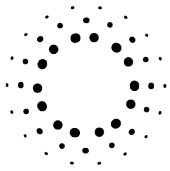

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Study of Entanglement Measures Using Path Integrals

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STUDY OF ENTANGLEMENT MEASURES USING PATH INTEGRALS

Dissertação de Mestrado apresentada ao Instituto de Física Teórica do Câmpus de São Paulo, da Universidade Estadual Paulista "Júlio de Mesquita Filho", como parte dos requisitos para obtenção do título Mestra em Física, Especialidade Física Teórica.

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Resumo

Revisamos métodos para representar medidas de emaranhamento em um sistema quântico bipartite em termos de integrais de caminho da formulação de Feynman da mecânica quântica. Usamos como medidas de emaranhamento a entropia linear e a segunda entropia de Rényi, ambas definidas em termos de uma matriz densidade reduzida associada a uma das partes do sistema bipartite. A representação da matriz densidade reduzida como uma integral de trajétória é obtida de duas maneiras distintas. A primeira faz uso explícito da função de onda do estado fundamental. A segunda toma o limite de temperatura zero de uma distribuição térmica. Exemplificamos o emprego desses métodos num problema de dois osciladores harmônicos acoplados. Por fim, formulamos um esquema pertubativo que expressa as medidas de emaranhamento como integrais de trajetória representando valores esperados e elementos de matriz de termos responsáveis pelo emaranhamento na lagrangiana do sistema. Esse método permite empregar técnicas numéricas bem estabelecidas para simular integrais de trajetória, como a quantização estocástica e o método de Monte Carlo.

Palavras-chave: Informação quântica; Integrais de trajetória; Perturbação (Matemática); Correlações entre partículas.

Área do conhecimento: Física teórica.

Abstract

We review methods to represent entanglement measures in a bipartite quantum system in terms of path integrals of Feynman's representation of quantum mechanics. We employ as entanglement measures the linear entropy and the second Rényi entropy, both defined in terms of a reduced density matrix associated with one part of the bipartite system. The path integral representation of the reduced density matrix is obtained in two different ways. The first makes explicit use of ground state wave function. The second takes the zero temperature limit of a thermal distribution. We exemplify the use of these methods in a problem of two coupled harmonic oscillators. Finally, we formulate a perturbative scheme that expresses the entanglement measures as path integrals representing expectation values and matrix elements of terms responsible for the entanglement in the Lagrangian of the system. This method is suited for direct use of well established numerical techniques to simulate path integrals, as the stochastic quantization and the Monte Carlo method.

Keywords: Quantum information; Path integrals; Perturbation theory; Particle correlations.

Fields of Knowledge: Theoretical physics.

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Chapter 1

Introduction

Quantum information theory is a prominent research area in theoretical physics, with applications ranging from solid state physics to gauge-gravity duality [1, 2, 3]. This master dissertation concerns continuous variables and entanglement in bipartite Hilbert spaces. Our primary goal is to present a pedagogical introduction to the subject, with emphasis on the use of path integral methods to quantify entanglement. Our main focus is on two commonly used entanglement measures, the linear entropy and the second Rényi entropy. Both entropies are defined in terms of a reduced density matrix associated with one part of the bipartite system, obtained from the full density matrix by tracing over the degrees of freedom of the other part of the bipartite system. For small and finite dimensional systems, we can fully diagonalize the density matrix analytically or using exact diagonalization methods, and then obtain the desired entanglement measures. Even in these cases there are many open questions in quantum information theory, e.g. the problem of a separability criteria for mixed states [4, 5]. In this dissertation we restrict to pure bipartite states. In quantum field theory applications of quantum information, one is often interested in the entanglement between spatial regions or momentum modes, in which the subsystems are defined as an interval or a region [6, 7, 8, 9]. Path integrals are commonly used in this context. They are very suitable for discretization and numerical computations, and allow us to easily manipulate expectation values and matrix elements. Moreover, there exist powerful numerical methods to compute those quantities, such as Monte Carlo methods and stochastic quantization [10, 11].

The most common entanglement measures, as the entanglement entropy and

the Rényi entropies, are not expressible in terms of expectation values of products of the dynamical variables of the system, or correlation functions. Therefore, those traditional numerical methods are not straightforward to use to compute these entanglement measures. Our second goal in this dissertation is to formulate a perturbative method, valid for weakly entangled systems, by which the linear entropy and the second Rényi entropy can be expressed as path integrals of expectation values and matrix elements of terms responsible for the entanglement in the Lagrangian of the system.

We use a simple model of two coupled harmonic oscillators to illustrate the different techniques to compute entanglement between particles. The model is also used to illustrate the use of our perturbative technique to express the entanglement measures in terms of expectation values. The perturbative method is valid beyond the two coupled oscillator model, being applicable to systems with more complicated interactions or more particles, and also to quantum field theory. We tried to keep our expressions in a general form and used the coupled oscillator model to illustrate the different steps involved in the method.

In chapter 2, we introduce important concepts in quantum information theory [12, 13] that will be useful in the other chapters. First, we explain the difference between pure/mixed states, and define what is an entangled state; in this part we use qubits to explore such definitions. Then we discuss fundamental concepts of the quantum theory, such as locality and realism, along with the Einstein-Podolsky-Rosen paradox and Bell inequality. The rest of this chapter is dedicated to more computational topics: the Schmidt decomposition and many entanglement measures - entanglement entropy, Rényi entropies and linear entropy.

By far, the entanglement entropy, or von Neumann entropy, is the most requested entanglement measure in condensed matter and high energy physics due to its interesting theoretical properties, such as the area law [14]. It is defined as $S(\rho) = -\mathrm{Tr}(\rho \log \rho)$, and the $\log \rho$ in this expression results in several difficulties regarding the calculations. Fortunately, there are ways to circumvent this

problem, which we discuss in chapter 2: one can use the replica trick, or find approximations to the entanglement entropy. More specifically, the linear entropy and the second Rényi entropy are useful lower approximations to the entanglement entropy. These entanglement measures depend on $\mathrm{Tr}(\rho^2)$, and have the advantage that they can be experimentally probed [15, 16], while the same is not true for the entanglement entropy.

The standard way to compute the entanglement entropy between the two parts of a pure ground state requires that we solve two eigenvalue problems: one for the Hamiltonian, in order to find the ground state,

$$H\left|\Psi_0\right\rangle = E_0\left|\Psi_0\right\rangle, \tag{1.1}$$

and the other for density matrix, which has the form $\rho = \left|\Psi_0\right\rangle\left\langle\Psi_0\right|$ for a pure state, in order to find its eigenvalues $\{\lambda_n\}$,

$$\rho\left|\lambda_n\right\rangle = \lambda_n\left|\lambda_n\right\rangle. \tag{1.2}$$

With the density matrix eigenvalues in hands, it is straightforward to compute any entanglement measure. Infinite dimensional systems that can be analytically solved in that manner are rare; an example of an analytically solvable model is the system of two coupled harmonic oscillators. In the end of chapter 2, we use the standard method to analytically diagonalize this system, then compute and compare all the entanglement measures introduced through the chapter.

In chapter 3, we review the Feynman path integral formulation of quantum mechanics [17] in real and imaginary time — in field theory jargon, these correspond to Minkowski and in Euclidean time, respectively. A path integral representation of the transition amplitude $\left\langle x_f\, T\middle|x_i\, 0\right\rangle$ consists on splitting the total time T in small pieces and integrating over all possible intermediate positions x_j that the particle can occupy at the intermediate time t_j. This gives the many possible quantum trajectories, and they contribute differently to the transition amplitude: the contribution of each trajectory is proportional to the exponential of the action. We show how to express transition amplitudes, matrix elements and expectation

values with path integrals. In the end of chapter 3, we analytically perform the calculations for the case of a free particle, and for a simple quantum harmonic oscillator.

In chapter 4, we discuss our first technique, in which we express the wave function and the density matrix with path integrals. This method is based on the fact that all states converge to the ground state after evolution through a large amount of time, $T \to \infty$, as long as the initial state has non zero overlap with the ground state [1, 18]. We take advantage of this fact to represent the ground state wave function and density matrix using path integrals. However, these path integrals have special boundary conditions that prevents us from taking the replica trick limit in a straightforward way. In this chapter we will discuss these special boundary conditions, and then compute the second Rényi entropy and the linear entropy for the case of coupled harmonic oscillators.

In chapter 5, we present another technique to obtain the density matrix with path integrals. Differently from the method present in chapter 4, with this method we find an expression to the density matrix involving only one path integral. The key point is that a pure state can be obtained as the zero temperature limit, i.e. inverse temperature $\beta \to \infty$, of a thermal distribution mixed state [8, 9]. We apply this technique to write the trace of different powers of the reduced density matrix, which appear in the Rényi entropies and in the linear entropy. The path integrals that appear in this technique also have interesting boundary conditions, similar to those in chapter 4.

The advantage of the method presented in chapter 5 is that all expressions relevant to the entanglement measures involve half the amount of path integrals we had in chapter 4 because the density matrix itself will have the form of an evolution operator. However, this method does not allow us to access the state wavefunction. Once again, we compute the second Rényi entropy and the linear entropy for the system of coupled harmonic oscillators.

The original contribution of this work is presented in chapter 6, in which we formulate a perturbative approach to compute the linear entropy and the second

Rényi entropy. The key idea is to use the parameter that entangles the particles in the Lagrangian of the system as a perturbative parameter, and perform an expansion in the path integral representation of the reduced density matrix. Then we carry out the derivation of the trace of the square of a reduced density matrix corresponding to one part of the bipartite system, $\mathrm{Tr}_A(\rho_A^2)$, which appears in the definitions of the entanglement measures of interest. We find generic expressions, valid for arbitrary bipartite systems, and make use of the two coupled harmonic oscillator model to illustrate the findings. We show, in particular, that the zero-order (unentangled) and first-order expressions leads to the expected result for this model. We comment on the use of different analytical and numerical methods to compute the derived expressions for a generic model [10, 11, 19].

Lastly, in chapter 7, we summarize our study, make our final considerations, and discuss perspectives for future works.

Chapter 2

Brief Review of Quantum Information Theory

The existence of entanglement makes quantum mechanics fundamentally distinct from classical mechanics. Quantum entanglement is the key concept used by quantum information theory in the development of a quantum computer, with its qubits and quantum gates. More recently, there is also a growing interest in applications of quantum information concepts to condensed matter and high energy physics, e.g. for the detection of quantum phase transitions. These systems are often large and require novel techniques in order to make entanglement calculations possible.

The aim of this chapter is to present the basic concepts of quantum information theory that are needed for the development of our study, which are the density matrix and ways to quantify entanglement. We also discuss key aspects of quantum mechanics foundations using the EPR paradox and Bell's theorem.

2.1 Density matrix

In quantum mechanics, we usually deal with pure states, those which can be represented by a ket $|\psi\rangle$ in the Hilbert space $\mathcal{H}$. The density matrix, also called state operator, of a pure state is defined as

$$\rho_{pure} = |\psi\rangle \langle\psi| . \tag{2.1}$$

The density matrix is an Hermitian operator and with positive eigenvalues and has unit trace. For mixed states the eigenvalues are interpreted as probabilities.

In order to extract physics from the density matrix we have understand how to obtain expectation values of physical observables and the evolution of the density matrix. The expectation value of an observable $\hat{O}$ in terms of density matrix is

$$\begin{aligned} \langle \hat{O} \rangle &= \langle \psi | \hat{O} | \psi \rangle && (2.2) \\ &= \langle \psi | \psi \rangle \langle \psi | \hat{O} | \psi \rangle && (2.3) \\ &= \mathrm{Tr}\big(\rho \hat{O}\big), && (2.4) \end{aligned}$$

in the second line we have inserted $\langle \psi | \psi \rangle = 1$ and then recognized $\rho = |\psi\rangle \langle \psi|$. The evolution of the density operator can be derived from the Schrödinger equation; it is given by

$$i \frac{\partial \rho}{\partial t} = [H, \rho]. \tag{2.5}$$

There are some physical states in the Hilbert space that cannot be represented by a single ket, those are called mixed states. They can only be represented by a density matrix of the form

$$\rho_{mixed} = \sum_i p_i |\psi_i\rangle \langle \psi_i| . \tag{2.6}$$

A mixed state is obtained when we prepare a state $|\psi_i\rangle$ with probability p_i. For example, if we prepare $N/2$ electrons with spin up and $N/2$ electrons with spin down, then the state of one electron is a mixed state with probability 50% to have spin up and 50% to have spin down,

$$\rho = \frac{1}{2} |\uparrow\rangle \langle \uparrow| + \frac{1}{2} |\downarrow\rangle \langle \downarrow| . \tag{2.7}$$

Here $|\uparrow\rangle$ and $|\downarrow\rangle$ denote the eigenstates of σ_z with eigenvalue $+1$ and -1, respectively. This is very different from a system of N electrons of unknown spin, in which an electron is described by the pure state

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle + |\downarrow\rangle \right) . \tag{2.8}$$

Both states give the same expectation value for σ_z, $\langle\sigma_z\rangle = 0$, but show different expectation values for σ_x. The mixed state has $\langle\sigma_x\rangle = 0$, and the pure state is an eigenstate of σ_x, with $\langle\sigma_x\rangle = +1$. This happens because the probabilities in the mixed state 2.7 are classical, so it is an incoherent superposition of states, while in the pure state 2.8 we have a coherent superposition. Another way to understand is that the mixed state was prepared out of eigenstates of σ_z because we put together $N/2$ electrons with spin up with $N/2$ with spin down, therefore the mixed state must have zero expectation value for σ_x.

For a bipartite Hilbert space it can happen that the total state, the one describing both parts, is pure, but the state of each part is mixed. As an example, suppose we have two electrons $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ and they are in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle), \tag{2.9}$$

the 2-qubit $|\uparrow\uparrow\rangle$ stands for $|\uparrow\rangle_A \otimes |\uparrow\rangle_B$, similarly for $|\downarrow\downarrow\rangle$. In order to show that the A and B electrons cannot be expressed as pure states, we will try to write their total state 2.9 in the form $|\tilde{\psi}\rangle = |\psi\rangle_A \otimes |\psi\rangle_B$ and see that it is impossible.

Using the most general form for the pure states of each electron, $|\psi\rangle_A = a_1|\uparrow\rangle + a_2|\downarrow\rangle$ and $|\psi\rangle_B = b_1|\uparrow\rangle + b_2|\downarrow\rangle$, we obtain the following total state

$$|\tilde{\psi}\rangle = a_1 b_1 |\uparrow\uparrow\rangle + a_1 b_2 |\uparrow\downarrow\rangle + a_2 b_1 |\downarrow\uparrow\rangle + a_2 b_2 |\downarrow\downarrow\rangle . \tag{2.10}$$

Now we have to match these coefficients with the ones in 2.9 in order to have $|\psi\rangle = |\tilde{\psi}\rangle$. We need all the following equations to be satisfied:

$$a_1 b_1 = \frac{1}{\sqrt{2}},\ a_1 b_2 = 0,\ a_2 b_1 = 0,\ a_2 b_2 = \frac{1}{\sqrt{2}}, \tag{2.11}$$

but this is not possible as it requires some coefficients to be zero and not zero at the same time. We come to the conclusion that although the total state is a pure, the individual state of each electron is not a pure state.

When $|\psi\rangle \neq |\psi\rangle_A \otimes |\psi\rangle_B$, we say the parts A and B of the Hilbert space are entangled. Later we will define ways to quantify how strong the entanglement between two particles is. The fact that the joint state cannot be separated implies

that these particles are correlated. In this case, operators acting locally on one part of the Hilbert space can change the state of the other part.

Although the particles A and B of the example do not have their own pure states, each of them have a mixed state which can be represented by a density matrix. For a bipartite Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, the density matrix of part A is obtained by tracing out the degrees of freedom of B in the density matrix ρ of the full system,

$$\rho_A \coloneqq \mathrm{Tr}_B\, \rho. \tag{2.12}$$

In our example $\rho = |\psi\rangle \langle\psi|$, with $|\psi\rangle$ given in 2.9. Then the state of one electron is

$$\rho_A = \langle\uparrow|_B \rho\, |\uparrow\rangle_B + \langle\downarrow|_B \rho\, |\downarrow\rangle_B \tag{2.13}$$

$$= \frac{1}{2}(|\uparrow\rangle \langle\uparrow| + |\downarrow\rangle \langle\downarrow|), \tag{2.14}$$

here we are omitting the sub-indices, but we must remember that the qubits in this expression are in $\mathcal{H}_A$. The density matrix describing the B electron can be obtained in the same way, and in this case ρ_A and ρ_B are the same because the state of the full system in a pure state.

2.2 EPR paradox and Bell's theorem

In 1935, Einstein, Podolski and Rosen, EPR for short, wrote a paper [20] in which they discuss whether quantum mechanics was a complete theory, meaning that it describes all elements of physical reality. They define an element of physical reality as every property of the system that can be predicted with unit probability without disturbing the system.

Their conclusion was that either quantum mechanics is not a complete theory or physical quantities described by non-commuting operators do not have physical reality at the same time. For EPR it was not reasonable that two non-commuting physical quantities were not simultaneously real, therefore they believed that quantum mechanics was an incomplete theory.

The two main assumptions they make in their paper about nature are realism and locality. Realism is the statement that physical quantities have reality, i.e. definite values, even if they cannot be measured at the same time. Locality concerns the fact that we can separate two parts of a system in such a way that they no longer influence each other.

Today we are able to perform experiments that show quantum mechanics is right in that matter, and indeed non-commuting operators do not have simultaneous reality if we use their definition of reality. We say quantum mechanics is not a locally realistic theory. In what follows we present the Bell's theorem, which consists in an useful inequality derived when we assume local realism, and then see how quantum mechanics breaks it.

Suppose someone named Charlie performs an experiment on Earth to prepare two particles, then he gives one particle to Alice and the other to Bob. After that Alice and her particle take a spaceship and go to a lab somewhere very distant from Earth where she can perform experiments. Alice randomly chooses to measure either the property P_Q or P_R of her particle, these properties can only have outcomes ± 1. In his lab on Earth, Bob also randomly selects between properties P_S and P_T to measure, which again can only return ± 1. In the beginning of the experiment they have synchronized their clocks in such a way that the measurements are going to be causally disconnected events.

