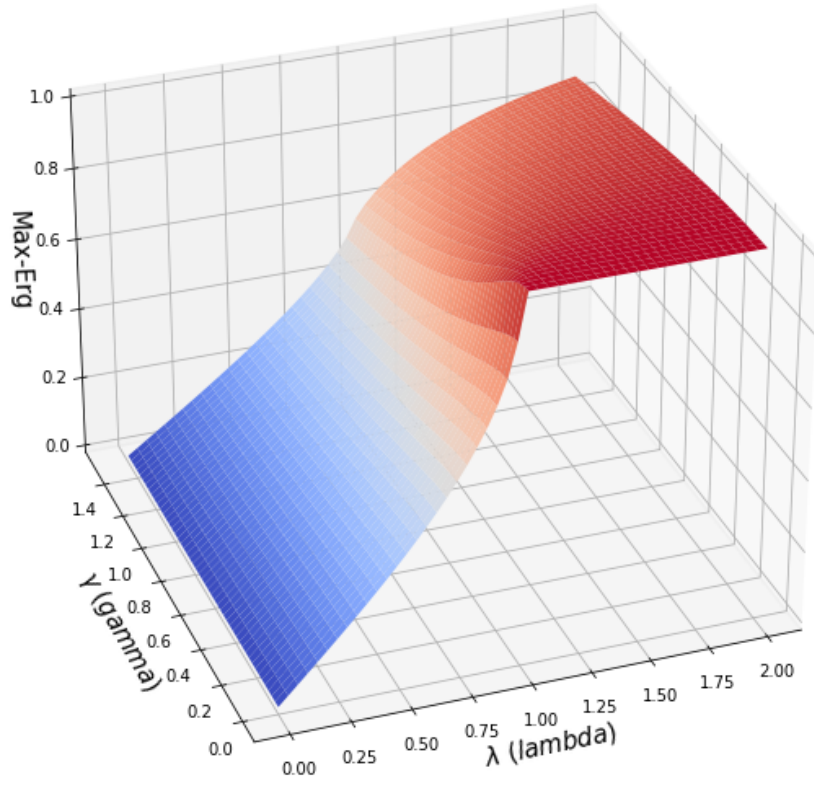## 4.1.5 Graphs

L=1, Analitical

Figure 4.1: For One Site, the Max-Ergotropy corresponds to the $g_0 = \langle \sigma_1^z \rangle$ coefficient.
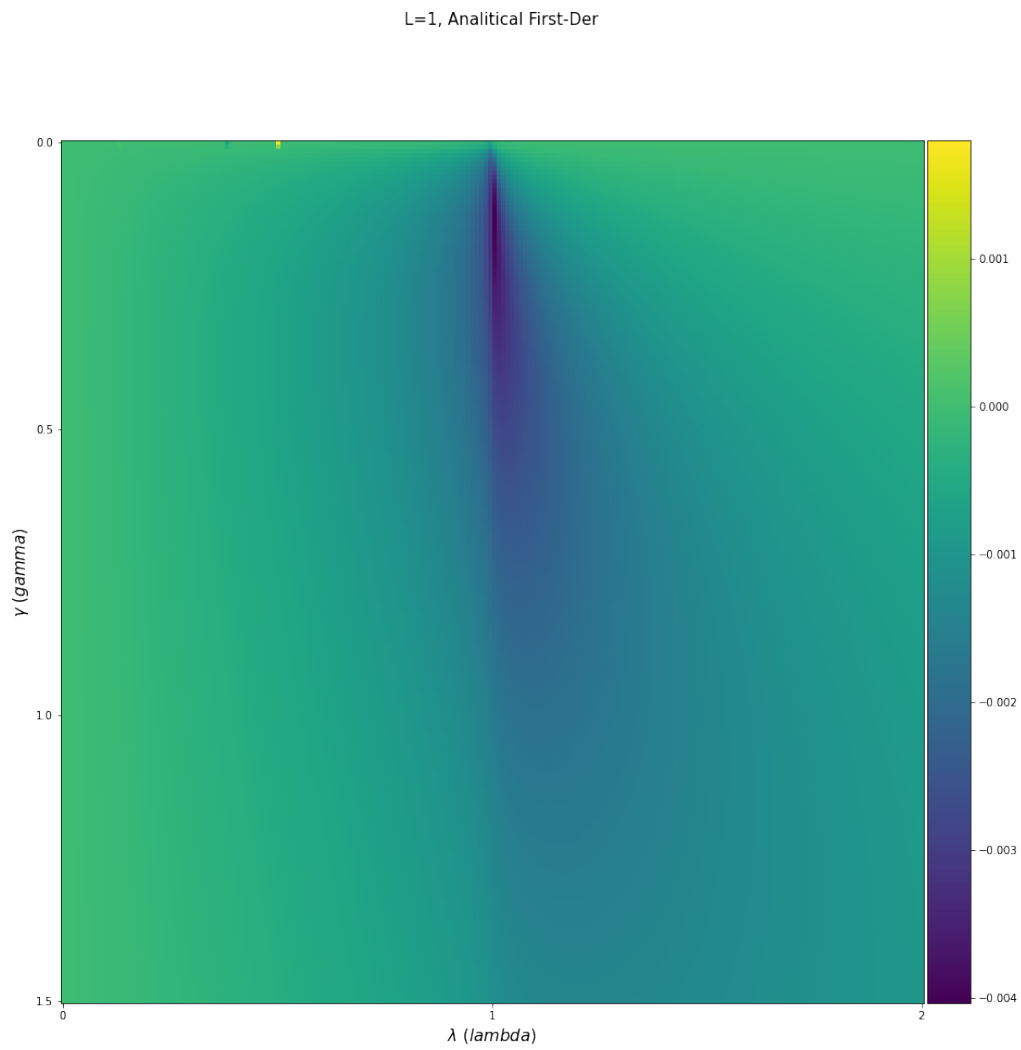
Figure 4.2: First-Derivative one-site Max-Ergotropy (g_0)

4.2 Two sites

4.2.1 Eigenvalues

Eigenvalues of the correlation matrix

$$\nu_\pm = \sqrt{\left(\frac{g_1 - g_{-1}}{2}\right)^2 + g_0^2} \pm \left|\frac{g_1 + g_{-1}}{2}\right| \tag{4.33}$$

With $\nu_- < \nu_+$.

These eigenvalues can be interpreted as occupation numbers for the fermionic modes [FCA+14] [LRV03]:

$$\langle \hat{c}_m \hat{c}_n \rangle = 0, \quad \langle \hat{c}_m^\dagger \hat{c}_n \rangle = \delta_{mn} \frac{1 + \nu_m}{2} \quad m, n = +, - \tag{4.34}$$

Where the $\hat{c}$ operators are particular combinations of the Majorana operators that diagonalize the correlation matrix.

Eigenvalues of the density matrix:

$$p_{\pm\pm} = (1 \pm \nu_-)(1 \pm \nu_+)/4 \tag{4.35}$$

4.2.2 Reduced Density Matrix

We want to calculate the density matrix for 2 adjacent sites in the infinite XY chain. We'll need the expectations values on the ground state for:

$$\rho_{\mu_1\mu_2} = \langle \sigma_1^{\mu_1} \sigma_2^{\mu_2} \rangle \quad \mu_1, \mu_2 = 0, x, y, z \tag{4.36}$$

Using the inverse transformations of 4.2 :

$$\sigma_1^z = -i\breve{a}_1\breve{a}_2 \quad \sigma_2^z = -i\breve{a}_3\breve{a}_4 \tag{4.37}$$

$$\sigma_1^x = \breve{a}_1 \quad \sigma_2^x = -i\breve{a}_1\breve{a}_2\breve{a}_3 \tag{4.38}$$

$$\sigma_1^y = \breve{a}_2 \quad \sigma_2^y = -i\breve{a}_1\breve{a}_2\breve{a}_4 \tag{4.39}$$

The correlation matrix for the first 4 Majorana operators is (4.7 , 4.10):

$$\langle \breve{a}_m\breve{a}_n \rangle = \delta_{mn} + i\left(\Gamma_2^A\right)_{mn}, \quad m, n = 1, 2, 3, 4 \tag{4.40}$$

$$\Gamma_2^A = \begin{bmatrix} \Pi_0 & \Pi_1 \\ -\Pi_1^T & \Pi_0 \end{bmatrix} = \begin{bmatrix} 0 & g_0 & 0 & g_1 \\ -g_0 & 0 & -g_{-1} & 0 \\ 0 & g_{-1} & 0 & g_0 \\ -g_1 & 0 & -g_0 & 0 \end{bmatrix} \tag{4.41}$$

$$g_l = \frac{1}{2\pi} \int_0^{2\pi} d\phi\, e^{-il\phi} \frac{\lambda - \cos\phi + i\gamma\sin\phi}{|\lambda - \cos\phi + i\gamma\sin\phi|} \tag{4.42}$$

Now we have all we need to calculate the coefficients of the 2-site density matrix in the pauli basis on the ground state (4.36) using Wick's theorem.

The Hamiltonian 4.1 has a symmetry:

$$\left(\prod_l \sigma_i^z\right) H \left(\prod_l \sigma_i^z\right) = H \tag{4.43}$$

That allows us to say that:

$$\rho_{\mu_1 \cdots \mu_L} = \langle \sigma_1^{\mu_1} \cdots \sigma_L^{\mu_L} \rangle = 0 \quad \text{if the sum of } \mu = x \text{ and } \mu = y \text{ is odd} \tag{4.44}$$

For example in our case $(L = 2)$: $\rho_{x0} = \rho_{zy} = 0$
The only non-vanishing terms are:

$$\rho_{00} \quad \rho_{xx} \quad \rho_{yy} \quad \rho_{xy} \quad \rho_{yx} \quad \rho_{zz} \quad \rho_{z0} \quad \rho_{0z} \tag{4.45}$$