Let us refer to the outcomes of the experiments as Q, R, S and T and analyze the expression $QS + RS + RT - QT$. It is important to call the attention to the fact Bell assumes all the physical properties mentioned have reality at the same time, therefore P_R has a definite unknown value R even if P_Q was the one measured. The expression for the outcomes can be rewritten as

$$(R + Q)S + (R - Q)T \tag{2.15}$$

and since R, $Q = \pm 1$ we have either $R + Q = 0$ or $R - Q = 0$. Then we are left with $(R + Q)S$ or $(R - Q)T$ and since each can only assume the values ± 2 we

come to the conclusion that

$$QS + RS + RT - QT = \pm 2. \tag{2.16}$$

Now assume we have a probability $p(q,r,s,t)$ to obtain $Q = q$, $R = r$, $S = s$ and $T = t$. The expectation value $\langle QS + RS + RT - QT \rangle$ then satisfies the following inequality,

$$\langle QS + RS + RT - QT \rangle = \sum_{q,r,s,t} p(q,r,s,t)\,(qs + rs + rt - qt) \tag{2.17}$$

$$\leq \sum_{q,r,s,t} p(q,r,s,t) \times 2. \tag{2.18}$$

The sum of the probabilities gives unity and on the left hand side we put the expectation value in every term of the sum. The result is called Bell inequality,

$$\langle QS \rangle + \langle RS \rangle + \langle RT \rangle - \langle QT \rangle \leq 2, \tag{2.19}$$

and again we stress that it was derived assuming local realism.

Now we will compute the left hand side of the Bell inequality for the entangled pair 2.9 introduced in the last section,

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle). \tag{2.20}$$

Moreover, the experiments that can be performed by Alice and Bob are going to be Stern-Gerlach experiments. As required from the theorem, these measurements can only give ± 1 outcomes. We use the same letters as before to define the operators that are going to be measured,

$$Q = \hat{S}_z \otimes \mathbb{1}_B\,, \tag{2.21}$$

$$R = \hat{S}_x \otimes \mathbb{1}_B\,, \tag{2.22}$$

$$S = \mathbb{1}_A \otimes \frac{1}{\sqrt{2}}(\hat{S}_x + \hat{S}_z), \tag{2.23}$$

$$T = \mathbb{1}_A \otimes \frac{1}{\sqrt{2}}(\hat{S}_x - \hat{S}_z), \tag{2.24}$$

$$\tag{2.25}$$

where $\hat{S}_z = \frac{1}{2}\sigma_z$ and $\hat{S}_x = \frac{1}{2}\sigma_x$. Remember that the arrows in $|\psi\rangle$ refer to the eigenstates of σ_z, therefore the effect of $\hat{S}_z$ is to extract the eigenvalue and $\hat{S}_x$ flips the arrow.

It is straightforward to compute the expectation values in the expression $\langle QS\rangle + \langle RS\rangle + \langle RT\rangle - \langle QT\rangle$. Here show the calculations for $\langle QS\rangle$:

$$\langle QS\rangle = \langle\psi| Q \left[\frac{1}{2}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\right] \tag{2.26}$$

$$= \langle\psi| \left[\frac{1}{2}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\right] \tag{2.27}$$

$$= \frac{1}{\sqrt{2}}. \tag{2.28}$$

The other expectation values are $\langle RS\rangle = \frac{1}{\sqrt{2}}$, $\langle RT\rangle = \frac{1}{\sqrt{2}}$ and $\langle QT\rangle = \frac{-1}{\sqrt{2}}$. This gives the violation of Bell inequality,

$$\langle QS\rangle + \langle RS\rangle + \langle RT\rangle - \langle QT\rangle = 2\sqrt{2}. \tag{2.29}$$

The violation by $2\sqrt{2}$ is the largest value allowed for this Hilbert space and the state 2.9 is one of the four Bell states, which are maximally entangled 2-qubits. For entangled states of the form $|\psi\rangle_{full} \neq |\psi\rangle_A \otimes |\psi\rangle_B$ one can always find observables Q, R, S and T such that the Bell inequality does not hold.

The violation of Bell inequality has already been verified experimentally and it demonstrates that either the assumption of realism or locality in the EPR paper is wrong. Most physicists believe realism is the assumption that does not hold, meaning that quantum mechanics is a complete theory. Moreover, quantum mechanics allows correlations which are fundamentally different from the classical ones. Classical correlations are consequence of lack of knowledge about the state, but this is not the case for entanglement.

2.3 Schmidt decomposition

The Schmidt decomposition is a useful tool in quantum information because it allow us to write the state of two particles in a single sum. According to this

theorem, a pure state on a bipartite Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ can always be written in the form

$$|\Psi\rangle = \sum_{k=1}^{\min(d_A,d_B)} \sqrt{\lambda_k} \left|\phi_k^A\right\rangle \otimes \left|\chi_k^B\right\rangle, \tag{2.30}$$

where d_A and d_B are the dimensions of $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, λ_k are the Schmidt coefficients, they are non-negative numbers and $\sum_k \lambda_k = 1$ and $\{\phi_k, \chi_k\}$ are called Schmidt modes.

Here we derive the theorem for $\mathcal{H}_A$ and $\mathcal{H}_B$ with a discrete and finite basis, but the result holds even if this is not the case. For this kind of Hilbert spaces the most general form of a two-particles pure state is

$$|\Psi\rangle = \sum_{i=1}^{d_A} \sum_{j=1}^{d_B} c_{ij} |\phi_i\rangle \otimes |\chi_j\rangle, \tag{2.31}$$

where the $\{|\phi_i\rangle\}$ are the basis vectors that span the Hilbert space $\mathcal{H}_A$ and $\{|\chi_i\rangle\}$ span $\mathcal{H}_B$. The elements c_{ij} define the $d_A \times d_B$ complex matrix M. This matrix can be expressed as $M = U\Lambda V^\dagger$ using the singular value decomposition (SVD), where U and V are unitary matrices and Λ is a diagonal matrix.

To demonstrate the SVD note that $M^\dagger M$ is an Hermitian matrix, therefore it has real eigenvalues and can be diagonalized by an unitary matrix V

$$V^\dagger M^\dagger M V = D, \tag{2.32}$$

the diagonal matrix D carries the eigenvalues which we suppose are all non-zero. The other unitary matrix is $U \coloneqq MVD^{-\frac{1}{2}}$,

$$U^\dagger U = D^{-\frac{1}{2}} \left(V^\dagger M^\dagger M V\right) D^{-\frac{1}{2}} = \mathbb{1}. \tag{2.33}$$

Then we define the diagonal matrix $\Lambda \coloneqq D^{\frac{1}{2}}$ with non-negative matrix elements $\{\sqrt{\lambda_k}\}$ and find that $M = U\Lambda V^\dagger$, indeed

$$U\Lambda V^\dagger = \left(MVD^{-\frac{1}{2}}\right) D^{\frac{1}{2}} V^\dagger = M. \tag{2.34}$$

Now we can continue the Schmidt decomposition of 2.31 by expressing the matrix elements of $M = U\Lambda V^\dagger$ as $c_{ij} = \sum_k u_{ik}\sqrt{\lambda_k}\, v^*_{kj}$, then

$$|\Psi\rangle = \sum_{k=1}^{\min(d_A,d_B)} \sqrt{\lambda_k} \left(\sum_{i=1}^{d_A} u_{ik} |\phi_i\rangle\right) \otimes \left(\sum_{j=1}^{d_B} v^*_{kj} |\chi_j\rangle\right) \tag{2.35}$$

$$= \sum_{k=1}^{\min(d_A,d_B)} \sqrt{\lambda_k} \left|\phi^A_k\right\rangle \otimes \left|\chi^B_k\right\rangle . \tag{2.36}$$

In the last line we have redefined the vectors in order to get rid of the sums over i and j. The new vectors $\left|\phi^A_k\right\rangle$ and $\left|\chi^B_k\right\rangle$ are the Schmidt modes and the normalization $\langle\Psi|\Psi\rangle = 1$ implies $\sum_k \lambda_k = 1$. This last result allows to interpret the λ_k as probabilities in the two particles density matrix.

When the Hilbert space does not have a discrete and finite basis we will have to manage integrals to decompose the kernel that appears instead of the matrix M, but the result of the Schmidt decomposition still has the same form as 2.40, with a sum over discrete Schmidt coefficients and modes.

2.4 Quantifying entanglement

In this section, we discuss some of the many different ways to quantify entanglement. There is a great variety of entanglement measures, which satisfy different properties. Here we present the entanglement entropy, Rényi entropies, purity and the linear entropy. The entanglement entropy can be obtained from the Rényi entropy using a very useful technique called the replica trick. Moreover, under some circumstances we can use the second Rényi entropy and the linear entropy to approximate the entanglement entropy.

2.4.1 Entanglement measures

In classical information theory, the **Shannon entropy** H is a way to quantify the amount of uncertainty regarding a random variable x when the outcomes $\{x_i\}$, also called events, are observed to happen with probability $\{p_i\}$ with $i = 1, \ldots, N$

for some $N \in \mathbb{N}$. The Shannon entropy is defined as

$$H(x) := -\sum_i p_i \log(p_i), \tag{2.37}$$

the sum is over the possible outcomes and p_i is the probability associated with the event x_i. In order to motivate this expression, we present some properties it satisfies and which should be natural for a function representing information.

The Shannon entropy does not depend on the labels of the events, only on their probabilities. This is a necessary property because if we change the name of our variables then nothing regarding the amount of information should change. Moreover the information gained when two independent events happen is the sum of the individual information obtained by each event.

Since $H(x)$ quantifies the amount of information obtained when x is observed, it is natural to expect that very likely events contribute less. In the extreme example when $p_x = 1$, we should learn nothing when x is observed because it already has unit probability to occur. Indeed in this case $H(x) \to 0$ and therefore there is no uncertainty regarding the variable x. The $-\log(x)$ makes $H(x)$ a non-negative function that decreases monotonically in the probabilities.

As we discussed in section 2.2, quantum correlations (entanglement) are very different from the classical ones because they are not necessarily consequence of our ignorance about the system. For this reason, entropy in quantum mechanics is a way to quantify entanglement, not a way to quantify uncertainty about a quantum state.

The eigenvalues of the density matrix are analogous to the probabilities of the events in classical information and a quantum generalization of the Shannon entropy should be given in terms of the density matrix. This generalization is the von Neumann entropy, also known as **entanglement entropy**, and it is defined as

$$S(\rho) := -\operatorname{Tr}(\rho \log \rho), \tag{2.38}$$

where the trace is over the Hilbert space ρ belongs. Note that if the eigenvalues

$\{p_i\}$ of the density matrix are known, then the von Neumann entropy becomes

$$S(\rho) = -\sum_i p_i \log p_i, \tag{2.39}$$

which is the same as the expression for the Shannon entropy. The entanglement entropy of a pure state is always zero: since the density matrix $\rho = |\phi\rangle \langle\phi|$ is diagonal in this basis, $\log(\rho) = \log(1) |\phi\rangle \langle\phi| = 0$ and then $S(\rho) = 0$.

Moreover, if ρ is a pure state in a bipartite Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, then it is true that $S(\rho_A) = S(\rho_B)$, where ρ_A and ρ_B are the reduced density matrices. This is not the case when ρ is mixed as it can be entangled with another Hilbert space $\mathcal{H}_C$. We can see that $S(\rho_A) = S(\rho_B)$ for a pure state using the Schmidt decomposition derived in section 2.3. The general form of a pure state in a bipartite Hilbert space is

$$|\Psi\rangle = \sum_n \sqrt{\lambda_n} |\phi_n\rangle \otimes |\chi_n\rangle , \tag{2.40}$$

where λ_n are the Schmidt coefficients, $|\phi_n\rangle$ and $|\chi_n\rangle$ are the Schmidt modes. The Schmidt coefficients are all non-negative and their sum is unity. The density matrix of this state then is given by

$$\rho = \sum_{m,n} \sqrt{\lambda_m \lambda_n} \; (\, |\phi_m\rangle \langle\phi_n| \,) \otimes (\, |\chi_m\rangle \langle\chi_n| \,) , \tag{2.41}$$

then to compute $S(\rho_A)$ and $S(\rho_B)$ we need the reduced density matrices for parts A and B. These can are obtained by taking partial traces of ρ,

$$\rho_A = \mathrm{Tr}_B \, \rho = \sum_n \lambda_n |\phi_n\rangle \langle\phi_n| \tag{2.42}$$

$$\rho_B = \mathrm{Tr}_A \, \rho = \sum_n \lambda_n |\chi_n\rangle \langle\chi_n| . \tag{2.43}$$

Since both have the same eigenvalues, they also have the same entanglement entropy

$$S(\rho_A) = S(\rho_B) = -\sum_n \lambda_n \log(\lambda_n). \tag{2.44}$$

When $\mathcal{H}_A$ and $\mathcal{H}_B$ are finite dimensional Hilbert spaces, entanglement entropy has an upper limit. With the purpose to derive this upper limit we introduce a Lagrange multiplier ξ together with the condition of unit trace for the density matrix. Therefore the expression we want to maximize is

$$F(\rho_A, \xi) = -\sum_n \lambda_n \log(\lambda_n) - \xi \left(\sum_n \lambda_n - 1 \right). \tag{2.45}$$

Now we impose the conditions $\frac{\partial F}{\partial \xi} = 0$ and $\frac{\partial F}{\partial \lambda} = 0$ for all $\lambda \in \{\lambda_n\}$ to obtain the equations

$$\begin{cases} -\log(\lambda) - 1 - \xi = 0, \text{ for all } \lambda \in \{\lambda_n\} \\ -\sum_n \lambda_n + 1 = 0. \end{cases} \tag{2.46}$$

Solving the first equation we find that all λ_n are equal to $\lambda = e^{-1-\xi}$. Suppose that the Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ have dimensions d_A and d_B, respectively. Using only the fact that all λ_n are equal and that the sum over n goes up to $d = \min(d_A, d_B)$, we obtain from the second equation that $\lambda = 1/d$. Then we put this result in the entanglement entropy expression to find

$$S(\rho_A)_{\max} = -\log(d). \tag{2.47}$$

The states that reach this upper limit are called maximally mixed states, e.g. the Bell states for the 2-qubit system. The maximally mixed states have the following general form

$$\rho_A = \sum_n \lambda \left|\phi_n\right\rangle \left\langle\phi_n\right|, \tag{2.48}$$

with $\lambda = 1/d$. Here we use the expression for the reduced density matrix with the Schmidt decomposition.

In several theories the entanglement entropy satisfies an area law, meaning that it scales with the boundary between the spaces entangled. Area laws are object of intense study in the theoretical physics community of many different fields, from black hole entropy in holography to topological entanglement entropy in quantum many-body physics.

Although the entanglement entropy has many interesting features, the computation of $\log(\rho)$ is often a big problem as it requires diagonalization of the density matrix. There are techniques to circumvent this problem, one of them if using the Rényi entropy and the replica trick.

The **Rényi entropy** depends on a parameter α, which assumes natural values $\alpha > 1$, and it is defined as

$$S_\alpha(\rho) := \frac{1}{1-\alpha} \log(\mathrm{Tr}\, \rho^\alpha). \tag{2.49}$$

The different Rényi entropies will satisfy different properties depending on α. Since the trace indicated in this definition is taken over the density matrix, which has eigenvalues $\lambda_n \geq 0$, and $\alpha \geq 1$, the Rényi entropies are always non-negative, but in general they are not bounded from above. Furthermore, these entropies are usually easier to be obtained as they depend only on powers of the density matrix and require no diagonalization.

In the special limit $\alpha \to 1$ the Rényi entropy reproduces the entanglement entropy, but in order to take this limit we need to consider an analytic continuation of α. When we try $\alpha \to 1$ on the definition of $S_\alpha(\rho)$ in 2.49, both numerator and denominator go to zero, so we can use L'Hôpital's rule to write

$$\lim_{\alpha\to 1} S_\alpha(\rho) = -\lim_{\alpha\to 1} \frac{1}{\mathrm{Tr}(\rho^\alpha)} \frac{d}{d\alpha} \left[\mathrm{Tr}(\rho^\alpha)\right]. \tag{2.50}$$

The limit of $1/\,\mathrm{Tr}(\rho^\alpha)$ gives unit because we assume the density matrix ρ is normalized to unit. The derivative can be obtained by its definition:

$$\lim_{\alpha\to 1} S_\alpha(\rho) = -\lim_{\alpha\to 1} \lim_{\Delta\to 0} \frac{\mathrm{Tr}\left(\rho^{\alpha+\Delta}\right) - \mathrm{Tr}(\rho^\alpha)}{\Delta} \tag{2.51}$$

$$= -\lim_{\alpha\to 1} \lim_{\Delta\to 0} \sum_j \lambda_j^\alpha \frac{(\lambda_j^\Delta - 1)}{\Delta}, \tag{2.52}$$

where λ_j are the eigenvalues of the density matrix ρ. When $\Delta \to 0$, numerator and denominator go zero, so we use L'Hôpital's rule again. In order to take the

derivative of the numerator, we write $\lambda_j = e^{b_j}$ with b_j real, and obtain

$$\lim_{\alpha\to 1} S_\alpha(\rho) = -\lim_{\alpha\to 1}\lim_{\Delta\to 0}\sum_j e^{b_j\alpha}\frac{(e^{b_j\Delta}-1)}{\Delta} \tag{2.53}$$

$$= -\sum_j b_j e^{b_j} \tag{2.54}$$

$$= -\sum_j \lambda_j \log\lambda_j \tag{2.55}$$

$$= S(\rho). \tag{2.56}$$

Finally we obtained the proof that the Rényi entropy gives the entanglement entropy in the limit $\alpha \to 1$,

$$S(\rho) = \lim_{\alpha\to 1} S_\alpha(\rho) = \lim_{\alpha\to 1}\frac{1}{1-\alpha}\log[\mathrm{Tr}\,\rho^\alpha]. \tag{2.57}$$

The trace in this expression is taken in the Hilbert space ρ belongs, thus $\mathrm{Tr}\,\rho^\alpha$ is a number. For example, if we are dealing with the coordinate of a particle with $\rho = \rho(x, x')$, then we can insert $\alpha - 1$ identities in $\mathrm{Tr}\,\rho^\alpha$ to write

$$\mathrm{Tr}\,\rho^\alpha = \int dx_1 \int dx_2 \cdots \int dx_\alpha\, \rho(x_1, x_2)\rho(x_2, x_3)\ldots\rho(x_\alpha, x_1). \tag{2.58}$$

The integral over dx_1 comes from the trace. The technique 2.57 of using multiple powers of the density matrix to compute the Rényi entropies and then take $\alpha \to 1$ to obtain the entanglement entropy is called **replica trick**.

At last, the purity and the linear entropy of a quantum state are also another important entanglement measures. The purity of a quantum state is defined as

$$\mathcal{K}(\rho) := \mathrm{Tr}\left(\rho^2\right), \tag{2.59}$$

and it has the physical interpretation of how much the state ρ deviates from a pure state. If ρ is a pure state, then it is true that $\rho^2 = \rho$, therefore in this case $\mathcal{K}(\rho)$ gives unit, which is the upper bound of the purity. The lower bound is achieved by the maximally mixed state, which for a finite dimensional Hilbert space has the form 2.48. In this case we have

$$\mathcal{K}(\rho) = \sum_n \lambda^2 = \frac{1}{d}\ , \tag{2.60}$$

where d is the dimension of the Hilbert space. For an infinite dimensional Hilbert space, we can write

$$0 \leq \mathcal{K}(\rho) \leq 1. \tag{2.61}$$

The purity of a quantum state is an entanglement measure that decreases when entanglement increases. The complement of this entanglement measure is called impurity, or **linear entropy**, and it is defined by

$$S_L(\rho) \coloneqq 1 - \mathrm{Tr}\Big(\rho^2\Big). \tag{2.62}$$

For an infinite dimensional Hilbert space, the linear entropy will have the same bounds as $\mathcal{K}(\rho)$, i.e.

$$0 \leq S_L(\rho) \leq 1. \tag{2.63}$$

If the Hilbert space has a finite dimension d, the upper bound is replaced by $1 - 1/d$. The linear entropy is a more intuitive entanglement measure as it is increases when the entanglement between the parties increase. Moreover, similarly to the Rényi entropies, it is common to find the purity or the linear entropy in the literature: they do not necessarily require diagonalization and therefore are easier to compute than the entanglement entropy.

2.4.2 Approximations

Although we have defined the linear entropy independently of the strength of the entanglement, it can be viewed also a first order approximation of the entanglement entropy, when we use a power series representation for $\log(\rho)$ that appears in the definition 2.38 of the entanglement entropy. For a real number x, we can write

$$\log(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \dots, \tag{2.64}$$

which is a convergent series if $|x| < 1$. Since the density matrix is a diagonalizable matrix with eigenvalues ranging from 0 to 1, we are allowed to write

$$\log(\rho) = \log[1 + (\rho - 1)] = (\rho - 1) - \frac{(\rho-1)^2}{2} + \frac{(\rho-1)^3}{3} - \dots \quad . \tag{2.65}$$

Therefore a first order approximation gives

$$\log(\rho) \approx \rho - 1, \tag{2.66}$$

and using this expression in the entanglement entropy 2.38 we obtain

$$S(\rho) \approx \mathrm{Tr}[\,\rho\,(\rho-1)] = 1 - \mathrm{Tr}\left(\rho^2\right) = S_L(\rho). \tag{2.67}$$

Note that the linear entropy has also a straighforward relation to the second Rényi entropy, which is obtained by computing 2.49 with parameter $\alpha = 2$,

$$S_L(\rho) = 1 - e^{-S_2(\rho)}. \tag{2.68}$$

Indeed the approximation of the entanglement entropy can also be obtained with the replica trick. We have already shown that the entanglement entropy is obtained as the limit $\alpha \to 1$ of the Rényi entropy 2.57. If we use equation 2.50 to represent the Rényi entropy, then

$$S(\rho) = -\lim_{\alpha\to 1} \frac{1}{\mathrm{Tr}(\rho^\alpha)} \frac{d}{d\alpha} \left[\mathrm{Tr}(\rho^\alpha)\right]. \tag{2.69}$$

The limit in the denominator gives unit, and since the α parameter can only take natural values and we are interested in the limit $\alpha \to 1$, the best approximation we can make for the derivative is:

$$\frac{d}{d\alpha}\left[\mathrm{Tr}(\rho^\alpha)\right] \approx \frac{\mathrm{Tr}\left(\rho^2\right) - \mathrm{Tr}\left(\rho^1\right)}{2-1}. \tag{2.70}$$

Using that approximation we find once again that

$$S(\rho) \approx 1 - \mathrm{Tr}\left(\rho^2\right) = S_L(\rho) = 1 - e^{-S_2(\rho)}. \tag{2.71}$$

2.5 Coupled harmonic oscillators I

Let us consider a system of two particles of Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, and with evolution given by the Hamiltonian

$$H = \frac{1}{2}\left[p_A^2 + p_B^2 + k(x_A^2 + x_B^2) + g(x_A - x_B)^2\right]. \tag{2.72}$$

This is a system of coupled harmonic oscillators, and the term proportional to g is coupling the two particles. We are going to compute the entanglement between the particles when the full system is in the ground state. For this calculations we will diagonalize the reduced density matrix of particle A, and then use its eigenvalues in the expression 2.39 for the entanglement entropy $S(\rho_A)$.

First we find the wavefuntion, and therefore the density matrix of the total system. We use the center of mass and relative coordinate variables

$$x_\pm = \frac{1}{\sqrt{2}}(x_A \pm x_B), \tag{2.73}$$

$$\omega_+ = \sqrt{k} \text{ and } \omega_- = \sqrt{k+2\,g}, \tag{2.74}$$

together with the standard identification $p_x \to -i\frac{\partial}{\partial x}$ to rewrite H as the Hamiltonian of two decoupled two harmonic oscillators:

$$H = \frac{1}{2}\left(-\frac{\partial^2}{\partial x_-^2} - \frac{\partial^2}{\partial x_+^2} + \omega_+^2 x_+^2 + \omega_-^2 x_-^2\right). \tag{2.75}$$

The ground state wavefunction can be obtained from the eigenvalue problem for the Hamiltonian,

$$\frac{1}{2}\left(-\frac{\partial^2}{\partial x_-^2} - \frac{\partial^2}{\partial x_+^2} + \omega_+^2 x_+^2 + \omega_-^2 x_-^2\right)\Psi = E\Psi. \tag{2.76}$$

Since H is the Hamiltonian of two decoupled harmonic oscillators with frequencies ω_+ and ω_-, the ground state energy is $E = \frac{1}{2}(\omega_+ + \omega_-)$. Now we put this energy in the equation and solve it to find that the normalized ground state wavefunction is

$$\Psi = \frac{(\omega_+\omega_-)^{\frac{1}{4}}}{\sqrt{\pi}} \exp\left[-\frac{1}{2}(\omega_+ x_+^2 + \omega_- x_-^2)\right]. \tag{2.77}$$

Once we have the wavefunction, it is straightforward to write the density matrix. However we are interested in the entanglement between particles that occupy positions x_A and x_B, not on the entanglement between their center of mass and relative coordinates. Actually the x_+ and x_- coordinates are not entangled at all because there is no interaction term between them in the Hamiltonian. When

we change variables we are also changing the Hilbert space partition, this is why entanglement can disappear.

After we go back to the original x_A and x_B coordinates in the ground state wavefunction, we compute the density matrix of particle A by taking the trace over the Hilbert space $\mathcal{H}_B$,

$$\rho_A(x,x') = \langle x| \operatorname{Tr}_B(|\Psi\rangle\langle\Psi|)\,|x'\rangle \tag{2.78}$$

$$= \int_{-\infty}^{\infty} dx_b\, \Psi(x,x_b)\Psi^*(x',x_b) \tag{2.79}$$

$$= \frac{\sqrt{\omega_+\omega_-}}{\pi}\int_{-\infty}^{\infty} dx_b\, \exp\left\{-\frac{1}{2}\left[\omega_+(x+x_b)^2+\omega_-(x'-x_b)^2\right]\right\}. \tag{2.80}$$

Performing the integration over dx_B and introducing new constants γ and η defined below, we obtain

$$\rho_A(x,x') = \sqrt{\frac{\gamma-\eta}{\pi}}\,\exp\left[-\frac{\gamma}{2}(x^2+x'^2)+\eta xx'\right], \tag{2.81}$$

where

$$\eta = \frac{(\omega_+-\omega_-)^2}{4(w_++w_-)} \text{ and } \gamma = \frac{2\omega_+\omega_-}{(w_++w_-)}+\eta. \tag{2.82}$$

In general it is hard to find the eigenvalues of a density matrix such as 2.81, but in this case this can be done analytically. The eigenvalues λ_n of the reduced density matrix ρ_A are obtained from the eigenvalue problem equation

$$\int dx'\,\rho_A(x,x')f_n(x') = \lambda_n\, f_n(x), \tag{2.83}$$

where $f_n(x)$ is the eigenfunction corresponding to the eigenstate λ_n. The equation is easier to solve when we we use the identity

$$\sum_n \frac{w^n}{n!}H_n(x)H_n(y) = \frac{1}{\sqrt{1-4w^2}}\,\exp\left\{\frac{2w\,[2w(x^2+y^2)-2xy]}{4w^2-1}\right\}, \tag{2.84}$$

which is valid for $|w|<1/2$, to express the density matrix as

$$\rho_A(x,x') = \sqrt{\frac{\alpha}{\pi}}\,(1-z)\,e^{-\frac{\alpha}{2}(x^2+x'^2)}\sum_n \frac{z^n}{2^n n!}H_n(\sqrt{\alpha}x)H_n(\sqrt{\alpha}x'), \tag{2.85}$$

where $\alpha = \sqrt{\omega_+\omega_-}$ and

$$z = \frac{\eta}{\alpha+\gamma}\,. \tag{2.86}$$

Then with the orthogonality relation for the Hermite polynomials

$$\int_{-\infty}^{\infty} du\, e^{-u^2} H_n(u) H_m(u) = \sqrt{\pi}\, 2^n\, n!\, \delta_{n,m}, \tag{2.87}$$

we find the eigenfunctions and eigenvalues of the density matrix

$$f_n(x) = H_n(\sqrt{\alpha}x)\, e^{-\frac{\alpha}{2}x^2} \text{ and} \tag{2.88}$$

$$\lambda_n = (1-z)z^n, \tag{2.89}$$

where $n = 0, 1, 2, \ldots$. Once we have the eigenvalues, it is straightforward to calculate the entropies. We use the expression 2.39 to compute the entanglement entropy between the particles

$$S(\rho_A) = -(1-z)\left(\log(1-z)\sum_n z^n + \log(z)\sum_n n\, z^n\right) \tag{2.90}$$

$$= -(1-z)\left[\log(1-z)\sum_n z^n + \log(z)\sum_n \left(\frac{d}{dz}z^{n+1} - z^n\right)\right] \tag{2.91}$$

$$= -(1-z)\left\{\frac{\log(1-z)}{1-z} + \log(z)\left[\frac{d}{dz}\left(\frac{z}{1-z}\right) - \frac{1}{1-z}\right]\right\} \tag{2.92}$$

$$= -\log(1-z) - \frac{z}{1-z}\log(z). \tag{2.93}$$

The Rényi entropies, defined in equation 2.49, are also easy to compute when we have the eigenvalues. In order to compute the n-th Rényi entropy we need the following trace

$$\mathrm{Tr}_A(\rho_A^n) = \sum_j \left[(1-z)\, z^j\right]^n \tag{2.94}$$

$$= \frac{(1-z)^n}{1-z^n}\,. \tag{2.95}$$

In particular, the second Rényi entropy is given by

$$S_2(\rho_A) = -\log\left[\frac{(1-z)^2}{1-z^2}\right] \tag{2.96}$$

$$= -\log(1-z) + \log(1+z) \tag{2.97}$$

or, in terms of the ω_+ and ω_- parameters,

$$S_2(\rho_A) = -\log\left(\frac{2\sqrt{\omega_+\omega_-}}{\omega_+ + \omega_-}\right). \tag{2.98}$$

Moreover, the entanglement entropy can also be obtained using the Rényi entropy in the limit $\alpha \to 1$. In this case we use equation 2.57 to find

$$S(\rho_A) = \lim_{\alpha\to 1} \frac{1}{1-\alpha} \log \mathrm{Tr}\left(\sum_n \lambda_n^\alpha\right) \tag{2.99}$$

$$= \lim_{\alpha\to 1} \frac{1}{1-\alpha} \left[\alpha \log(1-z) - \log(1-z^\alpha)\right] \tag{2.100}$$

$$= -\log(1-z) - \frac{z}{1-z}\log(z). \tag{2.101}$$

Finally, with the expression for the trace $\mathrm{Tr}_A(\rho_A^2)$ we can compute the linear entropy defined in 2.62. In terms of the z parameter we obtain

$$S_L(\rho_A) = 1 - \mathrm{Tr}_A(\rho_A^2) = \frac{2z}{1+z}\ , \tag{2.102}$$

and in terms of the ω_+ and ω_- parameters the linear entropy is

$$S_L(\rho_A) = \frac{(\sqrt{\omega_+} - \sqrt{\omega_-})^2}{\omega_+ + \omega_-}\ . \tag{2.103}$$

If we try to express the entanglement entropy in terms of the parameters ω_+ and ω_-, or in terms of the Hamiltonian 2.72 parameters k and g, we will find a very complicated function. In Fig. 2.1 we show how the entanglement entropy curve looks like as a function of g for different values of k. In all cases, $S(\rho_A) = 0$ when the interaction parameter g vanishes, and the curves grow logarithmically with g. We can see that the curves take even longer to grow when the parameter k is increased - entanglement as a function of k, with fixed g, decreases exponentially. Moreover, since we are dealing with continuous coordinates there are infinite space modes and the entanglement entropy has no upper bound.

Now we want to compare the entanglement measures using the parameter z defined in equation 2.86. Before analysing the plots in Fig. 2.2, we remind that z is bounded. The lower bound, $z = 0$, is reached when $\eta = 0$, and with the definition of η given in equation 2.82, we find that $\eta = 0$ implies $\omega_+ = \omega_-$. The last equality holds only when $g = 0$, therefore $z = 0$ when the particles are not entangled at all. Moreover, the upper bound, $z = 1$, is achieved when the numerator equals the denominator, i.e. when $\eta = \alpha + \gamma$. From the definitions

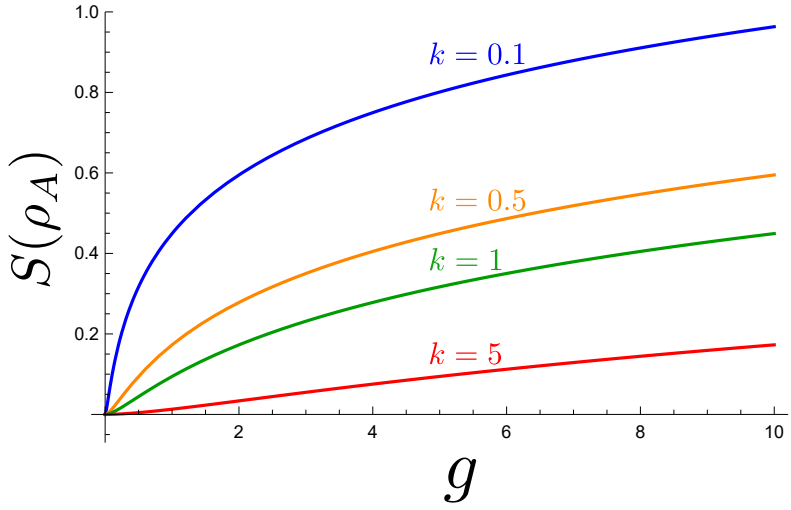

Figura 2.1: Entanglement entropy for the coupled harmonic oscillator 2.72 in terms of the interaction parameter g for different values of the parameter k, which is the square of the frequency that traps the particles.

$\gamma = \eta + \frac{2\omega_+\omega_-}{\omega_+ + \omega_-}$ and $\alpha = \sqrt{\omega_+\omega_-}$, we find that $z = 1$ when $k = 0$. Therefore, we have $z = 1$ when the only potential acting on the particles is the one proportional to g, which generates the entanglement.

In Fig. 2.2, we have the entanglement entropy, the second Rényi entropy and the linear entropy as function of the parameter z. As expected, when $z = 0$, i.e. $g = 0$, all the entropies vanish because particles A and B are not entangled anymore. Moreover, the entanglement entropy and the second Rényi entropy diverge to $+\infty$ when $z \to 1$, which corresponds to the $k \to 0$ limit. This limit corresponds to a system where there is only the mutual interaction, proportional to $(x_A - x_B)^2$. The wave function in this case will still be a Gaussian in the x_- coordinate, and a wave packet in the x_+ coordinate. The wave function for the center of mass x_+ spreads out to infinity with norm equal to unit.

On the other hand, as we have discussed in previous sections, the linear entropy remains finite everywhere, and reaches its maximum when $z = 1$. Another aspect of these plots is that the linear entropy and the Rényi entropy can only be considered as good approximations to the entanglement entropy when z is close

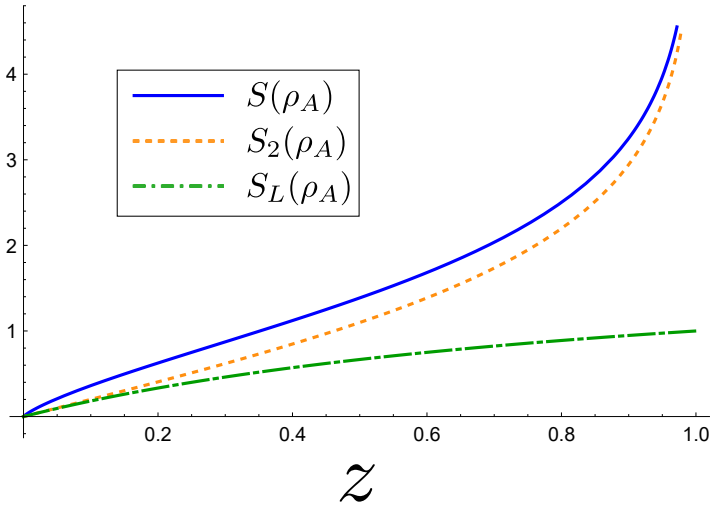

Figura 2.2: Entanglement entropy, second Rényi entropy and linear entropy for the coupled harmonic oscillator 2.72 in terms of the parameter $z = \eta/(\alpha + \gamma)$, which is bounded between 0 and 1. We have these bounds in z because the terms η, α and γ are non negative, and because $\gamma = \eta + (2\omega_+\omega_-)/(\omega_+ + \omega_-)$. All entropies vanish when $z \to 0$ or, in terms of the Hamiltonian parameters, when $g \to 0$.

to zero, i.e. when the entanglement strength is small.

Chapter 3

Path Integrals

Quantum mechanics has different equivalent formulations, the most common are the Schrödinger and Heisenberg formulations. In this chapter, we present the Feynman path integrals, which allow us to describe the basic objects of the quantum theory. The path integrals are a natural environment for discretization, and there are several numerical methods to compute them, e.g. Monte Carlo and stochastic quantization.

3.1 Derivation and basic properties

In quantum mechanics and quantum field theory, the transition amplitude between two states is often a useful quantity. Consider a non-relativistic particle in $1+1$ dimensions that evolves through the Hamiltonian H, at time t_f its state in the Schrödinger picture is given by

$$\left|\psi(x,t_f)\right\rangle = e^{-iH(t_f-t_i)}\left|\psi(x,t_i)\right\rangle, \tag{3.1}$$

which is the solution of the Schrödinger equation for a time-independent Hamiltonian. In the case that the Hamiltonian is time-dependent we need to write the exponential as a time-ordered product, considering that H is approximately constant in small periods of time.

The wavefunction $\psi(x,t_f) \equiv \left\langle x\middle|\psi(t_f)\right\rangle$ can be expressed in terms of transition amplitudes by inserting a complete set in space,

$$\psi(x,t_f) = \int_{-\infty}^{\infty} dy\, \langle x|\, e^{-iH(t_f-t_i)}\, |y\rangle\, \psi(y,t_i). \tag{3.2}$$

In this equation the wavefuntion $\psi(x, t_f)$ is obtained as the sum of contributions from wavefunctions at another time t_i coming from different positions, the contributions are proportional to the probability that the particle will evolve from position y to x. The transition amplitude $\langle x| \exp\left[-iH(t_f - t_i)\right] |y\rangle$ is our propagator, a Green's function that connects wavefunctions from different times.