We now use Wick's theorem:

$$\rho_{xx} = \langle \sigma_1^x \sigma_2^x \rangle = -i \langle \breve{a}_1 \breve{a}_1 \breve{a}_2 \breve{a}_3 \rangle$$
$$= -i \langle \breve{a}_1 \breve{a}_1 \rangle \langle \breve{a}_2 \breve{a}_3 \rangle + i \langle \breve{a}_1 \breve{a}_2 \rangle \langle \breve{a}_1 \breve{a}_3 \rangle - i \langle \breve{a}_1 \breve{a}_3 \rangle \langle \breve{a}_1 \breve{a}_2 \rangle = -i(-ig_{-1}) + 0 - 0$$
$$\rho_{yy} = -i \langle \breve{a}_2 \breve{a}_1 \breve{a}_2 \breve{a}_4 \rangle =$$
$$= -i \langle \breve{a}_2 \breve{a}_1 \rangle \langle \breve{a}_2 \breve{a}_4 \rangle + i \langle \breve{a}_2 \breve{a}_2 \rangle \langle \breve{a}_1 \breve{a}_4 \rangle - i \langle \breve{a}_2 \breve{a}_4 \rangle \langle \breve{a}_1 \breve{a}_2 \rangle = 0 + i(ig_1) - 0$$
$$\rho_{xy} = -i \langle \breve{a}_1 \breve{a}_1 \breve{a}_2 \breve{a}_4 \rangle =$$
$$= -i \langle \breve{a}_1 \breve{a}_1 \rangle \langle \breve{a}_2 \breve{a}_4 \rangle + i \langle \breve{a}_1 \breve{a}_2 \rangle \langle \breve{a}_1 \breve{a}_4 \rangle - i \langle \breve{a}_1 \breve{a}_4 \rangle \langle \breve{a}_1 \breve{a}_2 \rangle = 0 + i(ig_0 ig_1) - i(ig_1 ig_0)$$
$$\rho_{yx} = -i \langle \breve{a}_2 \breve{a}_1 \breve{a}_2 \breve{a}_3 \rangle =$$
$$= -i \langle \breve{a}_2 \breve{a}_1 \rangle \langle \breve{a}_2 \breve{a}_3 \rangle + i \langle \breve{a}_2 \breve{a}_2 \rangle \langle \breve{a}_1 \breve{a}_3 \rangle - i \langle \breve{a}_2 \breve{a}_3 \rangle \langle \breve{a}_1 \breve{a}_2 \rangle = ig_0 g_{-1} + 0 - ig_0 g_{-1}$$
$$\rho_{zz} = - \langle \breve{a}_1 \breve{a}_2 \breve{a}_3 \breve{a}_4 \rangle =$$
$$= - \langle \breve{a}_1 \breve{a}_2 \rangle \langle \breve{a}_3 \breve{a}_4 \rangle + \langle \breve{a}_1 \breve{a}_3 \rangle \langle \breve{a}_2 \breve{a}_4 \rangle - \langle \breve{a}_1 \breve{a}_4 \rangle \langle \breve{a}_2 \breve{a}_3 \rangle = -ig_0 ig_0 + 0 - (ig_1(-ig_{-1}))$$
$$\rho_{z0} = -i \langle \breve{a}_1 \breve{a}_2 \rangle = -i(ig_0) \quad \rho_{0z} = -i \langle \breve{a}_3 \breve{a}_4 \rangle = -i(ig_0) \quad \rho_{00} = 1$$
$$\tag{4.46}$$

So:
$$\rho_{00} = 1 \qquad \rho_{xx} = -g_{-1} \qquad \rho_{yy} = -g_1 \qquad \rho_{xy} = 0 \tag{4.47}$$

$$\rho_{yx} = 0 \qquad \rho_{zz} = g_0^2 - g_1 g_{-1} \qquad \rho_{z0} = \rho_{0z} = g_0$$

Using 4.8:

$$\rho_2 = \frac{1}{4}[(\sigma_1^0 \otimes \sigma_2^0) - g_{-1}(\sigma_1^x \otimes \sigma_2^x) - g_1(\sigma_1^y \otimes \sigma_2^y) + (g_0^2 - g_1 g_{-1})(\sigma_1^z \otimes \sigma_2^z) + g_0(\sigma_1^0 \otimes \sigma_2^z + \sigma_1^z \otimes \sigma_2^0)] \tag{4.48}$$

4.2.3 Ergotropy

$$\rho_2 = \frac{1}{4}[(\sigma_1^0 \sigma_2^0) - g_{-1}(\sigma_1^x \sigma_2^x) - g_1(\sigma_1^y \sigma_2^y) + (g_0^2 - g_1 g_{-1})(\sigma_1^z \sigma_2^z) + g_0(\sigma_1^0 \sigma_2^z + \sigma_1^z \sigma_2^0)] \quad (4.49)$$

$$\frac{1}{4}\mathbb{I} + \frac{1}{4}\begin{bmatrix} g_0^2 + 2g_0 - g_{-1}g_1 & & & g_1 - g_{-1} \\ & g_{-1}g_1 - g_0^2 & -g_1 - g_{-1} & \\ & -g_1 - g_{-1} & g_{-1}g_1 - g_0^2 & \\ g_1 - g_{-1} & & & g_0^2 - 2g_0 - g_{-1}g_1 \end{bmatrix} \quad (4.50)$$

For $\lambda \to \infty : g_l = \delta_{0,l}$

For the Ising Model ($\gamma = 1$) , $g_1 = 0$ at $\lambda = 0$, so that:

$$\rho_2 = \frac{1}{4}\left(\sigma_1^0 \sigma_2^0 + \sigma_1^x \sigma_2^x\right) \quad (4.51)$$

as we expect.

The eigenvalues of 4.50 are: (first two middle ones)

$$\frac{1}{4}\left\{\left(1 - g_0^2 + g_{-1}g_1 - g_{-1} - g_1\right), \left(1 - g_0^2 + g_{-1}g_1 + g_{-1} + g_1\right),\right.$$
$$\left.\left(1 + g_0^2 - g_{-1}g_1 - \sqrt{4g_0^2 + (g_1 - g_{-1})^2}\right), \left(1 + g_0^2 - g_{-1}g_1 + \sqrt{4g_0^2 + (g_1 - g_{-1})^2}\right)\right\}$$
$$(4.52)$$

$$\frac{1}{4}\left\{(1 + \nu_-)(1 - \nu_+), (1 - \nu_-)(1 + \nu_+)\right.$$
$$\left.(1 - \nu_-)(1 - \nu_+), (1 + \nu_-)(1 + \nu_+)\right\} \quad (4.53)$$

If we want to sort them, it's easy for $\gamma > 1$: (for $\gamma < 1$ there's a problem at low lambdas but we can solve it focusing only on the region $\lambda \simeq 1$)

Descending (up to down) order of the eigenvalues of the rdm: fig.4.3

$$\begin{aligned} &1/4(1 + \nu_-)(1 + \nu_+) \\ &1/4(1 - \nu_-)(1 + \nu_+) \\ &1/4(1 + \nu_-)(1 - \nu_+) \\ &1/4(1 - \nu_-)(1 - \nu_+) \end{aligned} \quad (4.54)$$

For now we consider $\lambda \simeq 1$ or we have troubles with ordering

Eigenvalues of 2 site Hamiltonian in ascending order:

$$\left\{-\frac{1}{2}\sqrt{\gamma^2 + 4\lambda^2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\sqrt{\gamma^2 + 4\lambda^2}\right\} \quad (4.55)$$

for $\gamma = 1$:

$$\left\{-\frac{1}{2}\sqrt{1 + 4\lambda^2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\sqrt{1 + 4\lambda^2}\right\} \quad (4.56)$$

Ergotropy:

$$\mathcal{W}(\rho, H) = E(\rho) - E(\rho_{pas}) = \sum_{j,k} r_j^{(\downarrow)} \varepsilon_k^{(\uparrow)} \left(\left|\left\langle r_j^{(\downarrow)}\big|\varepsilon_k^{(\uparrow)}\right\rangle\right|^2 - \delta_{jk}\right) \quad (4.57)$$
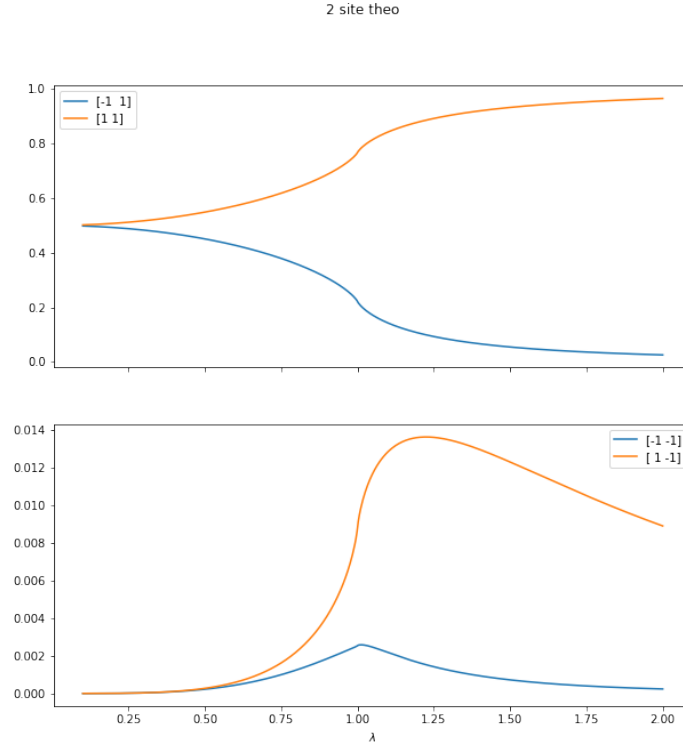
Figure 4.3: Eigenvalues of the two-site density matrix

$$E(\rho_{pas}) = \begin{bmatrix} 1/4(1+\nu_-)(1+\nu_+) \\ 1/4(1-\nu_-)(1+\nu_+) \\ 1/4(1+\nu_-)(1-\nu_+) \\ 1/4(1-\nu_-)(1-\nu_+) \end{bmatrix} \begin{bmatrix} -\frac{1}{2}\sqrt{\gamma^2+4\lambda^2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2}\sqrt{\gamma^2+4\lambda^2} \end{bmatrix} \quad (4.58)$$

$$E(\rho_{pas}) = -\frac{1}{4}\left(\sqrt{(g_{-1}-g_1)^2+4g_0^2}\left(\sqrt{\gamma^2+4\lambda^2}\right) - g_{-1} - g_1\right) \quad (4.59)$$

$$E(\rho_{pas}) = -\frac{1}{4}\left((\nu_++\nu_-)\left(\sqrt{\gamma^2+4\lambda^2}\right) + (\nu_+-\nu_-)\right) \quad (4.60)$$

$$E(\rho) = \frac{1}{4}\left((\gamma+1)g_{-1} - (\gamma-1)g_1 - 4g_0\lambda\right) \quad (4.61)$$

$\gamma = 1$:

$$E(\rho) = 1/2(g_{-1} - 2\lambda g_0) \quad (4.62)$$

Due to symmetry in H: $E(\rho_{pass})$ is $-E(\rho_{antipass})$

Ergotropy:

$$\frac{1}{4}\left(\sqrt{(g_{-1}-g_1)^2+4g_0^2}\sqrt{\gamma^2+4\lambda^2} + \gamma g_{-1} - \gamma g_1 - 4g_0\lambda\right) \quad (4.63)$$

for $\gamma = 1$:

$$\frac{1}{4}\left(\sqrt{(g_{-1}-g_1)^2+4g_0^2}\left(\sqrt{4\lambda^2+1}\right) + g_{-1} - 4g_0\lambda - g_1\right) \quad (4.64)$$