The evolution of position eigenstates carry the same exponential as the states, but with opposite sign. In order to obtain this result we first remind that the position operator in the Heisenberg picture is related to the one in the Schrödinger picture by

$$\hat{x}(t) = e^{iHt}\, \hat{x}\, e^{-iHt}, \tag{3.3}$$

where $\hat{x}$ denotes the position operator at the initial time which we choose to be $t_i = 0$. This equation can be obtained by assuming that the expectation value of $\hat{x}$ at time t is independent of the picture. The eigenvalue equation for this operator is

$$\hat{x}(t)\, |x\, t\rangle = x\, |x\, t\rangle\,, \tag{3.4}$$

where $|x\, t\rangle$ denotes the position eigenvector at time t which has eigenvalue x. Explicitly writing the time dependence gives

$$e^{iHt}\, \hat{x}\, e^{-iHt}\, |x\, t\rangle = x\, |x\, t\rangle \tag{3.5}$$

$$\hat{x}\, \left(e^{-iHt}\, |x\, t\rangle\right) = x\, \left(e^{-iHt}\, |x\, t\rangle\right), \tag{3.6}$$

therefore the term in parenthesis is the eigenvector of $\hat{x}$ with eigenvalue x. Using the eigenvalue equation and the fact that $\hat{x}$ is the operator at the initial time we have

$$e^{-iHt}\, |x\, t\rangle = |x\rangle \tag{3.7}$$

$$|x\, t\rangle = e^{iHt}\, |x\rangle\,. \tag{3.8}$$

In this way, we can write the transition amplitude as

$$\langle x| \exp\left[-iH(t_f - t_i)\right] |y\rangle = \langle x\, t_f | y\, t_i\rangle\,. \tag{3.9}$$

Now we derive the path integral expression for the propagator $\langle x\, t_f | y\, t_i \rangle$. The idea is that we will express the transition amplitude to go from (y, t_i) to (x, t_f) as the sum of all paths that connect these events. To identify these paths, we are going to split time and compute the contributions of the intermediate transitions. We will see that the most relevant paths to the path integral are the ones closer to the classical path, obtained by minimizing the action.

By splitting the time interval $t_f - t_i$ in N parts of size ϵ, i.e. $t_f - t_i = N\epsilon$,

$$\langle x\, t_f | y\, t_i \rangle = \langle x | \, e^{-iH\epsilon} \cdots e^{-iH\epsilon} \, | y \rangle \,, \tag{3.10}$$

we can insert $N-1$ complete sets between these exponentials and get

$$\langle x\, t_f | y\, t_i \rangle = \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1} \prod_{n=0}^{N-1} \langle x_{n+1} | \, e^{-iH\epsilon} \, | x_n \rangle \,, \tag{3.11}$$

where we identify $x_0 \equiv y$ and $x_N \equiv x$. Moreover, we insert N complete sets of momentum and take ϵ sufficiently small,

$$\langle x_{n+1} | \, e^{-iH\epsilon} \, | x_n \rangle = \int_{-\infty}^{\infty} dp_n \, \langle x_{n+1} | p_n \rangle \, \langle p_n | \, e^{-iH(\hat{x},\hat{p})\epsilon} \, | x_n \rangle \tag{3.12}$$

$$= \int_{-\infty}^{\infty} dp_n \, \langle x_{n+1} | p_n \rangle \, \langle p_n | x_n \rangle \, e^{-iH(x_n,p_n)\epsilon} \tag{3.13}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dp_n \, \exp\left\{ -i\epsilon \left[H(x_n, p_n) - p_n \left(\frac{x_{n+1} - x_n}{\epsilon} \right) \right] \right\}. \tag{3.14}$$

Therefore

$$\langle x_{n+1} | \, e^{-iH\epsilon} \, | x_n \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} dp_n \, \exp[i\epsilon \left(-p_n \dot{x}_n + H(x_n, p_n) \right)] \,, \tag{3.15}$$

where the dot in $\dot{x}_n$ denotes a time derivative. But before putting this expression in the full transition amplitude 3.11, note that if the Hamiltonian has the form

$$H = \frac{p^2}{2m} + V(x), \tag{3.16}$$

we can explicitly perform the integral over momentum,

$$\langle x_{n+1} | \, e^{-iH\epsilon} \, | x_n \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} dp_n \, \exp\left\{ -i\epsilon \left[\frac{p_n^2}{2m} + V(x_n) - p_n \left(\frac{x_{n+1} - x_n}{\epsilon} \right) \right] \right\} \tag{3.17}$$

$$= \left(\frac{m}{2\pi i \epsilon} \right)^{1/2} \exp\left\{ i\epsilon \left[\frac{m}{2} \left(\frac{x_{n+1} - x_n}{\epsilon} \right)^2 - V(x_n) \right] \right\}. \tag{3.18}$$

Back to the initial expression 3.11 for the transition amplitude, the product will become a sum in the exponential. Taking the continuum limit $\epsilon \to 0$ in the exponentials, we find $(x_{n+1} - x_n)/\epsilon \to \dot{x}_n$ and the sum becomes an integral. Then we identify the Lagrangian $\mathcal{L}$ that will appear in the exponential, and obtain the following for the transition amplitude,

$$\langle x\, t_f | y\, t_i \rangle = \left(\frac{m}{2\pi i\epsilon}\right)^{N/2} \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1}\, \exp\left\{ i \int_{t_i}^{t_f} dt\, \mathcal{L}(x, \dot{x}) \right\} \tag{3.19}$$

$$\equiv \int_{x(t_i)=y}^{x(t_f)=x} [\mathcal{D}x]\, \exp\left\{ i \int_{t_i}^{t_f} dt\, \mathcal{L}(x, \dot{x}) \right\}, \tag{3.20}$$

where we have enclosed in $[\mathcal{D}x]$ all the integration measures at intermediate times and we have explicitly written the boundary conditions. This is the path integral expression for the transition amplitude, which can be made shorter as just

$$\langle x\, t_f | y\, t_i \rangle = \int_{x(t_i)=y}^{x(t_f)=x} [\mathcal{D}x]\, e^{iI[x]}, \tag{3.21}$$

where $I[x]$ is the action for the Lagrangian $\mathcal{L}(x, \dot{x})$.

With the purpose of giving a reasonable physical interpretation to this expression, we perform Euclidean rotation in our time, i.e. we make $t \to t' = -i\tau$, with $\tau \in \mathbb{R}$. Then we assume the imaginary time is a line in the complex plane where time runs. This interpretation is valid as long as the quantity of interest has no poles in the complex plane.

Assuming the Lagrangian has the from

$$\mathcal{L}(x, \dot{x}) = \frac{m}{2} \left(\frac{\partial x}{\partial t}\right)^2 - V(x), \tag{3.22}$$

under the change of variables $\tau \equiv it$ the action becomes

$$I[x] = \int_{\tau_i}^{\tau_f} d(-i\tau) \left\{ \frac{m}{2} \left[\frac{\partial x}{\partial(-i\tau)}\right]^2 - V(x) \right\} \tag{3.23}$$

$$= i \int_{\tau_i}^{\tau_f} d\tau \left[\frac{m}{2} \left(\frac{\partial x}{\partial \tau}\right)^2 + V(x) \right] \tag{3.24}$$

$$\equiv i\, I_E[x], \tag{3.25}$$

where we define $I_E[x]$ as the Euclidean action. Using this expression, we obtain the Euclidean path integral

$$\langle x\,\tau_f | y\,\tau_i \rangle = \int_{x(\tau_i)=y}^{x(\tau_f)=x} [\mathcal{D}x]\; e^{-I_E[x]}. \tag{3.26}$$

This integral indicates that we sum over all the paths that connects (y, τ_i) to (x, τ_f), and the most relevant paths are the ones with highest weight $\exp(-I_E[x])$. Therefore, the largest contribution comes from the path that minimizes the action, i.e. the classical path. Moreover, paths around the classical path are going to be the most relevant ones for the exact calculation of the path integral.

Now we show two important path integrals tools that will be used through the rest of this work: how to split, or join, path integrals and how to compute matrix elements. In the transition amplitude $\langle x\,\tau_f | y\,\tau_i \rangle$, we can insert an identity at intermediate time τ. As a result we obtain

$$\langle x\,\tau_f | y\,\tau_i \rangle = \int_{-\infty}^{\infty} dq\, \langle x\,\tau_f | q\,\tau \rangle\, \langle q\,\tau | y\,\tau_i \rangle\,. \tag{3.27}$$

Then we express all the transition amplitudes using the path integral expression we already know,

$$\int_{x(\tau_i)=y}^{x(\tau_f)=x} [\mathcal{D}x]\; e^{-I_E[x]} = \int_{-\infty}^{\infty} dq \int_{x(\tau_i)=y}^{x(\tau)=q} [\mathcal{D}x]\; e^{-I_E[x]} \int_{x(\tau)=q}^{x(\tau_f)=x} [\mathcal{D}x]\; e^{-I_E[x]}. \tag{3.28}$$

This equation show us how one can split and join path integrals. The cost to split the transition amplitude at the intermediate time τ is that we have to put an integral over dq.

The matrix elements of an operator $\hat{O}(t)$ are obtained by inserting its eigenvalue $O(t)$ inside the path integral. For instance, if we want to compute the matrix elements $\langle x_f\,\tau_f | \,\hat{x}(t)\, | x_i\,\tau_i \rangle$ of the position operator $\hat{x}(t)$, then we put a complete set of position at the intermediate time t. Such manipulation allow us to extract the eigenvalue of the position operator

$$\langle x_f\,\tau_f | \,\hat{x}(t)\, | x_i\,\tau_i \rangle = \int_{-\infty}^{\infty} dx\; \langle x_f\,\tau_f | x\,t \rangle\, x(t)\, \langle x\,t | x_i\,\tau_i \rangle\,, \tag{3.29}$$

and then we use the integral to join the two path integrals that appear from the transition amplitudes on the RHS,

$$\langle x_f\, \tau_f |\, \hat{x}(t)\, | x_i\, \tau_i \rangle = \int_{x(\tau_i)=x_i}^{x(\tau_f)=x_f} [\mathcal{D}x]\; x(t)\, e^{-I_E[x]}\,. \tag{3.30}$$

Note that the above expression makes sense only if t is between times τ_i and τ_f. For the eigenvalue of $\hat{x}(t)$, we integrate the expression for $x_i = x_f$,

$$\langle \hat{x}(t) \rangle = \int dx \int_{x(\tau_i)=x}^{x(\tau_f)=x} [\mathcal{D}x]\; x(t)\, e^{-I_E[x]}\,. \tag{3.31}$$

Moreover, we can compute the matrix elements of a product of many operators, for instance $\langle x_f\, \tau_f |\, \hat{x}(t)\hat{x}(t')\, | x_i\, \tau_i \rangle$. Since our path integrals always evolve in the increasing time direction, we need to assure that the operators $\hat{x}(t)\hat{x}(t')$ are time ordered. For this purpose, we define the time-ordered product $T[\hat{x}(t)\hat{x}(t')]$, which gives $\hat{x}(t)\hat{x}(t')$ if $t > t'$, and $\hat{x}(t')\hat{x}(t)$ if $t' < t$. Then the matrix elements are obtained using the same idea of splitting the path integral in the intermediate times t and t',

$$\langle x_f\, \tau_f |\, T\left[\hat{x}(t)\hat{x}(t')\right]\, | x_i\, \tau_i \rangle = \int_{x(\tau_i)=x_i}^{x(\tau_f)=x_f} [\mathcal{D}x]\; x(t)x(t')\, e^{-I_E[x]}. \tag{3.32}$$

Although we have a time-ordered product on the LHS, the $x(t)$ and $x(t')$ in the RHS commute: they are just the eigenfunctions.

3.2 Free particle

In this subsection we compute the path integral for the free particle in $1+1$ dimensions,

$$H = \frac{p^2}{2m}. \tag{3.33}$$

To compute the propagator $\langle x\, t_f | y\, t_i \rangle$, we go back to the discretized expression of the path integral. We use equation 3.18 with $V(x) = 0$ in 3.11, but still do not take the continuum limit so the propagator becomes a product of many integrals

$$\langle x\, t_f | y\, t_i \rangle = \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1} \prod_{n=0}^{N-1} \left(\frac{m}{2\pi i\epsilon}\right)^{1/2} \exp\left[\frac{im}{2\epsilon}(x_{n+1} - x_n)^2\right] \tag{3.34}$$

$$\equiv \left(\frac{m}{2\pi i\epsilon}\right)^{1/2} I_{N-1}. \tag{3.35}$$

We defined in the last line a new object that encloses all integrals,

$$I_k = \left(\frac{m}{2\pi i\epsilon}\right)^{k/2} \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_k \, e^{\frac{im}{2\epsilon}(x_1-x_0)^2} \cdots e^{\frac{im}{2\epsilon}(x_{k+1}-x_k)^2}. \tag{3.36}$$

With this definition we use induction to prove that, for $k \in \mathbb{N}$,

$$I_k = \frac{1}{\sqrt{k+1}} \exp\left[\frac{im}{2\epsilon(k+1)}(x_{k+1}-x_0)^2\right]. \tag{3.37}$$

Starting with I_1,

$$I_1 = \left(\frac{m}{2\pi i\epsilon}\right)^{1/2} \int_{-\infty}^{\infty} dx_1 \exp\left\{\frac{im}{2\epsilon}\left[(x_1-x_0)^2 + (x_2-x_1)^2\right]\right\} \tag{3.38}$$

$$= \left(\frac{m}{2\pi i\epsilon}\right)^{1/2} \exp\left[\frac{im}{2\epsilon}(x_2^2+x_0^2)\right] \int_{-\infty}^{\infty} dx_1 \exp\left[\frac{im}{\epsilon}x_1^2 - \frac{im}{\epsilon}(x_2+x_0)x_1\right] \tag{3.39}$$

$$= \sqrt{\frac{1}{2}} \exp\left[\frac{im}{2\epsilon\cdot 2}(x_2-x_0)^2\right]. \tag{3.40}$$

The first step has the form we want, it matches with 3.37 with $k = 1$. Assuming 3.37 works for $k-1$, we show it also works for k:

$$I_k = \left(\frac{m}{2\pi i\epsilon}\right)^{1/2} \int_{-\infty}^{\infty} dx_k \, I_{k-1} \exp\left[\frac{im}{2\epsilon}(x_{k+1}-x_k)^2\right] \tag{3.41}$$

$$= \left(\frac{m}{2\pi i\epsilon k}\right)^{1/2} \int_{-\infty}^{\infty} dx_k \exp\left[\frac{im}{2\epsilon k}(x_k-x_0)^2 + \frac{im}{2\epsilon}(x_{k+1}-x_k)^2\right] \tag{3.42}$$

$$= \left(\frac{m}{2\pi i\epsilon k}\right)^{1/2} \exp\left[\frac{im}{2\epsilon k}(x_0^2 + k x_{k+1}^2)\right]$$

$$\times \int_{-\infty}^{\infty} dx_k \exp\left[\frac{im(k+1)}{2\epsilon k}x_k^2 - \frac{im}{2\epsilon k}(x_0 + k\, x_{k+1})x_k\right] \tag{3.43}$$

$$= \frac{1}{\sqrt{k+1}} \exp\left[\frac{im}{2\epsilon k}(x_{k+1}-x_0)^2\right]. \tag{3.44}$$

Now that we know the identity 3.37 is true for $k \in \mathbb{N}$, we use it with $k = N-1$ and go back to the propagator

$$\langle x\, t_f | y\, t_i\rangle = \left(\frac{m}{2\pi i\epsilon}\right)^{1/2} I_{N-1} \tag{3.45}$$

$$= \sqrt{\frac{m}{2\pi i\epsilon N}} \exp\left[\frac{im}{2\epsilon N}(x_N-x_0)^2\right]. \tag{3.46}$$

By definition, the product ϵN is equal to the difference $t_f - t_i$. Moreover $x_N = x_f$ and $x_0 = x_i$ are the coordinates of the endpoints, then we find that the propagator

of the free particle in $1+1$ dimensions is

$$\langle x\, t_f | y\, t_i \rangle = \sqrt{\frac{m}{2\pi i (t_f - t_i)}} \exp\left[\frac{im}{2(t_f - t_i)}(x_f - x_i)^2\right]. \tag{3.47}$$

To obtain the Euclidean propagator, we just change the real times for imaginary time $\tau = it$,

$$\langle x\, t_f | y\, t_i \rangle = \sqrt{\frac{m}{2\pi (\tau_f - \tau_i)}} \exp\left[\frac{-m}{2(\tau_f - \tau_i)}(x_f - x_i)^2\right]. \tag{3.48}$$

3.3 Harmonic oscillator

In this subsection we give another example and compute the propagator for the $1+1$ dimensional simple harmonic oscillator,

$$\langle x_f\, t_f | x_i\, t_i \rangle = \int_{x(t_i)=x_i}^{x(t_f)=x_f} [\mathcal{D}x] \exp\left[i \int_{t_i}^{t_f} dt \left(\frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2\right)\right]. \tag{3.49}$$

We split the paths as $x = x_{cl} + y$, where x_{cl} is the classical path that connects (x_i, t_i) and (x_f, t_f) and y is the quantum fluctuation from x_{cl}, it has boundary conditions $y(t_i) = 0$ and $y(t_f) = 0$ because x and x_{cl} coincide at the endpoints.

The classical path is defined as the solution that minimizes the action, which is found by solving the Lagrange-Euler equations with boundary conditions $x_{cl}(t_i) = x_i$ and $x_{cl}(t_f) = x_f$. The integration measure for the path integral has contributions only from the y paths, $[\mathcal{D}x] = [\mathcal{D}y]$, so we can put the terms that only involves x_{cl} outside the path integral. The action for the new variables is

$$\begin{aligned} I[x] &= I[x_{cl} + y] && (3.50)\\ &= \int_{t_i}^{t_f} dt \left[\left(\frac{1}{2}\dot{x}_{cl}^2 - \frac{1}{2}\omega^2 x_{cl}^2\right) + \frac{1}{2}\dot{y}^2 - \frac{1}{2}\omega^2 y^2 + \dot{x}_{cl}\dot{y} - \omega^2 x_{cl} y\right] && (3.51)\\ &= I[x_{cl}] + \int_{t_i}^{t_f} dt \left[\frac{1}{2}\dot{y}^2 - \frac{1}{2}\omega^2 y^2 + \dot{x}_{cl}\dot{y} - \omega^2 x_{cl} y\right]. && (3.52) \end{aligned}$$

The last two terms in the action vanish,

$$\int_{t_i}^{t_f} dt \left(\dot{x}_{cl}\dot{y} - \omega^2 x_{cl} y\right) = \int_{t_i}^{t_f} dt \left[\frac{d}{dt}\left(\dot{x}_{cl} y\right) - \ddot{x}_{cl} y - \omega^2 x_{cl} y\right] \tag{3.53}$$

$$= \left(\dot{x}_{cl} y\right)\Big|_{t_i}^{t_f} - \int_{t_i}^{t_f} dt \left(\ddot{x}_{cl} + \omega^2 x\right) y \tag{3.54}$$

$$= 0. \tag{3.55}$$

The first term is zero due to the boundary conditions for y and the second because x_{cl} solves the Lagrange-Euler equation $\ddot{x}_{cl} = -\omega^2 x_{cl}$. Then the transition amplitude becomes

$$\left\langle x_f\, t_f \middle| x_i\, t_i \right\rangle = e^{iI[x_{cl}]} \int_{y(t_i)=0}^{y(t_f)=0} [\mathcal{D}y] \exp\left[i \int_{t_i}^{t_f} dt \left(\frac{1}{2}\dot{y}^2 - \frac{1}{2}\omega^2 y^2\right)\right]. \tag{3.56}$$

The path integral over y is periodic, so it does not depend on the endpoints x_i and x_f. All the spatial part contributions come from the exponential fo the classical action.