4.2.4 Max-Ergotropy

Eigenvalues of the density matrix:

$$p_{\pm\pm} = (1 \pm \nu_-)(1 \pm \nu_+)/4 \tag{4.65}$$

Eigenvalues of 2 site Hamiltonian:

$$H = -\frac{1}{2}\left(\sigma^x\sigma^x + \lambda\sigma^z\sigma^0 + \lambda\sigma^0\sigma^z\right) = \begin{pmatrix} -\lambda & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & \lambda \end{pmatrix} \tag{4.66}$$

$$\left\{ -\frac{1}{2}\sqrt{1+4\lambda^2}, -\frac{1}{2}, \frac{1}{2}, , \frac{1}{2}\sqrt{1+4\lambda^2} \right\} \tag{4.67}$$

$$\mathcal{M}(\mathcal{I}) = 2\sum_{i=1}^{2}\left(p_i^{(\downarrow)} - p_{D-i+1}^{(\downarrow)}\right)\left|\epsilon_i^{(\uparrow)}\right|$$

$$\left(p_1^{(\downarrow)} - p_4^{(\downarrow)}\right)\left|\epsilon_1^{(\uparrow)}\right| + \left(p_2^{(\downarrow)} - p_3^{(\downarrow)}\right)\left|\epsilon_2^{(\uparrow)}\right| =$$

$$(1/4)\left[(1+\nu_-)(1+\nu_+) - (1-\nu_-)(1-\nu_+)\right]\left(\sqrt{1+4\lambda^2}\right) + \tag{4.68}$$

$$(1/4)\left[(1-\nu_-)(1+\nu_+) - (1+\nu_-)(1-\nu_+)\right] =$$

$$\frac{(\nu_+ + \nu_-)}{2}\left(\sqrt{1+4\lambda^2}\right) + \frac{\nu_+ - \nu_-}{2}$$

Normalized:

$$\mathfrak{M}(\mathcal{I}) = \frac{\mathcal{M}(\mathcal{I})}{2\left|\epsilon_1^{(\uparrow)}\right|} = \frac{(\nu_+ + \nu_-)}{2} + \frac{(\nu_+ - \nu_-)}{2\left(\sqrt{1+4\lambda^2}\right)} \tag{4.69}$$
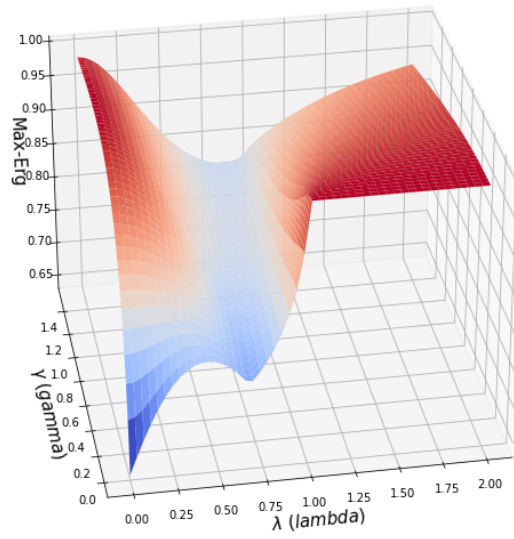
4.2.5 Graphs
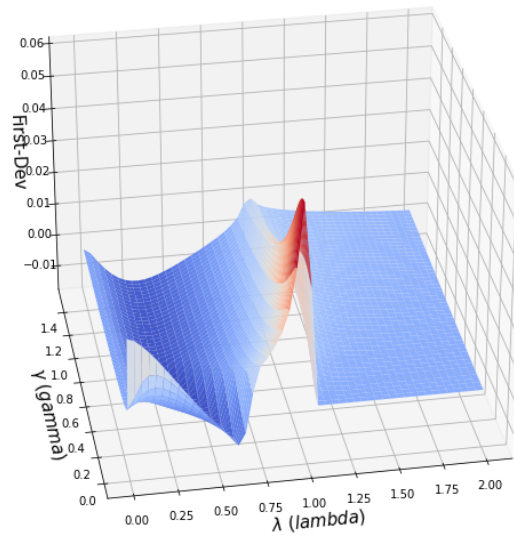
Figure 4.4: Max-Ergotropy
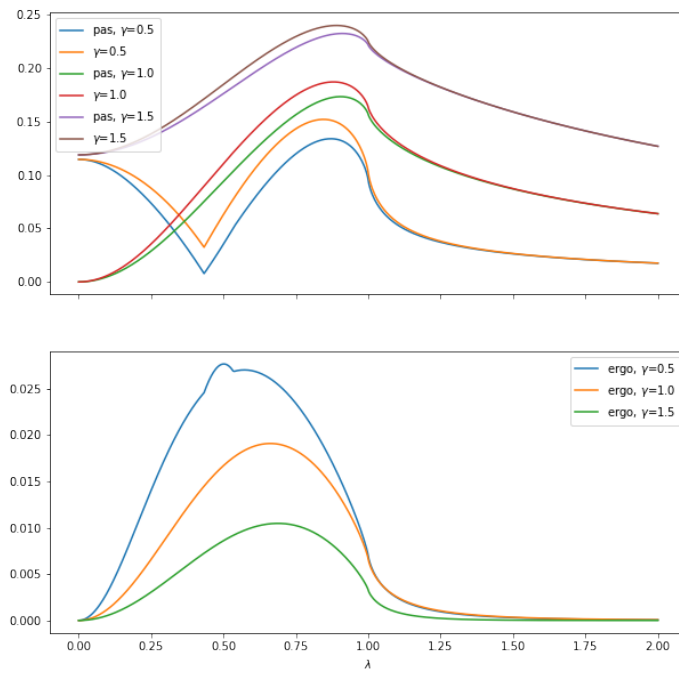

Figure 4.5: First-Derivative of the Max-Ergotropy

Figure 4.6: Ergotropy analitical calculation

4.3   Two distant sites

4.3.1   Eigenvalues

We have to change g_1 with g_d where d is the distance between sites. [FFIP08]

$$\nu_{\pm} = \sqrt{\left(\frac{g_d - g_{-d}}{2}\right)^2 + g_0^2} \pm \left|\frac{g_d + g_{-d}}{2}\right| \tag{4.70}$$

Eigenvalues of the density matrix:

$$p_{\pm\pm} = (1 \pm \nu_-)(1 \pm \nu_+)/4 \tag{4.71}$$

4.3.2   Reduced Density Matrix (difficult)

If we choose two distant sites at a distance d:

$$\rho_{\mu_1\mu_2} = \left\langle \sigma_1^{\mu_1} \sigma_2^0 \ldots \sigma_d^{\mu_d} \right\rangle = \left\langle \sigma_1^{\mu_1} \sigma_d^{\mu_d} \right\rangle \quad \mu_1, \mu_d = 0, x, y, z \tag{4.72}$$

$$\sigma_1^x = \breve{a}_1 \quad \sigma_1^y = \breve{a}_2 \quad \sigma_1^z = -i\breve{a}_1\breve{a}_2 \tag{4.73}$$

$$\sigma_d^z = -i\breve{a}_{2d-1}\breve{a}_{2d} \tag{4.74}$$

$$\sigma_d^x = \left(\prod_{m<d} -i\breve{a}_{2m-1}\breve{a}_{2m}\right)\breve{a}_{2d-1} \tag{4.75}$$

$$\sigma_d^y = \left(\prod_{m<d} -i\breve{a}_{2m-1}\breve{a}_{2m}\right)\breve{a}_{2d} \tag{4.76}$$

4.3.3   Max-Ergotropy

Eigenvalues of the density matrix:

$$p_{\pm\pm} = (1 \pm \nu_-)(1 \pm \nu_+)/4 \tag{4.77}$$

Eigenvalues of distant Hamiltonian:

$$H_{dist} = -(\lambda/2)(\sigma_l^z \sigma_{l+d}^0 + \sigma_l^0 \sigma_{l+d}^z) \tag{4.78}$$

$$\text{eigs} = \{-\lambda, 0, 0, \lambda\} \tag{4.79}$$

Normalized-Max-Ergo: (the two eigenvalues of the Hamiltonian are the same, so we simplify)

$$\mathfrak{M}(\mathcal{I}) = \sum_{i=1}^{2}\left(p_i^{(\downarrow)} - p_{D-i+1}^{(\downarrow)}\right) = \frac{(\nu_+ + \nu_-)}{2} + \frac{(\nu_+ - \nu_-)}{2} \tag{4.80}$$

4.4 More than two sites

We stress again [LR09] that the eigenvalues of the reduced density matrix can be calculated directly from the correlation matrix in the Majorana basis (4.6) because the basis coefficients stay the same after the Jordan Wigner Trasformation:

$$
\begin{aligned}
|\psi\rangle &= \sum_{i_1,i_2,\ldots,i_n} C^{i_1,i_2,\ldots,i_n} |i_1, i_2, \ldots, i_n\rangle \\
&= \sum_{i_1,i_2,\ldots,i_n} C^{i_1,i_2,\ldots,i_n} (a_1^\dagger)^{i_1} (a_2^\dagger)^{i_2} \ldots (a_n^\dagger)^{i_n} |\text{vac}\rangle
\end{aligned}
\tag{4.81}
$$

where the i's represent a spin basis and the a's are the fermionic creation operators
So using the correlation matrix for the Majorana fermions on the ground state (4.5, 4.6):

$$
\langle \breve{a}_m \breve{a}_n \rangle = \delta_{mn} + i \left(\Gamma^A\right)_{mn},
\tag{4.82}
$$

$$
\Gamma^A = \begin{bmatrix}
\Pi_0 & \Pi_1 & \cdots & \Pi_{N-1} \\
-\Pi_1^T & \Pi_0 & & \vdots \\
\vdots & & \ddots & \vdots \\
-\Pi_{N-1}^T & \cdots & \cdots & \Pi_0
\end{bmatrix}
\tag{4.83}
$$

We can calculate the eigenvalues of the reduced density matrix for any group of sites we want. Basically if we want the eigenvalues for the density matrix of L adiacent sites we have to:

1. diagonalize the appropriate Γ_L^A matrix

2. The diagonal matrix we obtain as the form:

$$
\Gamma_L^C = \bigoplus_{l=1}^{L} \begin{bmatrix} 0 & \nu_l \\ -\nu_l & 0 \end{bmatrix}
\tag{4.84}
$$

So, writing:

$$
\rho_L = \varrho_1 \otimes \cdots \otimes \varrho_L
\tag{4.85}
$$

The density matrix ρ_l has eigenvalues:

$$
p_{l\pm} = \frac{1 \pm \nu_l}{2}
\tag{4.86}
$$

3. The eigenvalues of ρ_L are obtained computing all the possible p_l products

4.4.1 Graphs

It's clear that only the first 2-3 eigenvalues are relevant.
I suppose we can stick with two sites density matrix for simulations.
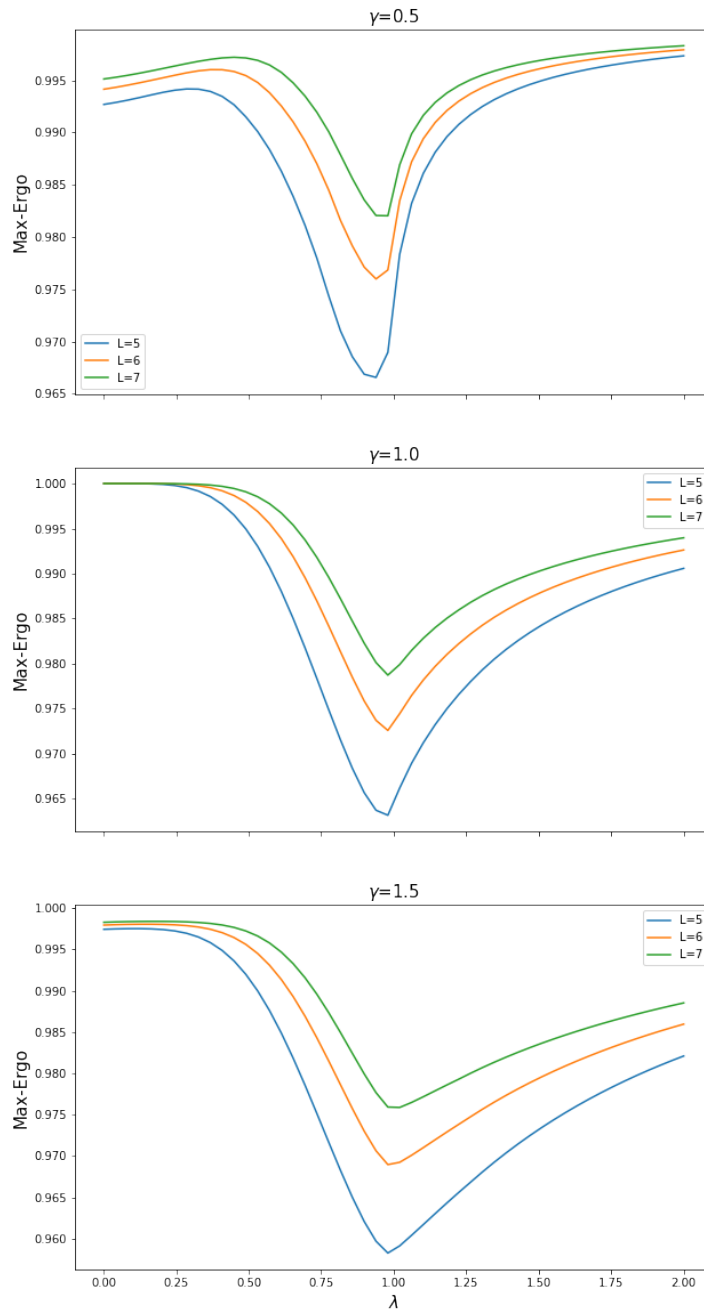
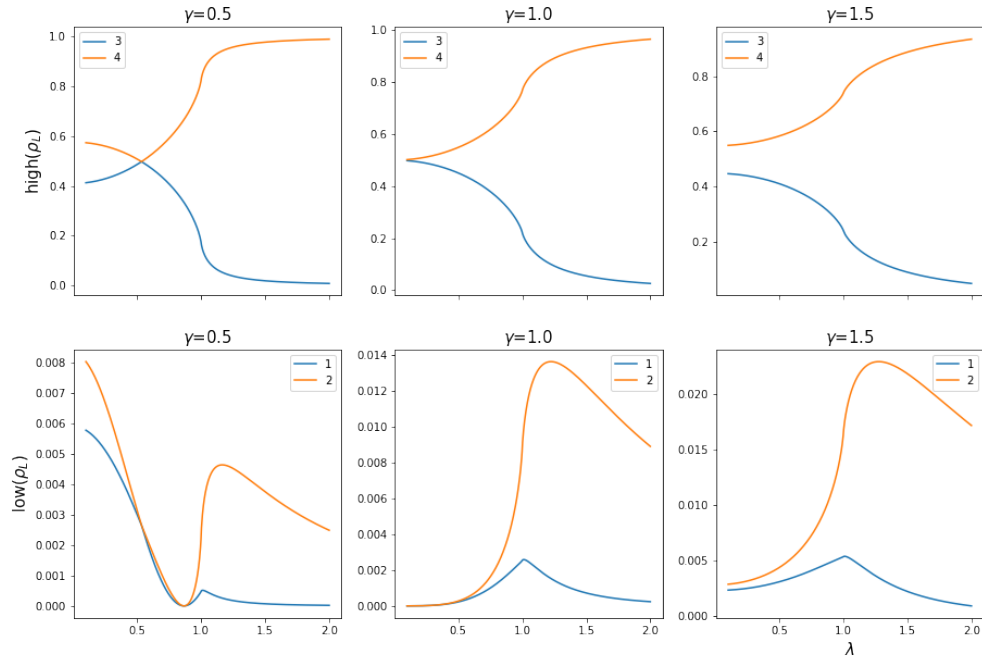Figure 4.7: Analitical Max-Ergotropy
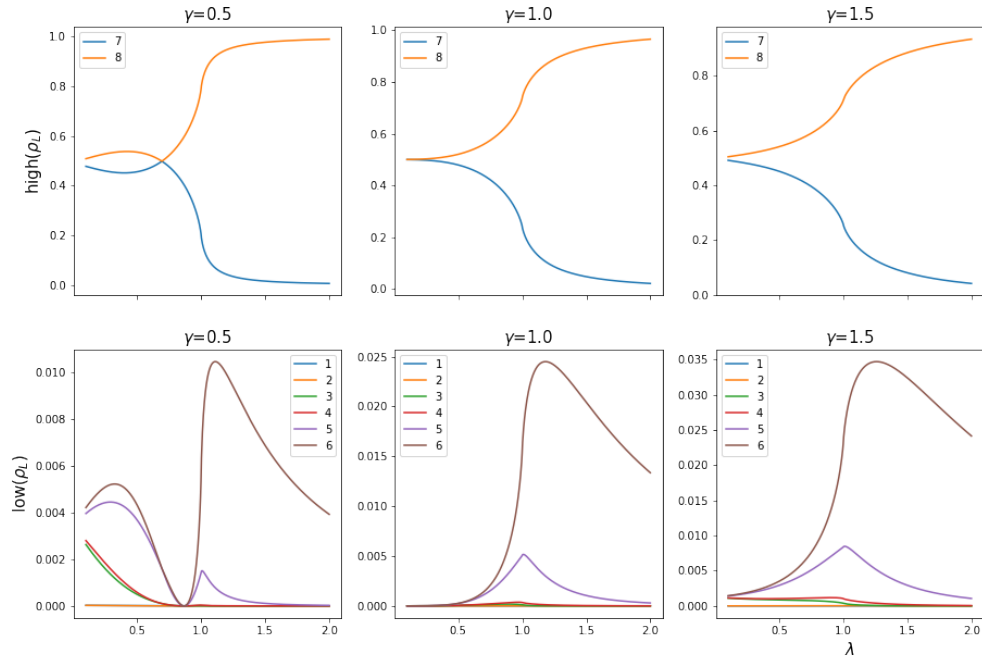
Figure 4.8: Eigenvalues of the 2-sites density matrix

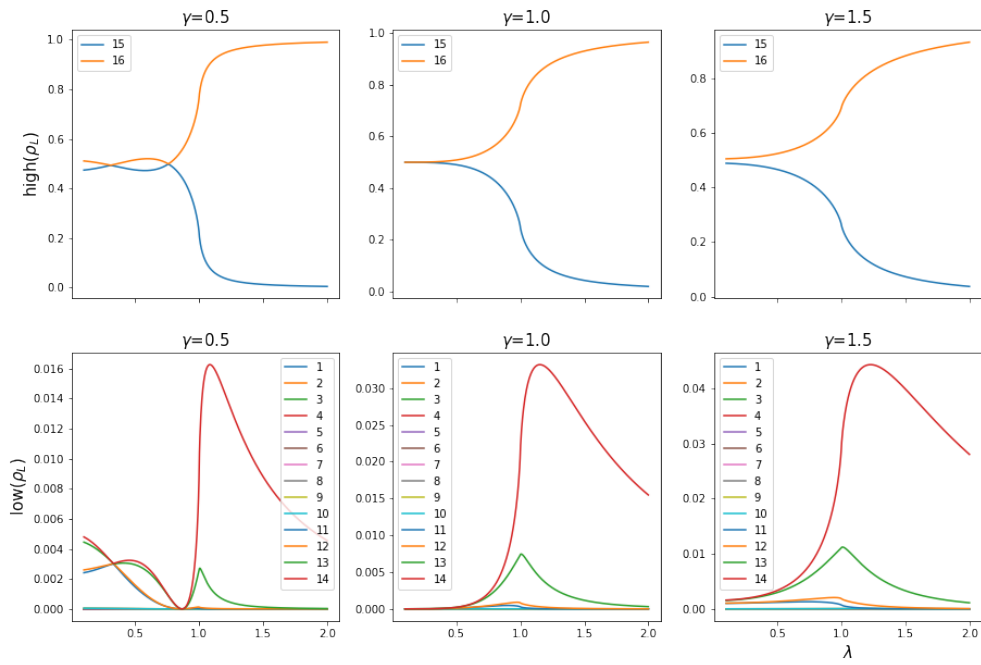Figure 4.9: Eigenvalues of the 3-sites density matrix

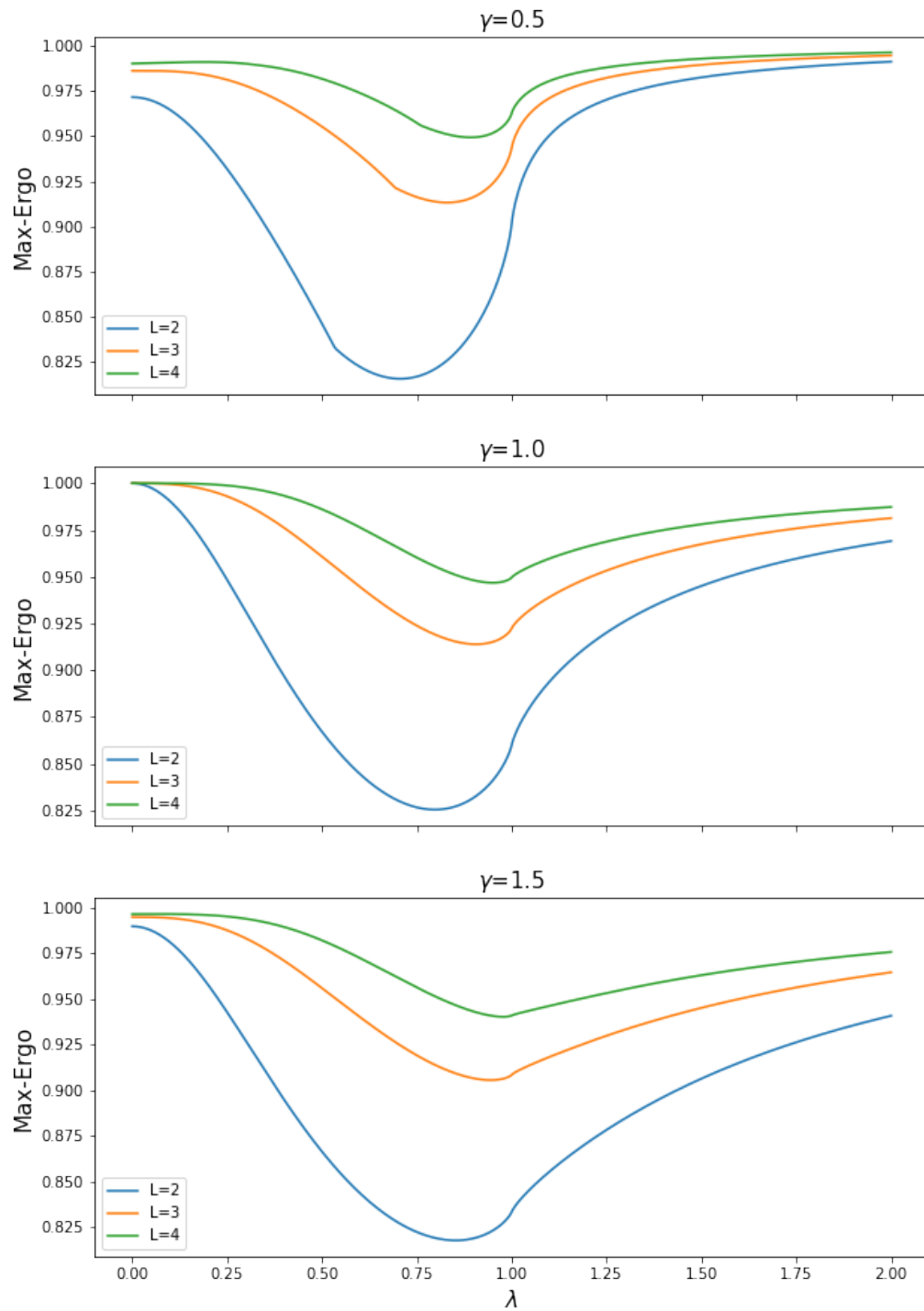Figure 4.10: Eigenvalues of the 4-sites density matrix