The classical path, solution to the Lagrange-Euler equation, is

$$x_{cl}(t) = A\cos(\omega t) + B\sin(\omega t), \tag{3.57}$$

with A and B determined by the boundary conditions. Since the equations of motion are invariant under time translation, the propagator can depend only on the difference of times $T = t_f - t_i$ and we can take the boundary conditions to be $x_{cl}(0) = x_i$ and $x_{cl}(T) = x_f$. Therefore the constants are

$$A = x_i \text{ and } B = \frac{x_f - x_i\cos(\omega T)}{\sin(\omega T)}. \tag{3.58}$$

Now we can obtain the classical action that appears on the transition amplitude expression,

$$I[x_{cl}] = \int_0^T dt \left(\frac{1}{2}\dot{x}_{cl} - \frac{1}{2}\omega^2 x_{cl}^2\right) \tag{3.59}$$

$$= -\frac{\omega}{4}\sin(2\omega T)(A^2 - B^2) - \omega\sin^2(\omega T)AB \tag{3.60}$$

$$= \frac{\omega}{2\sin(\omega T)}\left[(x_i^2 + x_f^2)\cos(\omega T) - 2x_i x_f\right]. \tag{3.61}$$

We write $\exp(iI[x_{cl}])$ to find that the transition amplitude is

$$\langle x_f\, t_f | x_i\, t_i \rangle = F(T) \exp\left\{ \frac{i\omega}{2\sin(\omega T)} \left[(x_i^2 + x_f^2)\cos(\omega T) - 2x_i x_f \right] \right\}, \tag{3.62}$$

where $F(T)$ is the periodic path integral for the quantum fluctuation $y(t)$,

$$F(T) = \int_{y(0)=0}^{y(T)=0} [\mathcal{D}y] \exp\left[i \int_0^T dt \left(\frac{1}{2}\dot{y}^2 - \frac{1}{2}\omega^2 y^2 \right) \right] \tag{3.63}$$

$$= \int_{y(0)=0}^{y(T)=0} [\mathcal{D}y] \exp\left[i \int_0^T dt \left(\frac{1}{2}\frac{d}{dt}(\dot{y}y) - \frac{1}{2}\ddot{y}y - \frac{1}{2}\omega^2 y^2 \right) \right] \tag{3.64}$$

$$= \int_{y(0)=0}^{y(T)=0} [\mathcal{D}y] \exp\left[i \int_0^T dt - \frac{1}{2} y \left(\frac{\partial^2}{\partial t^2} + \omega^2 \right) y \right]. \tag{3.65}$$

In order to perform this integral, we expand the quantum fluctuations in eigenfunctions of the operator $\hat{O} = -\frac{1}{2}\left(\frac{\partial^2}{\partial t^2} + \omega^2\right)$,

$$y(t) = \sum_n a_n y_n(t). \tag{3.66}$$

The eigenfunctions $y_n(t)$ are orthogonal and have eigenvalues λ_n,

$$y_n(t) = \sqrt{\frac{2}{T}} \sin\left(\frac{n\pi t}{T} \right) \tag{3.67}$$

$$\lambda_n = \frac{1}{2}\left[\left(\frac{n\pi}{T} \right)^2 - \omega^2 \right]. \tag{3.68}$$

Since all the coordinate dependence is in the a_n, the new integration measure of the path integral is just a product of the da_n times a normalization constant C. This normalization constant does not depend on ω, we will use this fact later to fix C. Gives these considerations,

$$F(T) = C \prod_{n=1}^{N} \int_{-\infty}^{\infty} da_n \exp\left\{ \frac{i}{T} \left[\left(\frac{n\pi}{T} \right)^2 - \omega^2 \right] \left[\int_0^T dt\, \sin^2\left(\frac{n\pi t}{T} \right) \right] a_n^2 \right\} \tag{3.69}$$

$$= C \prod_{n=1}^{N} \int_{-\infty}^{\infty} da_n \exp\left\{ \frac{i}{2} \left(\frac{n\pi}{T} \right)^2 \left[1 - \left(\frac{\omega T}{n\pi} \right)^2 \right] a_n^2 \right\} \tag{3.70}$$

$$= C \prod_{n=1}^{N} \left[\frac{T\sqrt{2\pi i}}{n\pi} \right] \prod_{n=1}^{N} \left[1 - \left(\frac{\omega T}{n\pi} \right)^2 \right]^{-1/2}. \tag{3.71}$$

We can include the first product in the constant C and it still does not depend on ω. Moreover, we take the continuum limit $N \to \infty$ in the second product and

obtain

$$F(T) = C\sqrt{\frac{\omega T}{\sin(\omega T)}}. \tag{3.72}$$

The constant C can be obtained by taking $\omega \to 0$. In this limit the function $F(T)$ is the same as for the free particle 3.47, then we fix

$$C = \sqrt{\frac{1}{2\pi i T}}. \tag{3.73}$$

Finally, the path integral for the quantum fluctuations is

$$F(T) = \sqrt{\frac{\omega}{2\pi i \sin(\omega T)}} \tag{3.74}$$

and the full expression for the propagator of the $1+1$ dimensional harmonic oscillator 3.62 in terms of $T = t_f - t_i$ is

$$\langle x_f\, t_f | x_i\, t_i \rangle = \sqrt{\frac{\omega}{2\pi i \sin(\omega T)}} \exp\left\{ \frac{i\omega}{2\sin(\omega T)} \left[(x_i^2 + x_f^2)\cos(\omega T) - 2x_i x_f \right] \right\}. \tag{3.75}$$

The Euclidean propagator, for $T = \tau_f - \tau_i$, is given by

$$\langle x_f\, \tau_f | x_i\, \tau_i \rangle = \sqrt{\frac{\omega}{2\pi \sinh(\omega T)}} \exp\left\{ \frac{-\omega}{2\sinh(\omega T)} \left[(x_i^2 + x_f^2)\cosh(\omega T) - 2x_i x_f \right] \right\}. \tag{3.76}$$

Chapter 4

Ground state path integral

In quantum information theory, one can obtain information about entanglement from the density matrix. As we have seen, for a pure state $|\phi\rangle$ the density matrix has a simple form $\rho = |\phi\rangle\langle\phi|$. In this chapter, we will show how to express entanglement in terms of path integrals, which is a suitable formalism to deal with large systems that can be discretized.

The cases we are interested are those with a pure ground state, and only the constituent parts can be mixed states. We start by deriving an expression for the wave function and density matrix in terms of path integrals for a generic two-particle Hamiltonian. Finally, we discuss how to compute the second Rényi entropy and the linear entropy without diagonalization using path integrals.

4.1 Wave function and density matrix

In chapter 3, we expressed transition amplitudes in terms of path integrals. Therefore in order to find how wave functions relate to path integrals, we will find an equation that links transition amplitudes to wave functions. To project out the ground state wave function from the transition amplitude, it is convenient to work with imaginary time, i.e. we perform a Wick rotation $t \to -i\tau$. In the jargon of field theory, we will work in Euclidean space. The Euclidean transition amplitude from events (y, τ_i) to (x, τ_f) can be written as

$$\langle x\,\tau_f | y\,\tau_i\rangle = \langle x|\, e^{-\hat{H}(\tau_f-\tau_i)}\,|y\rangle \tag{4.1}$$

$$= \sum_n \langle x|\, e^{-\hat{H}(\tau_f-\tau_i)}\,|n\rangle\,\langle n|y\rangle\,, \tag{4.2}$$

where the $|n\rangle$ are a complete set of eigenstates of the Hamiltonian $\hat{H}$ which, for convenience, is supposed to have a discrete spectrum only. Then, we act with the Hamiltonian on the energy eigenstate $|n\rangle$ to obtain the corresponding eigenvalue E_n, and thereby identify the coordinate-space wave functions, $\langle x|n\rangle \equiv \psi_n(x)$. Then, the transition amplitude can be written as

$$\langle x\,\tau_f|y\,\tau_i\rangle = \sum_n \psi_n(x)\,\psi_n^*(y)\,e^{-E_n(\tau_f-\tau_i)}. \tag{4.3}$$

We already know how to express Euclidean transition amplitudes in terms of path integrals, namely:

$$\langle x\,\tau_f|y\,\tau_i\rangle = \int_{x(\tau_i)=y}^{x(\tau_f)=x} [\mathcal{D}x(\tau)]\,e^{-I_E[x]}, \tag{4.4}$$

here $I_E[x]$ is the Euclidean action of the particle,

$$I_E[x] = \int_{\tau_i}^{\tau_f} d\tau\,\mathcal{L}_E(x)\,, \tag{4.5}$$

where $\mathcal{L}_E(x)$ is the Euclidean Lagrangian. Recall that the Euclidean Lagragian is the *sum* (not the difference) of the kinetic and potential energies. Since we are interested in the ground state wave function, it is useful to consider the limit when the time difference $\tau_f - \tau_i$ is very large, because the largest contribution for the exponential in 4.3 comes from the lowest energy when $\tau_f - \tau_i$ becomes very large. For convenience of notation, we take $\tau_f = 0$ and $\tau_i = -T$ with large T, in such a way that 4.3 becomes

$$\langle x\,0|y\,-T\rangle = \psi_0(x)\,\psi_0^*(y)\,e^{-E_0\,T}. \tag{4.6}$$

Moreover, we can always redefine the Hamiltonian as $H \to H - E_0$ to have a zero energy ground state. By simply writing $E_0 = 0$ and integrating this expression in y, we obtain

$$\int_{-\infty}^{\infty} dy\,\langle x\,0|y\,-T\rangle = \psi_0(x)\left(\int_{-\infty}^{\infty} dy\,\psi_0^*(y)\right). \tag{4.7}$$

The integral in the parenthesis is just a complex number, say z. Using the path integral expression in 4.4 for $\tau_i = -T$ and $\tau_f = 0$:

$$\langle x\,0|y\,-T\rangle = \int_{x(-T)=y}^{x(0)=x} [\mathcal{D}x]\,e^{-I_E[x]}, \tag{4.8}$$

we obtain for the ground-state wave function the following expression:

$$\psi_0(x) = \frac{1}{z}\int_{-\infty}^{\infty} dy \int_{x(-T)=y}^{x(0)=x} [\mathcal{D}x]\, e^{-I_E[x]}. \tag{4.9}$$

Another way to deal with the y on the path integral is to choose a constant value for it right from the beginning in 4.6, e.g. we can choose $y = c$. Then there is no need to integrate over y in what follows and $\psi^*(c)$ will be obtained afterwards through normalization. In this case the only tricky part is that we have to choose c such that $\psi_0(c)$ have finite overlap.

Now that we have the wave function, it is straightforward to obtain the density matrix elements. With the purpose of making the notation lighter, we omit the integral over the boundary condition at $x(-T) = c$ from the whole equation

$$\psi_0(x) = \frac{1}{z}\int_{x(-T)=c}^{x(0)=x} [\mathcal{D}x]\, e^{-I_E[x]}, \tag{4.10}$$

meaning that at the initial time $\tau = -T$ we sum over all possible initial positions or that we choose a constant value for y. For the complex conjugate, we start with the propagator $\langle y\, T|x\, 0\rangle$ and obtain

$$\psi_0^*(x) = \frac{1}{z'}\int_{x(0)=x}^{x(T)=c} [\mathcal{D}x]\, e^{-I_E[x]}. \tag{4.11}$$

The boundary condition at $\tau = T$ has to be the same as the one chosen for $\tau = -T$ in the wavefuntion, i.e. $x(T) = x(-T) = c$.

The matrix elements of the ground state density matrix $\rho = |\psi_0\rangle\langle\psi_0|$ in position representation are

$$\begin{aligned}
\rho(x, x') &= \psi_0(x)\psi_0^*(x') && (4.12)\\
&= \frac{1}{Z}\int_{x(-T)=c}^{x(0)=x} [\mathcal{D}x]\, e^{-I_E[x]} \int_{x(0)=x'}^{x(T)=c} [\mathcal{D}x]\, e^{-I_E[x]} && (4.13)\\
&\equiv \frac{1}{Z}\int_{x(-T)=c}^{x(0)=x} \int_{x(0)=x'}^{x(T)=c} [\mathcal{D}x]\, e^{-I_E[x]}, && (4.14)
\end{aligned}$$

where Z is the normalization factor and in the last line we defined a short notation for the product of two path integrals. In this expression if $x \neq x'$ then there is a discontinuity in the path integral at $\tau = 0$ because while one path integral

requires $x(0) = x'$, the other requires $x(0) = x$. For this reason we split $\tau = 0$ in two, $\tau = -\epsilon$ and $\tau = \epsilon$ in such a way that we can satisfy both conditions at different times,

$$\rho(x, x') = \frac{1}{Z} \int_{x(-T)=c}^{x(-\epsilon)=x} \int_{x(\epsilon)=x'}^{x(T)=c} [\mathcal{D}x]\, e^{-I_E[x]}. \tag{4.15}$$

As a notation, one can use Dirac deltas to express the density matrix as a full path integral from $-T$ to T with special boundary conditions inserted at $-\epsilon$ and ϵ,

$$\rho(x, x') = \frac{1}{Z} \int_{x(-T)=c}^{x(T)=c} [\mathcal{D}x]\, \delta[x(-\epsilon) = x]\, \delta[x(\epsilon) = x']\, e^{-I_E[x]}. \tag{4.16}$$

For bipartite Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ describing two particles, we need to generalize the last equations for $\Psi(x_A, x_B) \equiv \psi_0(x_A, x_B)$. Repeating the calculations above for a wave function describing two particles leads to

$$\Psi(x_A, x_B) = \frac{1}{z} \int_{x_A(-T)=c_A}^{x_A(0)=x_A} \int_{x_B(-T)=c_B}^{x_B(0)=x_B} [\mathcal{D}x_A]\, [\mathcal{D}x_B]\, e^{-I_E[x_A, x_B]}. \tag{4.17}$$

here the boundary conditions $x_A(-T) = x_A(T) = c_A$ and $x_B(-T) = x(T) = c_B$ can be either chosen or integrated. Moreover, in this case,

$$I_E[x_A, x_B] = \int_{-T}^{0} d\tau\, \mathcal{L}_E(x_A, x_B), \tag{4.18}$$

where $\mathcal{L}_E(x_A, x_B)$ is the Euclidean Lagrangian, i.e. the sum of the kinetic terms and the potentials.

In order to simplify the notation, we will use only one integral for both particles and the symbol $BC[x_A, x_B, \tau]$ to say that $x_A(\tau) = x_A$ and $x_B(\tau) = x_B$. Then the wave function and its complex conjugate for two particles are

$$\Psi(x_A, x_B) = \frac{1}{z} \int_{BC[c_A, c_B, -T]}^{BC[x_A, x_B, 0]} [\mathcal{D}x_A]\, [\mathcal{D}x_B]\, e^{-I_E[x_A, x_B]}, \tag{4.19}$$

$$\Psi^*(x_A, x_B) = \frac{1}{z'} \int_{BC[x_A, x_B, 0]}^{BC[c_A, c_B, T]} [\mathcal{D}x_A]\, [\mathcal{D}x_B]\, e^{-I_E[x_A, x_B]}. \tag{4.20}$$

Note that, for the complex conjugate, the integral inside the Euclidean action is from 0 to T, instead of the limits $-T$ to 0 that appear in the wave function.

The density matrix of the total system is $\rho = |\Psi\rangle\langle\Psi|$, and the reduced density matrix for particle A is obtained by tracing out the degrees of freedom of particle B. Thus the matrix elements in position representation of $\rho_A = \mathrm{Tr}_B\,\rho$ are

$$\rho_A(x,x') = \int_{-\infty}^{\infty} dx_B\, \Psi(x,x_B)\Psi^*(x',x_B) \tag{4.21}$$

$$= \frac{1}{Z}\int_{-\infty}^{\infty} dx_B \int_{BC[c_A,c_B,-T]}^{BC[x,x_B,-\epsilon]} \int_{BC[x',x_B,\epsilon]}^{BC[c_A,c_B,T]} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\, e^{-I_E[x_A,x_B]}. \tag{4.22}$$

Note that in this case the discontinuity in the path integral only happens for particle A. However, if the particles are entangled, it is wrong to say that the path integral for the path integral for A times the path integral for B. Therefore one cannot join the path integral of particle B at time $\tau = 0$ using the integral over dx_B. The density matrix of two particles in terms of path integrals is the product of a path integral from $-T$ to $-\epsilon$ and another from ϵ to T.

4.2 Trace of ρ_A^n

In order to compute the entanglement entropy from its definition 2.38, we would have to diagonalize the density matrix ρ to obtain $\log\rho$. This is a simple problem to solve for small and finite dimensional systems, but diagonalization is often hard to implement for infinite or large dimensional systems. For these cases it is easier to calculate the Rényi entropies from definition 2.49, or the linear entropy.

In section 2.4, we have demonstrated equation 2.57, which shows that in the limit $n \to 1$ the nth Rényi entropy $S_n(\rho_A)$ corresponds to the von Neumann entanglement entropy. Since we are interested in the entanglement between parts A and B in a bipartite Hilbert space with the full system in a pure ground state, the equivalent of equation 2.57 in this case is

$$S(\rho_A) = \lim_{n\to 1} S_n(\rho_A) = -\lim_{n\to 1}\frac{\partial}{\partial n}\log[\mathrm{Tr}_A(\rho_A^n)]. \tag{4.23}$$

Note that the log in $\log[\mathrm{Tr}_A(\rho_A^n)]$ is not problematic here because $\mathrm{Tr}_A(\rho_A^n)$ is a number, for this reason we do not have to worry about diagonalizations when using the replica trick. In what follows we focus on the trace of ρ_A^n, then specify

to $n = 2$, which is the power that appears in the second Rényi entropy and linear entropy. These entanglement measures are lower bound approximations to the entanglement entropy, as we have already discussed in 2.4.2.

For two particles in a quantum mechanics system, first we have to compute the reduced density matrix using the path integrals in equation 4.22, then for the $\mathrm{Tr}_A(\rho_A^n)$ we need to perform n integrals:

$$\mathrm{Tr}_A(\rho_A^n) = \int dx_1 \, \langle x_1 | \, \rho_A^n \, | x_1 \rangle \tag{4.24}$$

$$= \int dx_1 \int dx_2 \cdots \int dx_n \, \rho_A(x_1, x_2) \rho_A(x_2, x_3) \ldots \rho_A(x_n, x_1) \tag{4.25}$$

$$= \prod_{j=1}^{n} \int_{-\infty}^{\infty} dx_j \, \rho_A(x_j, x_{j+1}), \tag{4.26}$$

from the first to the second line we have inserted $n-1$ identities and in the third line we consider the identification $x_{n+1} \equiv x_1$. A generic term in the product is

$$\rho_A(x_j, x_{j+1}) = \frac{1}{Z} \int_{-\infty}^{\infty} dx_B \int_{BC[c_A, c_B, -T]}^{BC[x_j, x_B, -\epsilon]} \int_{BC[x_{j+1}, x_B, \epsilon]}^{BC[c_A, c_B, T]} \left[\mathcal{D}x_A^j\right] \left[\mathcal{D}x_B^j\right] e^{-I_E[x_A^j, x_B^j]}. \tag{4.27}$$

Now we specify for $n = 2$, i.e. $\mathrm{Tr}\left(\rho_A^2\right)$, which appears in the calculations of the purity, linear entropy and second Rényi entropy,

$$\mathrm{Tr}_A(\rho_A^2) = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \, \rho_A(x_1, x_2) \, \rho_A(x_2, x_1) \tag{4.28}$$

$$= \frac{1}{Z^2} \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2$$
$$\times \int_{BC[c_A, c_B, -T]}^{BC[x_1, y_1, -\epsilon]} \int_{BC[x_2, y_1, \epsilon]}^{BC[c_A, c_B, T]} \left[\mathcal{D}x_A^1\right] \left[\mathcal{D}x_B^1\right] e^{-I_E[x_A^1, x_B^1]}$$
$$\times \int_{BC[c_A, c_B, -T]}^{BC[x_2, y_2, -\epsilon]} \int_{BC[x_1, y_2, \epsilon]}^{BC[c_A, c_B, T]} \left[\mathcal{D}x_A^2\right] \left[\mathcal{D}x_B^2\right] e^{-I_E[x_A^2, x_B^2]}. \tag{4.29}$$

Next we will consider the coupled harmonic oscillator Hamiltonian and perform the calculations analytically, which can be done in this case. Before that, we review the main approximations to the entanglement entropy. One can use the second Rényi entropy as an approximation to the entanglement entropy, we obtain this expression starting from equation 4.23 and approximating the derivative as the difference $\log\left(\mathrm{Tr}_A \, \rho_A^2\right) - \log(\mathrm{Tr}_A \, \rho_A)$. One can also use the linear entropy

to approximate the entanglement entropy: in this case we write the $\log(\rho)$ as a power series and take only the first term, then $\log(\rho) \approx \rho - 1$. These approximations, however, are only valid for weak entanglement regime. In any case, the second Rényi entropy and the linear entropy are important entanglement measures that satisfy interesting properties listed in 2, and in some cases they can be probed experimentally.

4.3 Coupled harmonic oscillators II

In this section we revisit the example of coupled harmonic oscillators that has already been discussed in section 2.5. We will calculate again the quantities obtained in that section, but now using path integrals and no diagonalization.

The full system has Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ where A and B refers to the particles, it evolves through the Hamiltonian

$$H = \frac{1}{2}\left[p_A^2 + p_B^2 + k(x_A^2 + x_B^2) + g(x_A - x_B)^2\right], \tag{4.30}$$

and we are interested in the entanglement between the particles when the system is in the ground state. Since we are going to use path integrals, we should first compute the propagator for the coupled harmonic oscillators. If we use center of mass and relative coordinates $x_+ = (x_A + x_B)/\sqrt{2}$ and $x_- = (x_A - x_B)/\sqrt{2}$, the Hamiltonian decouples in two simple harmonic oscillators as in equation 2.75. We can use this fact to factorize the propagator for the coupled harmonic oscillator in two propagators of simple harmonic oscillators.

More precisely, the transition amplitude to have, in the time interval $T = \tau_f - \tau_i$, particle A going from x_i to x_f and particle B going from y_i to y_f is

$$\langle x_f\, y_f\, \tau_f | x_i\, y_i\, \tau_i \rangle_{\text{CHO}} = \langle x_{+f}\, \tau_f | x_{+i}\, \tau_i \rangle_{\text{SHO}} \times \langle x_{-f}\, \tau_f | x_{-i}\, \tau_i \rangle_{\text{SHO}} \quad , \tag{4.31}$$

where CHO stands for coupled harmonic oscillator and SHO for simple harmonic oscillator. The transition amplitude for a simple harmonic oscillator has already been computed in section 3.3, the Euclidean propagator is given in equation 3.76.

We use this expression for both x_+ and x_- coordinates and then go back to the original variables x and y, for particles A and B, to find that the coupled harmonic oscillator propagator is

$$\begin{aligned}\langle x_f\, y_f\, \tau_f | x_i\, y_i\, \tau_i \rangle_{\text{CHO}} = \frac{1}{2\pi}\sqrt{\frac{\omega_+\omega_-}{\sinh(\omega_+ T)\sinh(\omega_- T)}} \\ \times \exp\left\{-\frac{\omega_+}{4}\left[(x_i+y_i)^2+(x_f+y_f)^2\right]\coth(\omega_+ T)\right\} \\ \times \exp\left\{+\frac{\omega_+(x_i+y_i)(x_f+y_f)}{2\sinh(\omega_+ T)}\right\} \\ \times \exp\left\{-\frac{\omega_-}{4}\left[(x_i-y_i)^2+(x_f-y_f)^2\right]\coth(\omega_- T)\right\} \\ \times \exp\left\{+\frac{\omega_-(x_i-y_i)(x_f-y_f)}{2\sinh(\omega_- T)}\right\}, \end{aligned} \tag{4.32}$$

where $T = \tau_f - \tau_i$, $\omega_+ = \sqrt{k}$ and $\omega_- = \sqrt{k+2g}$. In what follows we will use a different notation for the CHO propagator in order to avoid confusion with the brackets,

$$\Delta^{\text{CHO}}[x_i\, y_i, \tau_i;\, x_f\, y_f,\, \tau_f] \equiv \langle x_f\, y_f\, \tau_f | x_i\, y_i\, \tau_i \rangle_{\text{CHO}}\,. \tag{4.33}$$

Now that we have the transition amplitude, we can apply the equations derived in section 4.1 to find the ground state wave function and the reduced density matrix using path integrals.

The ground state wave function for the coupled harmonic oscillators is obtained from equation 4.19. We must choose T to be very large in order to have only ground state contributions,

$$\Psi(x_A, x_B) = \frac{1}{z}\int_{BC[c_A,c_B,-T]}^{BC[x_A,x_B,0]} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\, e^{-I_E[x_A,x_B]} \tag{4.34}$$

$$= \frac{1}{z}\lim_{T\to\infty}\Delta^{\text{CHO}}[c_A\, c_B,\, -T;\, x_A\, x_B,\, 0], \tag{4.35}$$

here we have chosen the boundary conditions at $\tau = -T$ to be $x_A(-T) = c_A$ and $x_B(-T) = c_B$. We also have the same conditions at $\tau = T$, which will appear in

the conjugate wave function

$$\Psi^*(x_A, x_B) = \frac{1}{z'} \int_{BC[x_A,x_B,0]}^{BC[c_A,c_B,T]} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\, e^{-I_E[x_A,x_B]} \tag{4.36}$$

$$= \frac{1}{z'} \lim_{T\to\infty} \Delta^{\mathrm{CHO}}[x_A\, x_B,\, 0;\, c_A\, c_B,\, T], \tag{4.37}$$

in what follows we will denote all the normalization factors by $\mathcal{N}$, later they will be obtained using the fact that the density matrix has unit trace.

The reduced density matrix ρ_A of particle A is obtained by taking the trace over the coordinate x_B in the full system density matrix,

$$\rho_A(x, x') = \frac{1}{\mathcal{N}} \lim_{T\to\infty} \int dx_B\, \Delta^{\mathrm{CHO}}[c_A\, c_B,\, -T;\, x\, x_B,\, 0] \times \Delta^{\mathrm{CHO}}[x'\, x_B,\, 0;\, c_A\, c_B,\, T]. \tag{4.38}$$

We will denote by I_P the integral of the product of propagators, i.e.

$$I_P = \int dx_B\, \Delta^{\mathrm{CHO}}[c_A\, c_B,\, -T;\, x\, x_B,\, 0] \times \Delta^{\mathrm{CHO}}[x'\, x_B,\, 0;\, c_A\, c_B,\, T]. \tag{4.39}$$

After performing the integral we find that I_P has the following form

$$I_P = \exp\Big[c_1(x^2 + x'^2) + c_2(x + x') + c_3\, xx'\Big], \tag{4.40}$$

together with some normalization factors that we enclose in $\mathcal{N}$. The parameters in the exponential are given by

$$c_1 = \frac{\omega_-^2 \coth(\omega_- T)^2}{2\,\omega_- \coth(\omega_- T) + 2\,\omega_+ \coth(\omega_+ T)} - \frac{5}{8}\,\omega_- \coth(\omega_- T) - \frac{1}{8}\,\omega_+ \coth(\omega_+ T) \tag{4.41}$$

$$c_2 = \frac{\omega_-\,\omega_+\,\operatorname{csch}(\omega_- T)\,\operatorname{csch}(\omega_+ T)}{\omega_- \coth(\omega_- T) + \omega_+ \coth(\omega_+ T)} \times \left[(c_A + c_B)\cosh(\omega_- T) + (c_A - c_B)\cosh(\omega_+ T)\right] \tag{4.42}$$

$$c_3 = \frac{(\omega_- \coth(\omega_- T) - \omega_+ \coth(\omega_+ T))^2}{4\,(\omega_- \coth(\omega_- T) + \omega_+ \coth(\omega_+ T))}, \tag{4.43}$$

where $\coth(x) = 1/\tanh(x)$ and $\operatorname{csch}(x) = 1/\sinh(x)$ are inverse hyperbolic trigonometric functions. When x is large these functions give

$$\lim_{x\to\infty} \coth(x) = 1 \tag{4.44}$$

$$\lim_{x\to\infty} \operatorname{csch}(x) = 0, \tag{4.45}$$

therefore we just have to choose T large enough to have these limits valid. Then the parameters c_1, c_2 and c_3 in the integral I_p will give

$$c_1 \to -\frac{(\omega_-^2 + 6\omega_-\omega_+ + \omega_+^2)}{8(\omega_- + \omega_+)} \equiv -\frac{\gamma}{2} \tag{4.46}$$

$$c_2 \to 0 \tag{4.47}$$

$$c_3 \to \frac{(\omega_- - \omega_+)^2}{4(\omega_- + \omega_+)} \equiv \eta, \tag{4.48}$$

here we have identified the same γ and η parameters as in section 2.5. Now that we know how I_P behaves for large T, we can go back to the reduced density matrix expression to find

$$\rho_A(x, x') = \frac{1}{\mathcal{N}} \exp\Big[-\frac{\gamma}{2}(x^2 + x'^2) + \eta\, xx'\Big]. \tag{4.49}$$

We use the fact that $\mathrm{Tr}_A\, \rho_A = 1$ to fix the normalization factor:

$$\int_{-\infty}^{\infty} dx\, \rho_A(x, x) = 1 \Rightarrow \mathcal{N} = \sqrt{\frac{\pi}{\gamma - \eta}}. \tag{4.50}$$

Finally we obtain the normalized reduced density matrix for particle A,

$$\rho_A(x, x') = \sqrt{\frac{\gamma - \eta}{\pi}} \exp\Big[-\frac{\gamma}{2}(x^2 + x'^2) + \eta\, xx'\Big]. \tag{4.51}$$

This calculation is just a confirmation that our method works for the coupled harmonic oscillator Hamiltonian.

Now we are going to compute entanglement measures using this formalism. We use equation 4.29 to compute the trace $\mathrm{Tr}_A(\rho_A^2)$ that appears in the second Rényi entropy and the linear entropy,

$$\begin{aligned}\mathrm{Tr}_A(\rho_A^2) = \frac{1}{Z^2} \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \\ \times \Delta^{\mathrm{CHO}}[c_A\, c_B,\, -T;\, x_1\, y_1,\, 0] \times \Delta^{\mathrm{CHO}}[x_2\, y_1,\, 0;\, c_A\, c_B,\, T] \\ \times \Delta^{\mathrm{CHO}}[c_A\, c_B,\, -T;\, x_2\, y_2,\, 0] \times \Delta^{\mathrm{CHO}}[x_1\, y_2,\, 0;\, c_A\, c_B,\, T],\end{aligned} \tag{4.52}$$

where Z is the normalization factor obtained by imposing that the reduced density matrix has unit trace, i.e.

$$Z = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dy_1\, \Delta^{\mathrm{CHO}}[c_A\, c_B,\, -T;\, x_1\, y_1,\, 0] \times \Delta^{\mathrm{CHO}}[x_1\, y_1,\, 0;\, c_A\, c_B,\, T]. \tag{4.53}$$

Once we have the normalized reduced density matrix, it is straightforward to compute the trace,

$$\mathrm{Tr}_A(\rho_A^2) = \frac{\gamma-\eta}{\pi}\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \exp\left[-\gamma({x_1}^2+{x_2}^2)+2\,\eta\, x_1 x_2\right] \tag{4.54}$$

$$= \sqrt{\frac{\gamma-\eta}{\gamma+\eta}}. \tag{4.55}$$

Then we can use this result in the entanglement measures defined in equations 2.49, with the parameter equals 2, and 2.62. The second Rényi entropy $S_2(\rho_A)$ is given by,

$$S_2(\rho_A) = -\frac{1}{2}\log(\gamma-\eta)+\frac{1}{2}\log(\gamma+\eta) = -\log\left(\frac{2\sqrt{\omega_+\omega_-}}{\omega_++\omega_-}\right)\ , \tag{4.56}$$

and the linear entropy between the particles A and B, denoted by $S_L(\rho_A)$ is given by

$$S_L(\rho_A) = 1-\sqrt{\frac{\gamma-\eta}{\gamma+\eta}} = \frac{(\sqrt{\omega_+}-\sqrt{\omega_-})^2}{\omega_++\omega_-}\ . \tag{4.57}$$

In this way, we have re-derived all the results of previous sections, but with the advantage that this time no diagonalization was required. Instead, we found an representation of the density matrix with the path integrals, then we were allowed to compute the traces in the entanglement measures. The downside of this method are the arbitrary boundary conditions c_A and c_B, but we have discussed that could also be replaced by an integral.

Chapter 5

Thermal distribution density matrix

In this chapter, we present a different method to compute entanglement using path integrals. This method allow us to obtain the density matrix in a straightforward way, without bothering about the wavefunction. As we will see, this method reduces in half the number of path integrals we have to perform.

We use this method to compute the second Rényi entropy and the linear entropy. We illustrate how this method works in practice for the case of coupled harmonic oscillators. The results obtained reproduce the ones from other methods.

5.1 Ground state density matrix

As in the other chapters, we consider particles A and B that live in the bipartite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. We also suppose the full system is in the pure ground state $|0\rangle$ of the Hamiltonian H, thus it has density matrix $\rho = |0\rangle \langle 0|$.

We start this section with a claim: the density matrix ρ describing the two particles ground state can be expressed as the following limit of a thermal distribution

$$\rho = \lim_{\beta \to \infty} \frac{1}{Z(\beta)} e^{-\beta H}, \tag{5.1}$$

of inverse temperature β and with a partition function $Z(\beta) = \mathrm{Tr}\left(e^{-\beta H}\right)$.

In order to show that equation 5.1 indeed reproduces $\rho = |0\rangle \langle 0|$, we will work on the limit of the exponential in the RHS. By inserting a complete set of energy

eigenstates next to the exponential we find that

$$\lim_{\beta\to\infty} e^{-\beta H} = \lim_{\beta\to\infty} \sum_n e^{-\beta H} \left|n\right\rangle \left\langle n\right| \tag{5.2}$$

$$= \lim_{\beta\to\infty} \sum_n e^{-\beta E_n} \left|n\right\rangle \left\langle n\right| . \tag{5.3}$$

When $\beta \to \infty$ the largest contribution to this sum comes from $n = 0$. Therefore in this limit the largest contribution comes from E_0, which we can always set to zero by redefining the Hamiltonian. As a result, we obtain the ground state density matrix

$$\lim_{\beta\to\infty} e^{-\beta H} = \left|0\right\rangle \left\langle 0\right| . \tag{5.4}$$

This validates our claim, and we can use 5.1 as an equivalent expression to the ground state density matrix. The partition function $Z(\beta)$ in the limit $\beta \to \infty$ corresponds to a normalization that assures that the density matrix $\left|0\right\rangle \left\langle 0\right|$ has unit trace.

In equation 5.1 the density matrix is basically an evolution operator through the Hamiltonian H in the time interval β. Therefore it has a straightforward interpretation as a path integral, the matrix elements of the density matrix in the coordinate basis $\{\left|x_A x_B\right\rangle\}$ are

$$\left\langle x_f\, y_f\right| \rho \left|x_i\, y_i\right\rangle = \lim_{\beta\to\infty} \frac{1}{Z(\beta)} \left\langle x_f\, y_f\right| e^{-\beta H} \left|x_i\, y_i\right\rangle \tag{5.5}$$

$$= \lim_{\beta\to\infty} \frac{1}{Z(\beta)} \left\langle x_f\, y_f\, \beta\right| \left.x_i\, y_i\, 0\right\rangle . \tag{5.6}$$

We know that transition amplitudes can be expressed as path integrals through the equation

$$\left\langle x_f\, y_f\, \beta\right| \left.x_i\, y_i\, 0\right\rangle = \int_{x_A(0)=x_i}^{x_A(\beta)=x_f} \int_{x_B(0)=y_i}^{x_B(\beta)=y_f} \left[\mathcal{D}x_A\right] \left[\mathcal{D}x_B\right] e^{-I_E[x_A, x_B]}, \tag{5.7}$$

where x_A and x_B represent the coordinates of particles A and B, respectively. Moreover, $I_E[x_A, x_B]$ is the Euclidean action of the two particles,

$$I_E[x_A, x_B] = \int_0^\beta d\tau\, \mathcal{L}_E(x_A, x_B), \tag{5.8}$$

where τ is the imaginary time, and $\mathcal{L}_E(x_A, x_B)$ is the Euclidean Lagrangian: it is the sum of the kinetic terms and potentials for particles A and B.