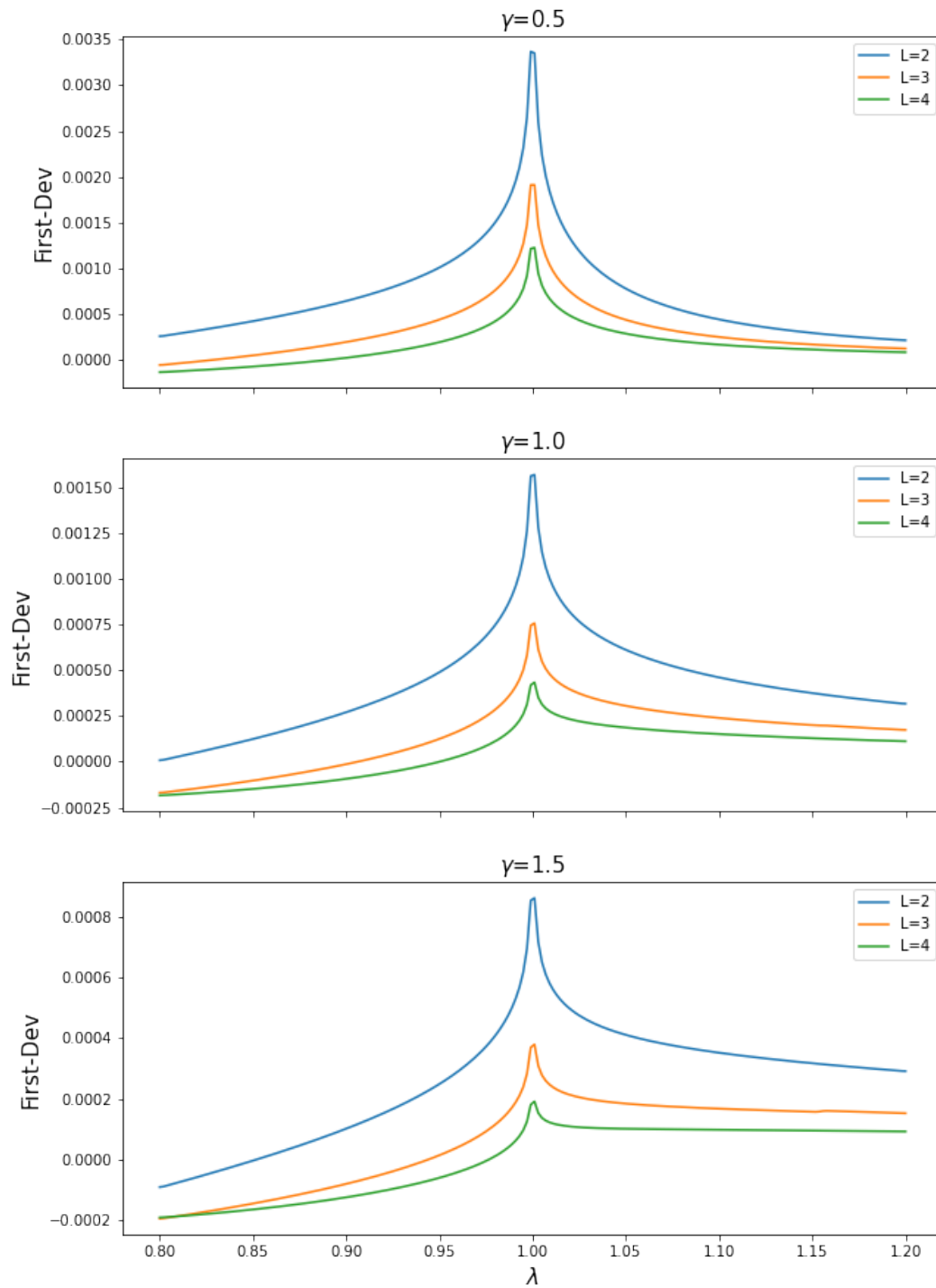Figure 4.11: Max-Ergotropy analitical calculations

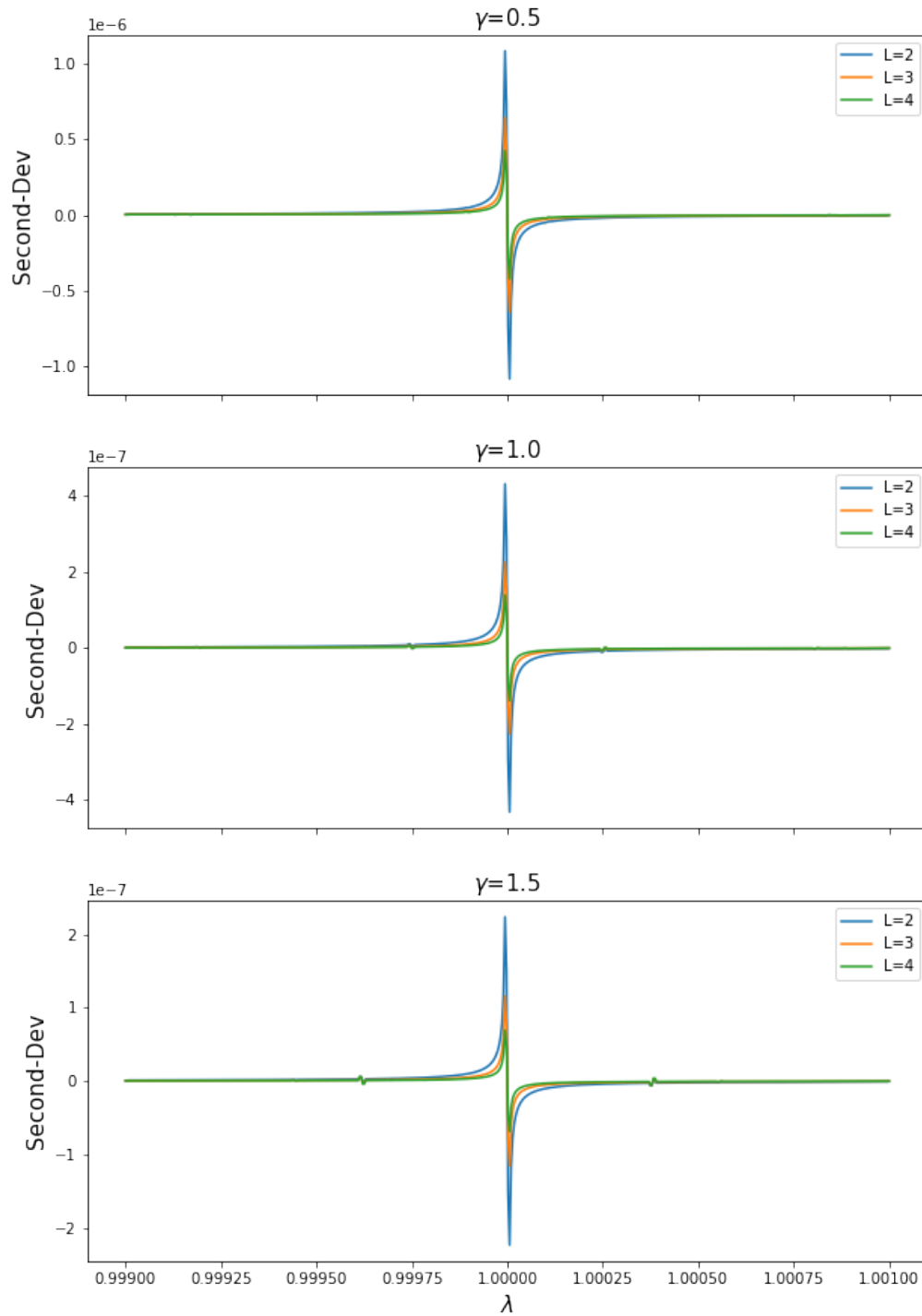Figure 4.12: Analitical First-Derivative-Max-Ergotropy

Figure 4.13: Analitical Second-Derivative-Max-Ergotropy

Chapter 5

Numerical Simulations

For simulations on two distant sites, it's difficult to access the wavefunction directly, but we can calculate the 8 correlators :

The Hamiltonian 4.1 has a symmetry:

$$\left(\prod_l \sigma_l^z\right) H \left(\prod_l \sigma_l^z\right) = H \tag{5.1}$$

That allows us to say that:

$$\rho_{\mu_1 \cdots \mu_L} = \left\langle \sigma_1^{\mu_1} \cdots \sigma_L^{\mu_L} \right\rangle = 0 \quad \text{if the sum of } \mu = x \text{ and } \mu = y \text{ is odd} \tag{5.2}$$

For example in our case ($L = 2$): $\rho_{x0} = \rho_{zy} = 0$

The only non-vanishing terms are:

$$\rho_{00} \quad \rho_{xx} \quad \rho_{yy} \quad \rho_{xy} \quad \rho_{yx} \quad \rho_{zz} \quad \rho_{z0} \quad \rho_{0z} \tag{5.3}$$

This could be interesting to understand the "range of correlations".

To simulate the Symmetry Breaking mechanism, we add a little magnetic field in the X direction, we distinguish between the "preserved symmetry" and "broken symmetry" simulations.

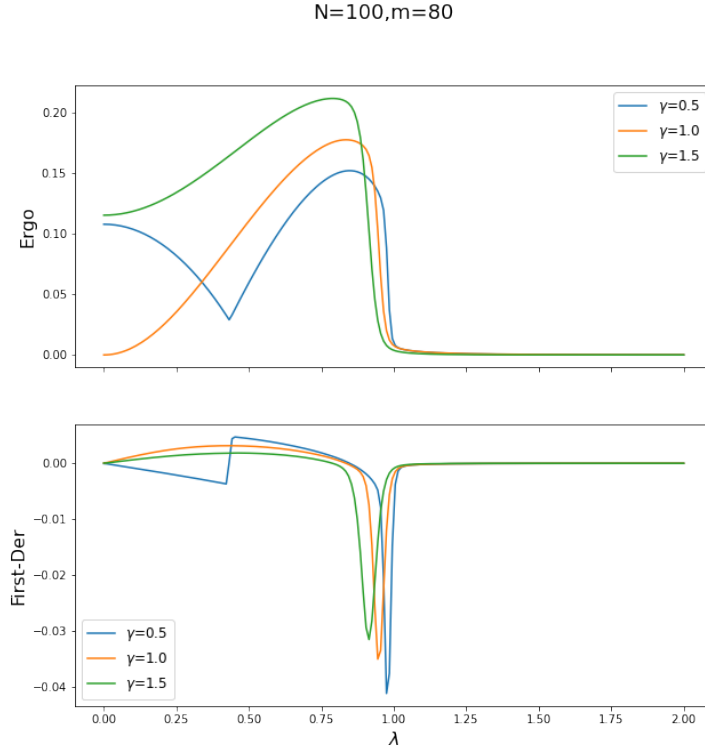## 5.1 Preserved Symmetry

N=100,m=80

Figure 5.1: Dmrg with preserved Symmetry, 100 sites, 80 states kept.
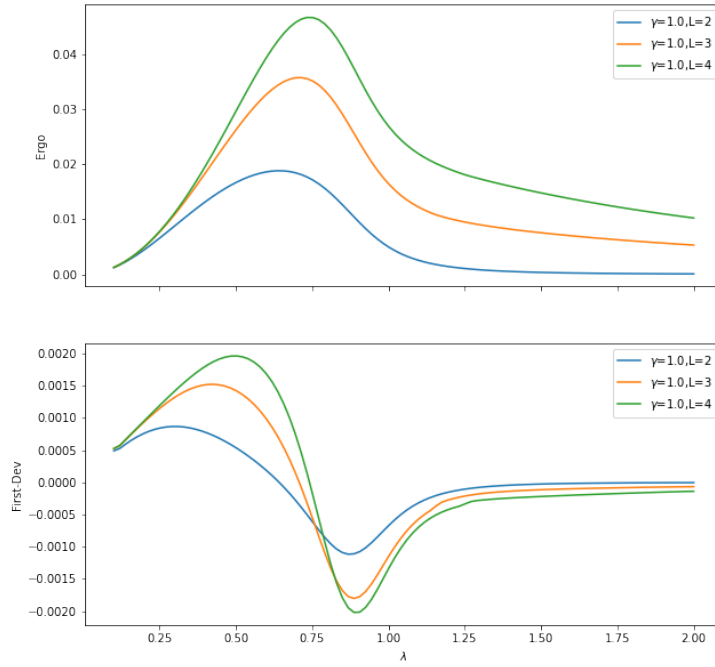
Figure 5.2: Two to four site Ergotropy, $E(\rho)$ and $E(pas)$, Lanczos 12 sites

5.2 Broken Symmetry

The factorizing field is found to be: $\lambda_f = \frac{\sqrt{(1-\gamma^2)}}{2}$

Figure 5.3: Two-site Ergotropy. Dmrg simulation on 60 sites and 40 states kept. Finite-size effects are visible. The factorization point leads to a non analyticity in the first-der.

N=100,m=80

Figure 5.4

N=60,m=40

Figure 5.5

Figure 5.6: Here we can see that the finite-size effect are negligible.

Chapter 6

Conclusions

conclusions

Appendix A

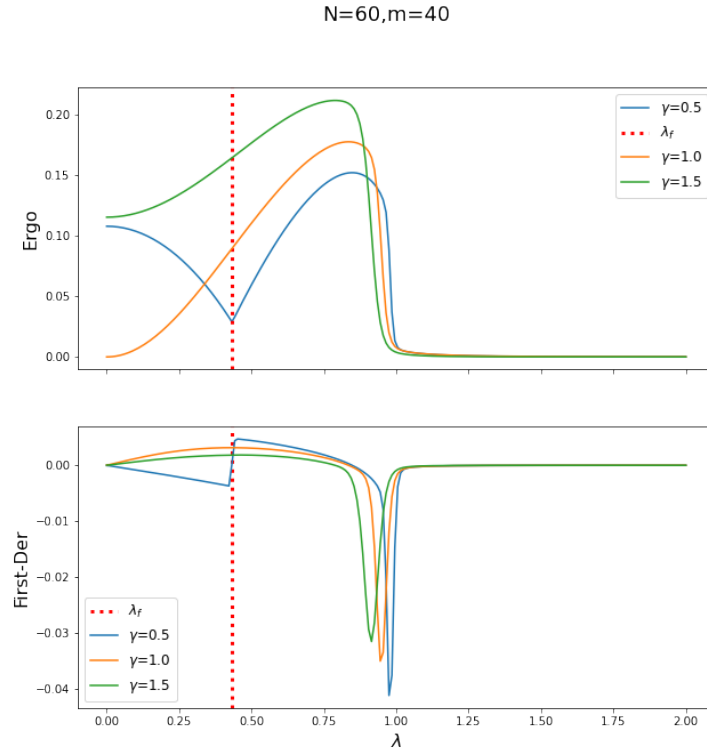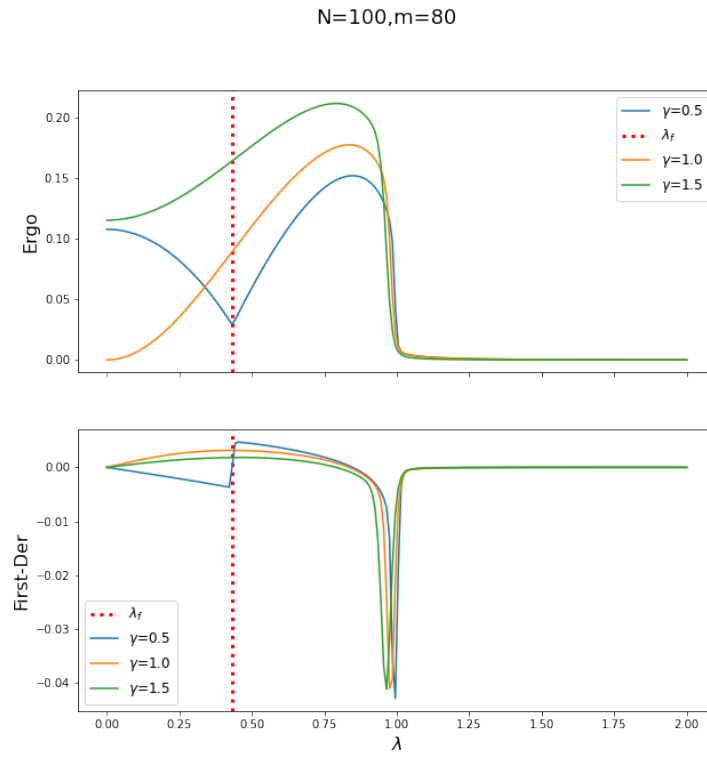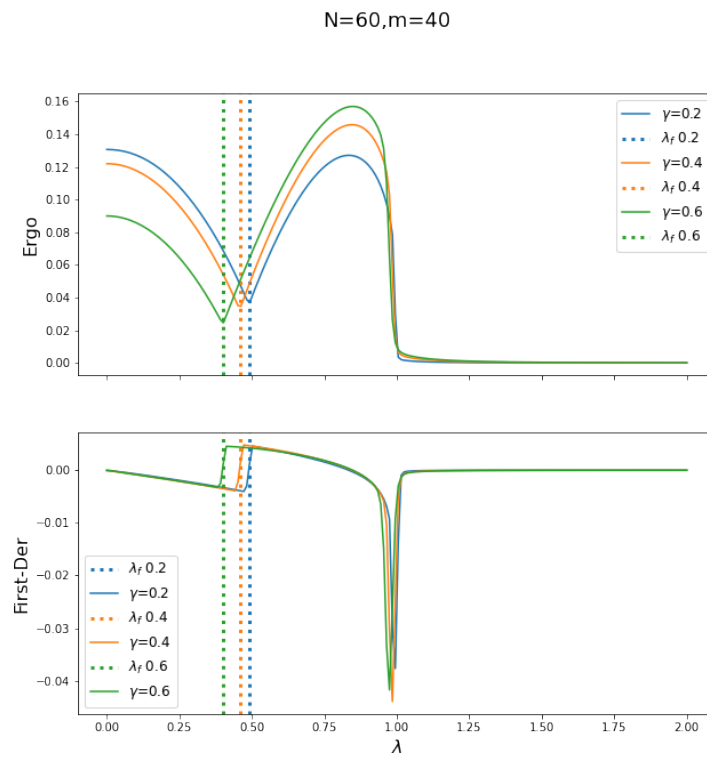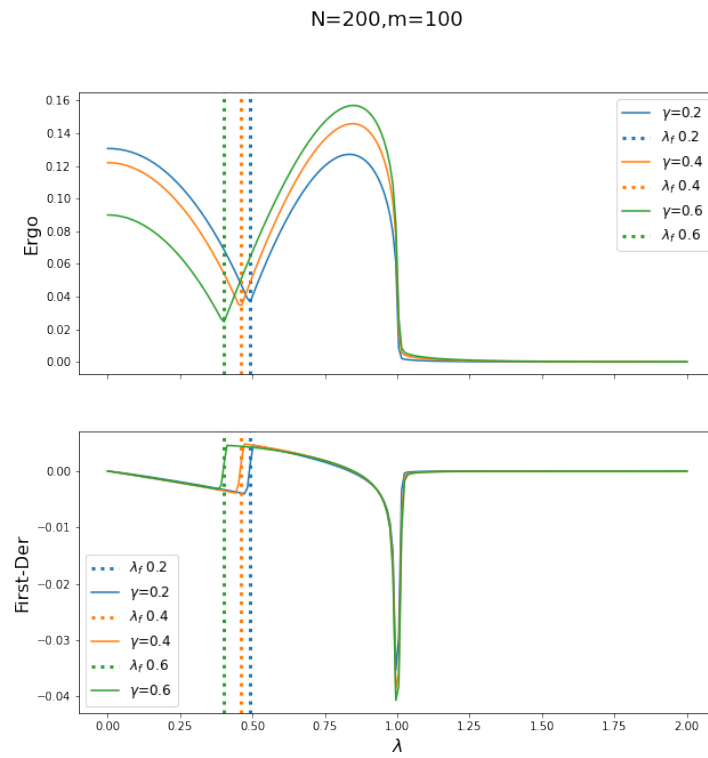# Correlation Matrix derivation

We switch to the momentum representation to exploit the translational symmetry with the help of 2N auxiliary Majorana operators:

$$
\begin{bmatrix} \check{d}_{2k-1} \\ \check{d}_{2k} \end{bmatrix} = \sqrt{\frac{2}{N}} \sum_{l=-\frac{N-1}{2}}^{\frac{N-1}{2}} \cos\frac{2\pi kl}{N} \begin{bmatrix} \check{a}_{2l-1} \\ \check{a}_{2l} \end{bmatrix} \tag{A.1}
$$

$$
\begin{bmatrix} \check{e}_{2k-1} \\ \check{e}_{2k} \end{bmatrix} = \sqrt{\frac{2}{N}} \sum_{l=-\frac{N-1}{2}}^{\frac{N-1}{2}} \sin\frac{2\pi kl}{N} \begin{bmatrix} \check{a}_{2l-1} \\ \check{a}_{2l} \end{bmatrix} \tag{A.2}
$$