Then we can use the path integral expression to the transition amplitude to find that the ground state density matrix ρ have matrix elements

$$\rho(x_f\, y_f; x_i\, y_i) = \lim_{\beta\to\infty} \frac{1}{Z(\beta)} \int_{x_A(0)=x_i}^{x_A(\beta)=x_f} \int_{x_B(0)=y_i}^{x_B(\beta)=y_f} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\, e^{-I_E[x_A,x_B]}, \tag{5.9}$$

where the normalization factor $Z(\beta)$, or partition function, is given in terms of path integrals as

$$Z(\beta) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{x_A(0)=x}^{x_A(\beta)=x} \int_{x_B(0)=y}^{x_B(\beta)=y} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\, e^{-I_E[x_A,x_B]}. \tag{5.10}$$

Moreover, the reduced density matrix ρ_A is obtained from the full density matrix by tracing out the degrees of freedom of particle B,

$$\rho_A(x, x') = \lim_{\beta\to\infty} \frac{1}{Z(\beta)} \int_{-\infty}^{\infty} dy \int_{x_A(0)=x}^{x_A(\beta)=x'} \int_{x_B(0)=y}^{x_B(\beta)=y} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\, e^{-I_E[x_A,x_B]}. \tag{5.11}$$

This equation allow us to compute the reduced density matrix as long as we have the path integral for the system that evolves with the Hamiltonian $H(x_A, x_B)$. In some cases it is hard to directly compute the path integral, but we can make a perturbative expansion on part of the exponential. These cases are explored in the next chapter, where we show how to use perturbative expansion to compute entanglement measures.

5.2 Rényi entropy and linear entropy

In this section, we are interested in calculating the second Rényi entropy and the linear entropy. For this reason, we will express the $\mathrm{Tr}_A(\rho_A^2)$ using the formalism with path integrals described in the previous section. The general expression for the trace is

$$\mathrm{Tr}_A(\rho_A^2) = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2\ \rho_A(x_1, x_2)\, \rho_A(x_2, x_1). \tag{5.12}$$

We use equation 5.11, where we express the reduced density matrix in terms of path integrals, in this trace to find that

$$\begin{aligned}\mathrm{Tr}_A(\rho_A^2) = \lim_{\beta\to\infty} \frac{1}{Z(\beta)^2} \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \\ \times \int_{x_A^1(0)=x_1}^{x_A^1(\beta)=x_2} \int_{x_B^1(0)=y_1}^{x_B^1(\beta)=y_1} \left[\mathcal{D}x_A^1\right] \left[\mathcal{D}x_B^1\right] e^{-I_E[x_A^1, x_B^1]} \\ \times \int_{x_A^2(0)=x_2}^{x_A^2(\beta)=x_1} \int_{x_B^2(0)=y_2}^{x_B^2(\beta)=y_2} \left[\mathcal{D}x_A^2\right] \left[\mathcal{D}x_B^2\right] e^{-I_E[x_A^2, x_B^2]} \,. \end{aligned} \tag{5.13}$$

This expression has too many elements to analyse. In order to simplify the calculations, we write trace as a ratio of two terms: the numerator is $Z_2(\beta)$, where we put all the integrals and path integrals with special boundary conditions, and denominator is the power of partition functions $Z(\beta)^2$. More specifically, we let

$$\mathrm{Tr}_A(\rho_A^2) = \lim_{\beta\to\infty} \frac{Z_2(\beta)}{Z(\beta)^2} \,, \tag{5.14}$$

with $Z_2(\beta)$ given by

$$\begin{aligned} Z_2(\beta) = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \\ \times \int_{x_A^1(0)=x_1}^{x_A^1(\beta)=x_2} \int_{x_B^1(0)=y_1}^{x_B^1(\beta)=y_1} \left[\mathcal{D}x_A^1\right] \left[\mathcal{D}x_B^1\right] e^{-I_E[x_A^1, x_B^1]} \\ \times \int_{x_A^2(0)=x_2}^{x_A^2(\beta)=x_1} \int_{x_B^2(0)=y_2}^{x_B^2(\beta)=y_2} \left[\mathcal{D}x_A^2\right] \left[\mathcal{D}x_B^2\right] e^{-I_E[x_A^2, x_B^2]} \,. \end{aligned} \tag{5.15}$$

Unfortunately, we cannot use the integrals over dx_j and dy_j to join the path integrals over A and over B separately because these particles may have their coordinates entangled in the action $I_E[x_A^j, x_B^j]$. Moreover, the denominator $Z(\beta)^2$ is just the squared of the term given in equation 5.10,

$$Z(\beta)^2 = \left[\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{x_A(0)=x}^{x_A(\beta)=x} \int_{x_B(0)=y}^{x_B(\beta)=y} \left[\mathcal{D}x_A\right] \left[\mathcal{D}x_B\right] e^{-I_E[x_A, x_B]}\right]^2 . \tag{5.16}$$

These expressions give us a way to compute the trace $\mathrm{Tr}_A(\rho_A^2)$ as long as we have the path integral for the two particles. Then we can use this quantity to compute the second Rényi entropy $S_2(\rho_A) = -\log[\mathrm{Tr}_A(\rho^2)]$ and the linear entropy $S_L(\rho_A) = 1 - \mathrm{Tr}_A(\rho_A^2)$.

5.3 Higher-order Rényi entropies

If we are interested in the other Rényi entropies, defined in equation 2.49, we have to work on the quantity $\mathrm{Tr}_A(\rho_A^n)$. In this case, we use the same idea of the last section and write this trace as a ratio. Note that in these traces we will always have a factor of $Z(\beta)^n$ in the denominator. Then, in order to focus solely in the path integrals with special boundary conditions, we define $Z_n(\beta)$ by the equation

$$\mathrm{Tr}_A(\rho_A^n) \equiv \lim_{\beta\to\infty} \frac{Z_n(\beta)}{Z(\beta)^n}\,. \tag{5.17}$$

The expression for $Z_n(\beta)$ corresponds to a partition function in the space with the size of n copies of the original space. The analogous to equation 5.15 for n copies is

$$Z_n(\beta) = \prod_{j=1}^{n} \int_{-\infty}^{\infty} dx_j \int_{-\infty}^{\infty} dy_j \int_{x_A^j(0)=x_j}^{x_A^j(\beta)=x_{j+1}} \int_{x_B^j(0)=y_j}^{x_B^j(\beta)=y_j} \left[\mathcal{D}x_A^j\right] \left[\mathcal{D}x_B^j\right] e^{-I_E[x_A^j, x_B^j]}, \tag{5.18}$$

together with the identification $1+n \equiv 1$. In that way, the boundary condition of the j-th copy at time $\tau = 0$ matches the condition of the $j+1$-th copy at time $\tau = \beta$. The Rényi entropies of higher order will naturally require us to perform more integrals.

5.4 Coupled harmonic oscillators III

In this section we use the methods derived in the previous sections of this chapter to compute the reduced density matrix, second Rényi entropy, and the linear entropy for the case of two coupled harmonic oscillators, which evolve with the Hamiltonian 2.72.

The coupled harmonic oscillators path integral is given by the propagator Δ^{CHO} in equations 4.33 and 4.32. We use this propagator in equation 5.11 to write the reduced density matrix,

$$\rho_A(x, x') = \lim_{\beta\to\infty} \frac{1}{Z(\beta)} \int dy\, \Delta^{\mathrm{CHO}}[x'\, y,\, 0;\, x\, y,\, \beta]. \tag{5.19}$$

Then we use equation 4.33 to write the propagator in an appropriate way to perform the dy integration,

$$\Delta^{\mathrm{CHO}}[x'\,y,\,0;\,x\,y,\,\beta] = a_0(\beta)\exp\Big[-a_1(\beta)y^2 + a_2(x,x',\beta)y + a_3(x,x',\beta)\Big], \quad (5.20)$$

with the parameters given by

$$a_0(\beta) = \frac{\sqrt{\omega_+\omega_-\mathrm{csch}(\beta\omega_-)\mathrm{csch}(\beta\omega_+)}}{2\pi} \quad (5.21)$$

$$\begin{aligned} a_1(\beta) =& + \frac{\omega_-}{2}\left[\coth(\beta\omega_-) - \mathrm{csch}(\beta\omega_-)\right] \\ &+ \frac{\omega_+}{2}\left[\coth(\beta\omega_+) - \mathrm{csch}(\beta\omega_+)\right] \end{aligned} \quad (5.22)$$

$$\begin{aligned} a_2(x,x',\beta) =& -\frac{\omega_+}{2}(x+x')\left[\coth(\beta\omega_+) - \mathrm{csch}(\beta\omega_+)\right] \\ &+ \frac{\omega_-}{2}(x+x')\left[\coth(\beta\omega_-) - \mathrm{csch}(\beta\omega_-)\right] \end{aligned} \quad (5.23)$$

$$\begin{aligned} a_3(x,x',\beta) =& \left[x^2 + x'^2\right]\left[-\frac{\omega_-}{4}\coth(\beta\omega_-) - \frac{\omega_+}{4}\coth(\beta\omega_+)\right] \\ &+ \frac{1}{2}xx'\left[\omega_-\mathrm{csch}(\beta\omega_-) + \omega_+\mathrm{csch}(\beta\omega_+)\right]. \end{aligned} \quad (5.24)$$

After performing the integral over the particle B coordinate, we obtain

$$\rho_A(x,x') = \lim_{\beta\to\infty}\frac{a_0(\beta)}{Z(\beta)}\sqrt{\frac{\pi}{a_1(\beta)}}\exp\left[\frac{a_2(x,x',\beta)^2}{4a_1(\beta)} + a_3(x,x',\beta)\right]. \quad (5.25)$$

The normalization factors next to the exponential will also appear in the end with the partition function $Z(\beta)$. Then we take the limit $\beta\to\infty$ inside the exponential, in this limit the inverse hyperbolic trigonometric functions behave as 4.44 and 4.45, therefore the parameters that appear in the exponential become

$$\lim_{\beta\to\infty} a_1(\beta) = \frac{1}{2}(\omega_- + \omega_+) \quad (5.26)$$

$$\lim_{\beta\to\infty} a_2(x,x',\beta) = \frac{1}{2}(\omega_- - \omega_+)(x+x') \quad (5.27)$$

$$\lim_{\beta\to\infty} a_3(x,x',\beta) = -\frac{1}{4}(\omega_- + \omega_+)\left(x^2 + x'^2\right). \quad (5.28)$$

After taking the limit inside the exponential, we find that the reduced density matrix ρ_A has matrix elements

$$\rho_A(x,x') = \mathcal{N}\exp\left[\frac{-\left(\omega_-^2 + 6\omega_-\omega_+ + \omega_+^2\right)}{8(\omega_- + \omega_+)}\left(x^2 + x'^2\right) + \frac{(\omega_- - \omega_+)^2}{4(\omega_- + \omega_+)}xx'\right], \quad (5.29)$$

where the factor $\mathcal{N}$ is defined as the limit of the partition function together with the factors multiplying the exponential,

$$\mathcal{N} \equiv \lim_{\beta\to\infty} \frac{a_0(\beta)}{Z(\beta)} \sqrt{\frac{\pi}{a_1(\beta)}}. \tag{5.30}$$

In terms of the parameters γ and η defined in 2.82 we see that this result matches exactly with the density matrices in equations 2.81 and 4.49 obtained from other methods,

$$\rho_A(x,x') = \mathcal{N} \exp\Big[-\frac{\gamma}{2}(x^2+x'^2)+\eta x x'\Big]. \tag{5.31}$$

We use the expression 5.10 to find the partition function $Z(\beta)$,

$$\begin{aligned} Z(\beta) &= \int dx \int dy\, \Delta^{\mathrm{CHO}}(x\,y,\,0;x\,y,\,\beta) && (5.32)\\ &= a_0(\beta)\sqrt{\frac{\pi}{a_1(\beta)}} \int dx\, \exp\left[\frac{a_2(x,x,\beta)^2}{4a_1(\beta)} + a_3(x,x,\beta)\right] && (5.33)\\ &= a_0(\beta)\sqrt{\frac{\pi}{a_1(\beta)}}\sqrt{\frac{\pi}{a_4(\beta)}}\,, && (5.34) \end{aligned}$$

where

$$a_4(\beta) = \frac{2\omega_-\omega_+}{\omega_+ \coth\left(\frac{\beta\omega_-}{2}\right) + \omega_- \coth\left(\frac{\beta\omega_+}{2}\right)}. \tag{5.35}$$

The hyperbolic function $\coth(x)$ goes to unit when x approaches infinity, this is useful when we take the limit $\beta \to \infty$. In the end, we have the following expression for the normalization factor,

$$\begin{aligned} \mathcal{N} &= \lim_{\beta\to\infty} \sqrt{\frac{a_4(\beta)}{\pi}} && (5.36)\\ &= \sqrt{\frac{2\omega_-\omega_+}{\pi(\omega_-+\omega_+)}} && (5.37)\\ &= \sqrt{\frac{\gamma-\eta}{\pi}}\,. && (5.38) \end{aligned}$$

Then the normalized reduced density matrix is

$$\rho_A(x,x') = \sqrt{\frac{\gamma-\eta}{\pi}} \exp\Big[-\frac{\gamma}{2}(x^2+x'^2)+\eta x x'\Big]. \tag{5.39}$$

Finally, in order to obtain the second Rényi entropy and linear entropy, we need to compute $\mathrm{Tr}_A(\rho_A^2)$. Once we know the reduced density matrix, it is straightforward to take this trace. The precise expression for the factor $Z_2(\beta)$ is

$$Z_2(\beta) = \int dx_1 \int dx_2 \int dy_1 \int dy_2 \times \Delta^{\mathrm{CHO}}[x_1\, y_1,\, 0;\, x_2\, y_1,\, \beta] \times \Delta^{\mathrm{CHO}}[x_2\, y_2,\, 0;\, x_1\, y_2,\, \beta]. \tag{5.40}$$

Since the propagator $\Delta^{\mathrm{CHO}}(x\, y,\, 0; x'\, y',\, \beta)$ of the coupled harmonic oscillators is invariant under the change $x \to x'$, the product of reduced density matrices $\rho_A(x_1, x_2)\rho_A(x_2, x_1)$ is actually the same as $\rho_A(x_1, x_2)^2$. After performing the integrals over the reduced density matrix, we find

$$\mathrm{Tr}_A(\rho_A^2) = \int dx_1 \int dx_2\, \rho_A(x_1, x_2)^2 \tag{5.41}$$

$$= \frac{\gamma - \eta}{\pi} \int dx_1 \int dx_2\, \exp\Big[-\gamma(x_1^2 + x_2^2) + 2\eta\, x_1 x_2\Big] \tag{5.42}$$

$$= \sqrt{\frac{\gamma - \eta}{\gamma + \eta}}. \tag{5.43}$$

In that way, we reproduced the same results as in other methods. The second Rényi entropy is given by $S_2(\rho_A) = -\frac{1}{2}\log(\gamma - \eta) + \frac{1}{2}\log(\gamma + \eta)$, while the linear entropy is $S_L(\rho_A) = 1 - \sqrt{\frac{\gamma-\eta}{\gamma+\eta}}$. The Rényi entropies of higher order can be calculated by taking the trace of higher powers of the reduced density matrix.

When we compare this method with the one developed in section 4.1, we immediately see that this time we had to use less path integrals to obtain the same results. In the other method, we had to write a path integral for the wavefunction and another one for its complex conjugate, but in the method used through this chapter we have only one path integral for the density matrix.

Moreover, in section 4.1 we had to choose special boundary conditions at the initial and final times and they had to be a point where wavefunction has finite overlap with the ground state, which is hard to guarantee if we do not know the wavefunction. We could avoid these issues in this method because the fundamental idea was to write the density matrix as the limit of an "evolution operator" $\exp(-\beta H)$. Then, by using this expression to write the ground state density

matrix, we could identify the path integrals in a much direct way than in the method of chapter 5.

Chapter 6

Perturbative expansion of entanglement

In this chapter, we use the idea of representing the ground state density matrix as a thermal distribution, which was presented in chapter 5, together with a perturbative expansion on the interaction part of the action to write the trace $\mathrm{Tr}_A(\rho_A^2)$ that appears in the second Rényi entropy and linear entropy. We analyse the different orders of this quantity in perturbation theory, and express it in terms of expectation values.

6.1 Density matrix and trace of ρ_A^2

In chapter 5, we propose a method to compute the second Rényi entropy and the linear entropy as path integral of expectation values. and eentanglement measures as expectations demonstrated that the ground state density matrix is given as the limit $\beta \to \infty$ of the thermal distribution $\exp[-\beta\, H(x_A, x_B)]$. We used this idea to derive equation 5.1, which gives the following representation to the ground state density matrix of two particles,

$$\rho(x'\,y';\,x\,y) = \lim_{\beta\to\infty} \frac{1}{Z(\beta)} \int_{x_A(0)=x}^{x_A(\beta)=x'} \int_{x_B(0)=y}^{x_B(\beta)=y'} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\, e^{-I_E[x_A,x_B]}\,, \tag{6.1}$$

where $Z(\beta)$ is the partition function of this state, defined as

$$Z(\beta) = \int dx \int dy \int_{x_A(0)=x}^{x_A(\beta)=x} \int_{x_B(0)=y}^{x_B(\beta)=y} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\, e^{-I_E[x_A,x_B]}\,, \tag{6.2}$$

and $I_E[x_A, x_B]$ is the Euclidean action, which is defined in terms of the Euclidean Lagrangian $\mathcal{L}_E(x_A, x_B)$ as

$$I_E[x_A, x_B] = \int_0^\beta d\tau\, \mathcal{L}_E(x_A, x_B), \tag{6.3}$$

where τ is the imaginary time, and the Euclidean Lagrangian is the sum of the kinetic and potential terms.

In this chapter we explore the cases in which the potential that causes entanglement has a weak coupling, which allows for a perturbative expansion. For this purpose, we consider the Euclidean Lagrangian has the form

$$\mathcal{L}_E(x_A, x_B) = \mathcal{L}_1(x_A) + \mathcal{L}_1(x_B) + g\,\mathcal{L}_2(x_A, x_B), \tag{6.4}$$

where $\mathcal{L}_1$ encloses the kinetic term, and the single-particle potentials. For simplicity, we suppose these single-particle potentials are the same for both particles. The term $\mathcal{L}_2$ is the interaction term, which has strength given by the constant g. The entanglement between particles A and B is created by $\mathcal{L}_2$, therefore g plays a main role in creating entanglement. Indeed, when $g = 0$ the particles A and B are not entangled at all.