With $0 \leq k \leq N/2$.

$$
\begin{aligned}
\check{d}_k^\dagger &= \check{d}_k, \quad \{\check{d}_k, \check{d}_q\} = \delta_{kq} \\
\check{e}_k^\dagger &= \check{e}_k, \quad \{\check{e}_k, \check{e}_q\} = \delta_{kq}
\end{aligned} \tag{A.3}
$$

Using the inverse relations:

$$
\begin{bmatrix} \check{a}_{2l-1} \\ \check{a}_{2l} \end{bmatrix} = \sqrt{\frac{2}{N}} \sum_{k=0}^{N/2} e^{-\frac{2\pi ikl}{N}} \begin{bmatrix} \check{d}_{2k-1} + i\check{e}_{2k-1} \\ \check{d}_{2k} + i\check{e}_{2k} \end{bmatrix} \tag{A.4}
$$

Substituting in 4.4:

$$
\begin{aligned}
H &= \frac{i}{2} \sum_{l=-\frac{N-1}{2}}^{\frac{N-1}{2}} \check{a}_{2l}\check{a}_{2l+1} + \lambda\check{a}_{2l-1}\check{a}_{2l} \\
&= \frac{i}{2} \sum_{l=-\frac{N-1}{2}}^{\frac{N-1}{2}} \frac{2}{N} \sum_{k_1=0}^{N/2} e^{\frac{2\pi ik_1 l}{N}} \left(\check{d}_{2k_1} - i\check{e}_{2k_1}\right) \sum_{k_2=0}^{N/2} e^{\frac{-2\pi ik_2(l+1)}{N}} \left(\check{d}_{2k_2-1} + i\check{e}_{2k_2-1}\right) \\
&\quad - \lambda\frac{i}{2}\frac{2}{N} \sum_{k_3=0}^{N/2} e^{\frac{2\pi ik_3 l}{N}} \left(\check{d}_{2k_3} - i\check{e}_{2k_3}\right) \sum_{k_4=0}^{N/2} e^{\frac{-2\pi ik_4 l}{N}} \left(\check{d}_{2k_4-1} + i\check{e}_{2k_4-1}\right)
\end{aligned} \tag{A.5}
$$

Summing on l first and noting that:

$$\frac{1}{N} \sum_{l=-\frac{N-1}{2}}^{\frac{N-1}{2}} e^{\frac{2\pi i (k_1 - k_2) l}{N}} = \delta_{k_1, k_2} \tag{A.6}$$

we obtain:

$$H = \sum_{k=0}^{N/2} H_k \tag{A.7}$$

with:

$$H_k = i \left(e^{-\frac{2\pi i k}{N}} - \lambda \right) \left(\check{d}_{2k} - i \check{e}_{2k} \right) \left(\check{d}_{2k-1} + i \check{e}_{2k-1} \right) \tag{A.8}$$

$$H_k = i \left(\cos \frac{2\pi k}{N} - i \sin \frac{2\pi k}{N} - \lambda \right) \left(\check{d}_{2k} \check{d}_{2k-1} + \check{e}_{2k} \check{e}_{2k-1} - i \check{e}_{2k} \check{d}_{2k-1} + i \check{d}_{2k} \check{e}_{2k-1} \right) \tag{A.9}$$

$$H_k = \frac{i \Lambda_k}{2} \begin{bmatrix} \check{d}_{2k-1} \\ \check{e}_{2k-1} \\ \check{d}_{2k} \\ \check{e}_{2k} \end{bmatrix}^T \begin{bmatrix} 0 & 0 & c_k & -s_k \\ 0 & 0 & s_k & c_k \\ -c_k & -s_k & 0 & 0 \\ s_k & -c_k & 0 & 0 \end{bmatrix} \begin{bmatrix} \check{d}_{2k-1} \\ \check{e}_{2k-1} \\ \check{d}_{2k} \\ \check{e}_{2k} \end{bmatrix} \tag{A.10}$$

$$\begin{aligned} \Lambda_k &\equiv \sqrt{\left(\cos \frac{2\pi k}{N} - \lambda \right)^2 + \sin^2 \frac{2\pi k}{N}} \\ c_k &\equiv \left(\lambda - \cos \frac{2\pi k}{N} \right) / \Lambda_k \\ s_k &\equiv \left(-\sin \frac{2\pi k}{N} \right) / \Lambda_k \end{aligned} \tag{A.11}$$

Since by construction $c_k^2 + s_k^2 = 1$, $\begin{bmatrix} 0 & 0 & c_k & -s_k \\ 0 & 0 & s_k & c_k \\ -c_k & -s_k & 0 & 0 \\ s_k & -c_k & 0 & 0 \end{bmatrix}^2 = -I$

So it exist an orthogonal transformation that defines new operators $\check{b}_p, -N \le p \le N-1$:

$$\begin{bmatrix} \check{b}_{-2k-1} \\ \check{b}_{-2k} \\ \check{b}_{2k-1} \\ \check{b}_{2k} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} u_k & v_k & u_k & -v_k \\ u_k & v_k & -u_k & v_k \\ v_k & -u_k & v_k & u_k \\ -v_k & u_k & v_k & u_k \end{bmatrix} \begin{bmatrix} \check{d}_{2k-1} \\ \check{e}_{2k-1} \\ \check{d}_{2k} \\ \check{e}_{2k} \end{bmatrix} \tag{A.12}$$

and puts the Hamiltonian in the block diagonal form (canonical form for a skew-symmetric matrix):

$$H = \frac{i}{2} \sum_{k=-\frac{N-1}{2}}^{\frac{N-1}{2}} \Lambda_k \left(\tilde{b}_{2k-1}\tilde{b}_{2k} - \tilde{b}_{2k}\tilde{b}_{2k-1} \right) = \frac{i}{2} \bigoplus_{k=-\frac{N-1}{2}}^{\frac{N-1}{2}} \Lambda_k \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \tag{A.13}$$

For one moment we switch to non-Hermitian fermionic operators:

$$\hat{b}_k \equiv \frac{\check{b}_{2k-1} + i\check{b}_{2k}}{2} \tag{A.14}$$

$$H = \sum_{k=-\frac{N-1}{2}}^{\frac{N-1}{2}} \Lambda_k \hat{b}_k^\dagger \hat{b}_k - \Lambda_k/2 \tag{A.15}$$

The second term is a constant and can be ignored.

Now since all $\Lambda_k > 0$ we can finally find the ground state imposing $b_k \left| \psi_g \right\rangle = 0$

From which also: $\hat{b}_k^\dagger \hat{b}_k \left| \psi_g \right\rangle = \hat{b}_k \hat{b}_k \left| \psi_g \right\rangle = 0$ and $b_k \hat{b}_k^\dagger \left| \psi_g \right\rangle = \left| \psi_g \right\rangle$

Using as always the inverse transformations we can calculate the correlation matrix on the ground state for the Majorana operators:

$$\begin{aligned}
< \check{b}_{2k-1}\check{b}_{2k} > &= i < \hat{b}_k \hat{b}_k^\dagger > = i \\
< \check{b}_{2k}\check{b}_{2k-1} > &= -i < \hat{b}_k \hat{b}_k^\dagger > = -i \\
< \check{b}_{2k}\check{b}_{2k} > &= < \check{b}_{2k-1}\check{b}_{2k-1} > = < \hat{b}_k \hat{b}_k^\dagger > = 1
\end{aligned} \tag{A.16}$$

In compact notation:

$$\left\langle \check{b}_p \check{b}_q \right\rangle = \delta_{pq} + i\Gamma_{pq}^B \tag{A.17}$$

$$\Gamma^B = \bigoplus_{k=-\frac{N-1}{2}}^{\frac{N-1}{2}} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \tag{A.18}$$

Now that we have the correlation matrix for the $\check{b}$ operators we have to go back to the $\check{a}$, that means we have to find the matrix W:

$$\check{b}_p = \sum_{m=-N}^{N-1} W_{pm}\check{a}_m, \quad -N+1 \le p \le N \tag{A.19}$$

The orthogonal transformation that defines the $\check{b}$ operators:

$$\begin{bmatrix} \check{b}_{-2k-1} \\ \check{b}_{-2k} \\ \check{b}_{2k-1} \\ \check{b}_{2k} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} u_k & v_k & u_k & -v_k \\ u_k & v_k & -u_k & v_k \\ v_k & -u_k & v_k & u_k \\ -v_k & u_k & v_k & u_k \end{bmatrix} \begin{bmatrix} \check{d}_{2k-1} \\ \check{e}_{2k-1} \\ \check{d}_{2k} \\ \check{e}_{2k} \end{bmatrix} \tag{A.20}$$

has coefficients $u_k = \cos(\theta_k/2)$, $v_k = \sin(\theta_k/2)$ such that:

$$
\begin{aligned}
u_k^2 - v_k^2 &= \cos(\theta_k) = \left(\lambda - \cos\frac{2\pi k}{N}\right)/\Lambda_k \\
2u_k v_k &= \sin(\theta_k) = \left(-\sin\frac{2\pi k}{N}\right)/\Lambda_k
\end{aligned}
\tag{A.21}
$$

For the sake of clarity we split the transformation A.20 in two even and odd parts:

$$
\begin{bmatrix} \check{b}_{-2k-1} \\ \check{b}_{-2k} \\ \check{b}_{2k-1} \\ \check{b}_{2k} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} u_k & v_k \\ u_k & v_k \\ v_k & -u_k \\ -v_k & u_k \end{bmatrix} \begin{bmatrix} \check{d}_{2k-1} \\ \check{e}_{2k-1} \end{bmatrix} + \frac{1}{\sqrt{2}} \begin{bmatrix} u_k & -v_k \\ -u_k & v_k \\ v_k & u_k \\ v_k & u_k \end{bmatrix} \begin{bmatrix} \check{d}_{2k} \\ \check{e}_{2k} \end{bmatrix}
\tag{A.22}
$$

and now using the definitions of $\check{d}$ and $\check{e}$ (A.1 , A.2):

$$
\begin{bmatrix} \check{b}_{-2k-1} \\ \check{b}_{-2k} \\ \check{b}_{2k-1} \\ \check{b}_{2k} \end{bmatrix} = \frac{1}{\sqrt{N}} \sum_{l=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left(\begin{bmatrix} u_k & v_k \\ u_k & v_k \\ v_k & -u_k \\ -v_k & u_k \end{bmatrix} \begin{bmatrix} \cos\frac{2\pi kl}{N} \\ \sin\frac{2\pi kl}{N} \end{bmatrix} \check{a}_{2l-1} + \begin{bmatrix} u_k & -v_k \\ -u_k & v_k \\ v_k & u_k \\ v_k & u_k \end{bmatrix} \begin{bmatrix} \cos\frac{2\pi kl}{N} \\ \sin\frac{2\pi kl}{N} \end{bmatrix} \check{a}_{2l} \right)
\tag{A.23}
$$

With this equation A.23 we can read the coefficients of W as defined in A.19.
The correlation matrix Γ^A for the operators $\check{a}$ is given by:

$$
\Gamma^A = W^T \Gamma^B W
\tag{A.24}
$$

Using the definition of Γ^B A.18:

$$
\Gamma^A_{mn} = \sum_{i,j} W^T_{mi} \Gamma^B_{ij} W_{jn} = \sum_{k=-\frac{N-1}{2}}^{\frac{N-1}{2}} W^T_{m,2k-1} W_{2k,n} - W^T_{m,2k} W_{2k-1,n} = \sum_{k=-\frac{N-1}{2}}^{\frac{N-1}{2}} W_{2k-1,m} W_{2k,n} - W_{2k,m} W_{2k-1,n}
\tag{A.25}
$$

Now using A.23 and A.25 we explicitly calculate an element of the correlation Γ^A :

$$< \check{a}_{2m-1}\check{a}_{2n} >= \Gamma^A_{2m-1,2n} = \sum_{k=-\frac{N-1}{2}}^{\frac{N-1}{2}} W_{2k-1,2m-1}W_{2k,2n} - W_{2k,2m-1}W_{2k-1,2n} =$$

$$\sum_{k=1}^{\frac{N-1}{2}} (W_{2k-1,2m-1}W_{2k,2n} - W_{2k,2m-1}W_{2k-1,2n} + W_{-2k-1,2m-1}W_{-2k,2n} - W_{-2k,2m-1}W_{-2k-1,2n}) +$$

$$W_{-1,2m-1}W_{0,2n} - W_{-1,2m-1}W_{0,2n} =$$

$$= \frac{2}{N} \sum_{k=1}^{\frac{N-1}{2}} \left(v_k \cos \frac{2\pi km}{N} - u_k \sin \frac{2\pi km}{N} \right) \left(v_k \cos \frac{2\pi kn}{N} + u_k \sin \frac{2\pi kn}{N} \right) +$$

$$\left(u_k \cos \frac{2\pi km}{N} + v_k \sin \frac{2\pi km}{N} \right) \left(v_k \sin \frac{2\pi kn}{N} - u_k \cos \frac{2\pi kn}{N} \right) - u_0^2 =$$

$$\frac{2}{N} \sum_{k=0}^{\frac{N}{2}} \cos(\theta_k) \cos \frac{2\pi k(m-n)}{N} - \sin(\theta_k) \sin \frac{2\pi k(m-n)}{N}$$

$$(A.26)$$

Now calling $\phi \equiv \frac{2\pi k}{N}$ and sending $N \to \infty$:

$$< \check{a}_{2m-1}\check{a}_{2n} >= \frac{1}{\pi} \int_0^\pi d\phi \frac{\lambda - \cos\phi}{|\lambda - \cos\phi + i\sin\phi|} \cos\phi(m-n) - \frac{1}{\pi} \int_0^\pi d\phi \frac{\sin\phi}{|\lambda - \cos\phi + i\sin\phi|} \sin\phi(m-n)$$

$$(A.27)$$

Wich can be written in the more compact form:

$$< \check{a}_{2m-1}\check{a}_{2n} >= \frac{1}{2\pi} \int_0^{2\pi} d\phi \ e^{-i\phi(n-m)} \frac{\lambda - \cos\phi + i\sin\phi}{|\lambda - \cos\phi + i\sin\phi|} \qquad (A.28)$$

Bibliography

[ABN04]   A. E. Allahverdyan, R. Balian, and Th. M. Nieuwenhuizen. Maximal work extraction from quantum systems, 2004.

[AF13]   Robert Alicki and Mark Fannes. Entanglement boost for extractable work from ensembles of quantum batteries. *Phys. Rev. E*, 87:042123, Apr 2013.

[AFOV08]   Luigi Amico, Rosario Fazio, Andreas Osterloh, and Vlatko Vedral. Entanglement in many-body systems. *Rev. Mod. Phys.*, 80:517–576, May 2008.

[AGP19]   Mir Alimuddin, Tamal Guha, and Preeti Parashar. Bound on ergotropic gap for bipartite separable states. *Phys. Rev. A*, 99:052320, May 2019.

[AKM$^+$19] Gian Marcello Andolina, Maximilian Keck, Andrea Mari, Vittorio Giovannetti, and Marco Polini. Quantum versus classical many-body batteries. *Phys. Rev. B*, 99:205437, May 2019.

[BGBE10]   Kristian Baumann, Christine Guerlin, Ferdinand Brennecke, and Tilman Esslinger. Dicke quantum phase transition with a superfluid gas in an optical cavity. *Nature*, 464(7293):1301–1306, April 2010.

[BM71a]   Eytan Barouch and Barry M. McCoy. Statistical mechanics of the XY model. iii. *Phys. Rev. A*, 3:2137–2140, Jun 1971.

[BM71b]   Eytan Barouch and Barry M. McCoy. Statistical mechanics of the *xy* model. ii. spin-correlation functions. *Phys. Rev. A*, 3:786–804, Feb 1971.

[BMD70]   Eytan Barouch, Barry M. McCoy, and Max Dresden. Statistical mechanics of the XY model. i. *Phys. Rev. A*, 2:1075–1092, Sep 1970.

[DC19]   Sebastian Deffner and Steve Campbell. Quantum thermodynamics: An introduction to the thermodynamics of quantum information, 2019.

[DCS18]   Gabriele De Chiara and Anna Sanpera. Genuine quantum correlations in quantum many-body systems: a review of recent progress. *Reports on Progress in Physics*, 81(7):074002, Jun 2018.

[FCA$^+$14]   Fabio Franchini, Jian Cui, Luigi Amico, Heng Fan, Mile Gu, Vladimir Korepin, Leong Chuan Kwek, and Vlatko Vedral. Local convertibility and the quantum simulation of edge states in many-body systems. *Physical Review X*, 4(4), Nov 2014.

[FFIP08]   P. Facchi, G. Florio, C. Invernizzi, and S. Pascazio. Entanglement of two blocks of spins in the critical ising model. *Phys. Rev. A*, 78:052302, Nov 2008.

[FGPP17]   Gianluca Francica, John Goold, Francesco Plastina, and Mauro Paternostro. Daemonic ergotropy: enhanced work extraction from quantum correlations. *npj Quantum Information*, 3(1), March 2017.

[Fra17]   Fabio Franchini. An introduction to integrable techniques for one-dimensional quantum systems. *Lecture Notes in Physics*, 2017.

[Gan07]   Wen Xiao Gang. *Quantum field theory of many-body systems: from the origin of sound to an origin of light and electrons.* Oxford University Press, Oxford, 2007.

[GMM10]   Jochen Gemmer, M. Michel, and Günter Mahler. *Quantum Thermodynamics.* Springer Berlin Heidelberg, 2010.

[Gol92]   Nigel Goldenfeld. *Lectures on phase transitions and the renormalization group.* Frontiers in physics 85. Addison-Wesley, 1992.

[GRMAR$^+$16]   F. J. Gómez-Ruiz, J. J. Mendoza-Arenas, F. J. Rodríguez, C. Tejedor, and L. Quiroga. Quantum phase transitions detected by a local probe using time correlations and violations of leggett-garg inequalities. *Phys. Rev. B*, 93:035441, Jan 2016.

[HT13]   E.M. Harrell and W. Thirring. *A Course in Mathematical Physics: Volume 4: Quantum Mechanics of Large Systems.* Springer Vienna, 2013.

[Hua]

[Kat62]   Shigetoshi Katsura. Statistical mechanics of the anisotropic linear heisenberg model. *Phys. Rev.*, 127:1508–1518, Sep 1962.

[KFIT17]   Jan Klaers, Stefan Faelt, Atac Imamoglu, and Emre Togan. Squeezed thermal reservoirs as a resource for a nanomechanical engine beyond the carnot limit. *Phys. Rev. X*, 7:031044, Sep 2017.

[LR09]   J I Latorre and A Riera. A short review on entanglement in quantum spin systems. *Journal of Physics A: Mathematical and Theoretical*, 42(50):504002, Dec 2009.

[LRV03]   J. I. Latorre, E. Rico, and G. Vidal. Ground state entanglement in quantum spin chains, 2003.

[LSM61]   Elliott Lieb, Theodore Schultz, and Daniel Mattis. Two soluble models of an antiferromagnetic chain. *Annals of Physics*, 16(3):407 – 466, 1961.

[MOA11]   Albert W. Marshall, Ingram Olkin, and Barry C. Arnold. *Inequalities: Theory of Majorization and its Applications*, volume 143. Springer, second edition, 2011.

[MSS10]   Sarah Mostame, Gernot Schaller, and Ralf Schützhold. Decoherence in a dynamical quantum phase transition. *Phys. Rev. A*, 81:032305, Mar 2010.

[NC11]   Michael A. Nielsen and Isaac L. Chuang. *Quantum Computation and Quantum Information: 10th Anniversary Edition*. Cambridge University Press, USA, 10th edition, 2011.

[OAFF02]   A. Osterloh, Luigi Amico, G. Falci, and Rosario Fazio. Scaling of entanglement close to a quantum phase transition. *Nature*, 416(6881):608–610, Apr 2002.

[ON02]   Tobias J. Osborne and Michael A. Nielsen. Entanglement in a simple quantum phase transition. *Phys. Rev. A*, 66:032110, Sep 2002.

[PW78]   W. Pusz and S. L. Woronowicz. Passive states and kms states for general quantum systems. *Comm. Math. Phys.*, 58(3):273–290, 1978.

[RDT+16]   J. Rossnagel, S. T. Dawkins, K. N. Tolazzi, O. Abah, E. Lutz, F. Schmidt-Kaler, and K. Singer. A single-atom heat engine. *Science*, 352(6283):325–329, Apr 2016.

[Sac11]   Subir Sachdev. *Quantum Phase Transitions*. Cambridge University Press, 2 edition, 2011.

[SZAW03]   Marlan O. Scully, M. Suhail Zubairy, Girish S. Agarwal, and Herbert Walther. Extracting work from a single heat bath via vanishing quantum coherence. *Science*, 299(5608):862–864, 2003.

[TRHA11]   B. Tomasello, D. Rossini, A. Hamma, and L. Amico. Ground-state factorization and correlations with broken symmetry. *EPL (Europhysics Letters)*, 96(2):27002, sep 2011.

[Voj03]   Matthias Vojta. Quantum phase transitions. *Reports on Progress in Physics*, 66(12):2069–2110, Nov 2003.

[Wil13]   Mark M. Wilde. *Quantum Information Theory*. Cambridge University Press, 2013.

[WSL04]   L.-A. Wu, M. S. Sarandy, and D. A. Lidar. Quantum phase transitions and bipartite entanglement. *Phys. Rev. Lett.*, 93:250404, Dec 2004.

[ZCZW19]   Bei Zeng, Xie Chen, Duan-Lu Zhou, and Xiao-Gang Wen. *Quantum Information Meets Quantum Matter*. Springer New York, 2019.