According to this separation of the Euclidean Lagrangian, we can write the exponential of the Euclidean action appearing in the path integral as a sum of three parts,

$$\exp\left(-I_E[x_A, x_B]\right) = \exp\left\{-\int_0^\beta d\tau\ \left[\mathcal{L}_1(x_A) + \mathcal{L}_1(x_B) + g\,\mathcal{L}_2(x_A, x_B)\right]\right\} \tag{6.5}$$

$$\equiv \exp\left(-I_1[x_A] - I_1[x_B] - g\,I_2[x_A, x_B]\right), \tag{6.6}$$

where I_1 and I_2 are the actions with respect to the Euclidean Lagrangians $\mathcal{L}_1$ and $\mathcal{L}_2$, respectively. We can use a power series to represent the exponential of the action I_2. In this case, the exponential becomes

$$\exp\left(-g\,I_2[x_A, x_B]\right) = 1 - g\int_0^\beta d\tau\,\mathcal{L}_2(x_A, x_B) + g^2\,\frac{1}{2!}\left[\int_0^\beta d\tau\,\mathcal{L}_2(x_A, x_B)\right]^2 + \dots, \tag{6.7}$$

which has a generic term proportional to g^n,

$$(-g)^n\,\frac{1}{n!}\left[\int_0^\beta d\tau\,\mathcal{L}_2(x_A, x_B)\right]^n. \tag{6.8}$$

Therefore, in the case that the parameter g, which generates entanglement, is sufficiently small, we can truncate the series at some power n. For example, the

lowest nontrivial order would be $\mathcal{O}(g)$ and given by

$$e^{-g\, I_2[x_A, x_B]} \approx 1 - g\, I_2[x_A, x_B]\,. \tag{6.9}$$

Although for the two coupled harmonic oscillators the $\mathcal{O}(g)$ term vanishes, as we will shown shortly ahead, for concreteness let us consider this first order approximation. At this order, the full density matrix of the bipartite system is given by

$$\begin{aligned}\rho(x'\,y';\,x\,y) \approx \lim_{\beta\to\infty} \frac{1}{Z(\beta)} \int_{x_A(0)=x}^{x_A(\beta)=x'} \int_{x_B(0)=y}^{x_B(\beta)=y'} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\, e^{-I_1[x_A]-I_1[x_B]} \\ \times\,(1 - g\, I_2[x_A, x_B])\ .\end{aligned} \tag{6.10}$$

Similarly, the partition function can be written as

$$\begin{aligned}Z(\beta) \approx \int dx \int dy \int_{x_A(0)=x}^{x_A(\beta)=x} \int_{x_B(0)=y}^{x_B(\beta)=y} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\, e^{-I_1[x_A]-I_1[x_B]} \\ \times\,(1 - g\, I_2[x_A, x_B])\ .\end{aligned} \tag{6.11}$$

These expressions, when compared to what we had in equations 6.1 and 6.2, have the feature that the actions of particles A and B in the exponential are now uncoupled.

For the reduced density matrix of particle A, we must trace out the degrees of freedom of particle B. After taking the trace, the first order approximation is then given by

$$\begin{aligned}\rho_A(x, x') \approx \lim_{\beta\to\infty} \frac{1}{Z(\beta)} \int dy \int_{x_A(0)=x}^{x_A(\beta)=x'} \int_{x_B(0)=y}^{x_B(\beta)=y} [\mathcal{D}x_A]\,[\mathcal{D}x_B] \\ \times\,(1 - g\, I_2[x_A, x_B])\ e^{-I_1[x_A]-I_1[x_B]}.\end{aligned} \tag{6.12}$$

As usual, the other quantity we are interested is the trace $\mathrm{Tr}_A(\rho_A^2)$ because it appears in the second Rényi entropy and linear entropy. The first order approximation

allows us to write this trace as

$$\begin{aligned}\mathrm{Tr}_A(\rho_A^2) \approx \lim_{\beta\to\infty} \frac{1}{Z(\beta)^2} \int dx_1 \int dx_2 \int dy_1 \int dy_2 \\ \times \int_{x_A(0)=x_1}^{x_A(\beta)=x_2} \int_{x_B(0)=y_1}^{x_B(\beta)=y_1} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\,(1-g\,I_2[x_A,x_B])\; e^{-I_1[x_A]-I_1[x_B]} \\ \times \int_{x_A(0)=x_2}^{x_A(\beta)=x_1} \int_{x_B(0)=y_2}^{x_B(\beta)=y_2} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\,(1-g\,I_2[x_A,x_B])\; e^{-I_1[x_A]-I_1[x_B]}.\end{aligned} \tag{6.13}$$

Here, there is a term $\mathcal{O}(g^2)$ that needs to be dropped. In the following sections, we will analyse the zeroth and first order approximations of this quantity. Note that in the denominator we have powers of the partition function $Z(\beta)$, which also depends on the parameters g. Therefore, in our analysis we have to take these powers of g into consideration when dealing with ρ, ρ_A and $\mathrm{Tr}_A(\rho_A^2)$. Once again, we will define the trace as the limit $\beta \to \infty$ of the ratio $Z_2(\beta)/Z(\beta)^2$, in that way we separately deal with $Z_2(\beta)$ and its path integrals with special boundary conditions,

$$\begin{aligned}Z_2(\beta) \equiv \int dx_1 \int dx_2 \int dy_1 \int dy_2 \\ \times \int_{x_A(0)=x_1}^{x_A(\beta)=x_2} \int_{x_B(0)=y_1}^{x_B(\beta)=y_1} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\,(1-g\,I_2[x_A,x_B])\; e^{-I_1[x_A]-I_1[x_B]} \\ \times \int_{x_A(0)=x_2}^{x_A(\beta)=x_1} \int_{x_B(0)=y_2}^{x_B(\beta)=y_2} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\,(1-g\,I_2[x_A,x_B])\; e^{-I_1[x_A]-I_1[x_B]}\,.\end{aligned} \tag{6.14}$$

6.2 Non-entangled limit: the zeroth order

In this section we analyse the trace $\mathrm{Tr}_A(\rho_A^2)$ in the zeroth order approximation, i.e. when the entanglement parameter vanishes. In this case, when we set $g = 0$ and denote the corresponding quantities with a superscript (0). For definiteness, we will make contact with the coupled harmonic oscillator problem; but it should be clear that the method is applicable to any problem for which the action can be

splitted as in Eq. (6.6). The zeroth-order partition function is given by

$$\begin{aligned} Z^{(0)}(\beta) &= \int dx \int dy \int_{x_A(0)=x}^{x_A(\beta)=x} \int_{x_B(0)=y}^{x_B(\beta)=y} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\; e^{-I_1[x_A]-I_1[x_B]} \\ &\equiv Z_A^{(0)}(\beta)\, Z_B^{(0)}(\beta)\,, \end{aligned} \tag{6.15}$$

where

$$Z_A^{(0)}(\beta) = \int dx \int_{x_A(0)=x}^{x_A(\beta)=x} [\mathcal{D}x_A]\; e^{-I_1[x_A]} = \int dx\, \Delta_A(x,\,0;\,x,\,\beta)\,, \tag{6.16}$$

$$Z_B^{(0)}(\beta) = \int dy \int_{x_B(0)=y}^{x_B(\beta)=y} [\mathcal{D}x_B]\; e^{-I_1[x_B]} = \int dy\, \Delta_B(y,\,0;\,y,\,\beta)\,, \tag{6.17}$$

where, as in previous chapters, we used the following notation for the propagators for the problem of the coupled harmonic oscillators:

$$\Delta_A(x,\,0;\,x',\,\beta) \equiv \int_{x_A(0)=x}^{x_A(\beta)=x'} [\mathcal{D}x_A]\, e^{-I_1[x_A]}\,, \tag{6.18}$$

$$\Delta_B(y,\,0;\,y',\,\beta) \equiv \int_{x_B(0)=y}^{x_B(\beta)=y'} [\mathcal{D}x_B]\, e^{-I_1[x_B]}. \tag{6.19}$$

The denominator of $\mathrm{Tr}_A(\rho_A^2)$ is just the square of $Z^{(0)}(\beta) = Z_A^{(0)}(\beta)\, Z_B^{(0)}(\beta)$.

Now we write zeroth order of the numerator $Z_2(\beta)$ of $\mathrm{Tr}_A(\rho_A^2)$. When we set $g = 0$ in equation 6.14, we obtain

$$\begin{aligned} Z_2^{(0)}(\beta) = \int dx_1 \int dx_2 \int dy_1 \int dy_2 \\ \times \int_{x_A(0)=x_1}^{x_A(\beta)=x_2} \int_{x_B(0)=y_1}^{x_B(\beta)=y_1} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\; e^{-I_1[x_A]-I_1[x_B]} \\ \times \int_{x_A(0)=x_2}^{x_A(\beta)=x_1} \int_{x_B(0)=y_2}^{x_B(\beta)=y_2} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\; e^{-I_1[x_A]-I_1[x_B]}\,, \end{aligned} \tag{6.20}$$

or, using the notation with propagators Δ_A and Δ_B,

$$Z_2^{(0)}(\beta) = \int dx_1 \int dx_2\, \Delta_A(x_1,\,0;\,x_2,\,\beta)\, \Delta_A(x_2,\,0;\,x_1,\,\beta) \left[\int dy\, \Delta_B(y,\,0;\,y,\,\beta)\right]^2. \tag{6.21}$$

In the ratio $Z_2^{(0)}(\beta)/Z^{(0)}(\beta)^2$, the parts that concern particle B will exactly cancel, but the same does not happen for particle A. The reason is that in $Z_2^{(0)}(\beta)$ the

trace over the propagator Δ_A is taken after the square, while in $Z^{(0)}(\beta)^2$ we first take the trace in Δ_A, and then we square this quantity.

In the zeroth order approximation, which corresponds to $g = 0$, we expect to find that ρ_A is a pure state because the particles are not entangled. Therefore, it should be the case that $\rho_A^2 = \rho_A$, and $\mathrm{Tr}_A(\rho_A^2) = 1$. However, what we see is that the terms $Z_2^{(0)}(\beta)$ and $Z^{(0)}(\beta)^2$ do not cancel, of course. The explanation is simple: we have to take zero temperature limit, or $\beta \to \infty$, as density matrix is a mixed state for a general β. Therefore, the correct statement for the non-entangled limit is

$$\mathrm{Tr}_A(\rho_A^2) = \lim_{\beta\to\infty} \frac{Z_2(\beta)}{Z(\beta)}\bigg|_{g=0} = 1. \tag{6.22}$$

We can verify this statement for the system of two coupled harmonic oscillators. In this case, the propagator Δ_A is the simple harmonic oscillator for particle A, which we have derived in chapter 3, and is given in equation 3.76. In our notation,

$$\begin{aligned}\Delta_A(x,\,0;x',\,\beta) =& \sqrt{\frac{\omega_+}{2\pi\sinh(\omega_+\beta)}} \\ &\times \exp\left\{\frac{-\omega_+}{2\sinh(\omega_+\beta)}\left[(x^2+x'^2)\cosh(\omega_+\beta) - 2xx'\right]\right\}.\end{aligned} \tag{6.23}$$

We recall that $\omega_+ = \sqrt{k}$, and k is a parameter in the single-particle part of the coupled harmonic oscillator Hamiltonian 2.72. The Euclidean Lagrangian in this case as the form,

$$\mathcal{L}_E(x_A, x_B) = \frac{1}{2}\left[\left(\frac{dx_A}{d\tau}\right)^2 + \left(\frac{dx_B}{d\tau}\right)^2 + k\,(x_A^2 + x_B^2) + g\,(x_A - x_B)^2\right]. \tag{6.24}$$

Then, the $\mathcal{L}_1$ and $\mathcal{L}_2$ parts, according to our definitions, are given by

$$\mathcal{L}_1(x) = \frac{1}{2}\left(\frac{dx}{d\tau}\right)^2 + \frac{1}{2}k\,x^2\,, \tag{6.25}$$

$$\mathcal{L}_2(x_A, x_B) = \frac{1}{2}\,(x_A - x_B)^2\,. \tag{6.26}$$

In such a way that $\mathcal{L}_E(x_A, x_B) = \mathcal{L}_1(x_A) + \mathcal{L}_1(x_B) + g\,\mathcal{L}_2(x_A, x_B)$. We will not need the $\mathcal{L}_2$ part in this case because here we are only interested in verifying equation 6.22 with the zeroth order of $\mathrm{Tr}_A(\rho_A^2)$.

As we have already discussed, the B part cancels in $\mathrm{Tr}_A(\rho_A^2)$. Therefore, we will compute only the A part of $Z_2^{(0)}(\beta)$ and $Z^{(0)}(\beta)$, and just write $f(B)$ for the part that concerns particle B. For the partition function $Z^{(0)}(\beta)$, we use the expression of the simple harmonic oscillator propagator to find

$$Z^{(0)}(\beta) = \sqrt{\frac{\omega_+}{2\pi \sinh(\omega_+\beta)}} \int dx \, \exp\left\{ \frac{-\omega_+[\cosh(\omega_+\beta) - 1]\, x^2}{\sinh(\omega_+\beta)} \right\} \times f(B) \tag{6.27}$$

$$= \frac{1}{2} \, \mathrm{csch}\left(\frac{\omega_+\beta}{2}\right) \times f(B)\,. \tag{6.28}$$

And for the factor $Z_2^{(0)}(\beta)$ we have

$$Z_2^{(0)}(\beta) = f(B)^2 \times \frac{\omega_+}{2\pi \sinh(\omega_+\beta)} \times \int dx_1 \int dx_2 \, \exp\left\{ \frac{-\omega_+}{\sinh(\omega_+\beta)} \left[(x_1^2 + x_2^2)\cosh(\omega_+\beta) - 2\, x_1 x_2 \right] \right\}. \tag{6.29}$$

$$= \frac{1}{2} \, \mathrm{csch}(\omega_+\beta) \times f(B)^2\,. \tag{6.30}$$

We immediately see that $[Z^{(0)}(\beta)]^2$ and $Z_2^{(0)}(\beta)$ do not exactly cancel, as ratio that appears is given by

$$\frac{Z_2^{(0)}(\beta)}{[Z^{(0)}(\beta)]^2} = \frac{\frac{1}{2}\,\mathrm{csch}(\omega_+\beta)}{\frac{1}{4}\,\mathrm{csch}\left(\frac{\omega_+\beta}{2}\right)^2} = \tanh\left(\frac{\omega_+\beta}{2}\right). \tag{6.31}$$

Now, since $\tanh(x)$ goes to one when $x \to \infty$, we obtain unit trace in the limit $\beta \to \infty$:

$$\mathrm{Tr}_A(\rho_A^2) = \lim_{\beta\to\infty} \left.\frac{Z_2(\beta)}{Z(\beta)^2}\right|_{g=0} = 1. \tag{6.32}$$

In this way we have verified what was stated earlier: in the limit where the particles are not entangled, i.e. $g = 0$, the reduced density matrix is a pure state, and consequently we have $\mathrm{Tr}_A(\rho_A^2) = \mathrm{Tr}_A(\rho_A) = 1$.

6.3 First order approximation

In this section, we write the first order approximation of the trace $\mathrm{Tr}_A(\rho_A^2)$. The results of last section are useful here because we need the zeroth order term of

both $Z_2(\beta)$ and $Z(\beta)^2$. Since we do not need to carry out the zeroth order term everywhere, we will define

$$Z_2(\beta) \approx Z_2^{(0)}(\beta) + g\, Z_2^{(1)}(\beta)\,, \tag{6.33}$$

$$Z(\beta) \approx Z^{(0)}(\beta) + g\, Z^{(1)}(\beta)\,. \tag{6.34}$$

In these expressions, the $Z^{(0)}(\beta)$ and $Z_2^{(0)}(\beta)$ refer to the terms calculated in the last section with $g = 0$, while $Z^{(1)}(\beta)$, and $Z_2^{(1)}(\beta)$ are going to be obtained in these section, they do not depend on g since g was pulled out explicitly. With this notation, in the denominator of the trace we will have the partition function squared. Neglecting the second order term, we have the denominator given by

$$Z(\beta)^2 = \left[Z^{(0)}(\beta)^2\right] + g\, \left[2\, Z^{(0)}(\beta) Z^{(1)}(\beta)\right]\,. \tag{6.35}$$

Before we go into the details of how $Z^{(1)}(\beta)$ and $Z_2^{(1)}(\beta)$ look like, we call attention to the fact that the trace we want to compute, $\mathrm{Tr}_A(\rho_A^2)$, is obtained as the limit of the ratio $Z_2(\beta)/Z(\beta)^2$. Therefore, it will involve many different powers of g,

$$\mathrm{Tr}_A(\rho_A^2) = \lim_{\beta\to\infty} \frac{Z_2^{(0)}(\beta) + g\, Z_2^{(1)}(\beta)}{Z^{(0)}(\beta)^2 + g\, \left[2\, Z^{(0)}(\beta)\, Z^{(1)}(\beta)\right]}\,. \tag{6.36}$$

We can obtain the first order approximation of this trace by expanding the denominator to $\mathcal{O}(g)$:

$$\mathrm{Tr}_A(\rho_A^2) = \lim_{\beta\to\infty} \left[Z_2^{(0)}(\beta) + g\, Z_2^{(1)}(\beta)\right] \left[\frac{1}{Z^{(0)}(\beta)^2} - g\, \frac{2\, Z^{(1)}(\beta)}{Z^{(0)}(\beta)^3}\right] \tag{6.37}$$

$$= \lim_{\beta\to\infty} \left[\frac{Z_2^{(0)}(\beta)}{Z^{(0)}(\beta)^2}\right] + g\, \left[\frac{Z_2^{(1)}(\beta)}{Z^{(0)}(\beta)^2} - \frac{2\, Z_2^{(0)}(\beta)\, Z^{(1)}(\beta)}{Z^{(0)}(\beta)^3}\right]\,. \tag{6.38}$$

Now we need to compute the terms $Z^{(1)}(\beta)$ and $Z_2^{(1)}(\beta)$ of this expression. Previously in this chapter, we have used the first order approximation of the exponential $\exp\left(-g\, I_2[x_A, x_b]\right)$ to write the partition function in equation 6.11,

$$Z(\beta) = \int dx \int dy \int_{x_A(0)=x}^{x_A(\beta)=x} \int_{x_B(0)=y}^{x_B(\beta)=y} [\mathcal{D}x_A]\, [\mathcal{D}x_B] \times \left(1 - g\, I_2[x_A, x_B]\right) e^{-I_1[x_A] - I_1[x_B]}\,. \tag{6.39}$$

The unit in this expression represents the term $Z^{(0)}(\beta)$ of last section, and the other term is the $Z^{(1)}(\beta)$ that we are interested,

$$Z^{(1)}(\beta) = -\int dx \int dy \int_{x_A(0)=x}^{x_A(\beta)=x} \int_{x_B(0)=y}^{x_B(\beta)=y} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\;\; I_2[x_A, x_B]\, e^{-I_1[x_A]-I_1[x_B]}\,. \tag{6.40}$$

In this form, it is easy to see that we have a term proportional to an expectation value of the coupled action, with respect to the variable x_B, written as a path integral. We recall that the coupled action $I_2[x_A, x_B]$ is given by

$$I_2[x_A, x_B] = \int_0^\beta d\tau\, \mathcal{L}_2(x_A, x_B). \tag{6.41}$$

Thus, we have an integral over $d\tau$ of the Euclidean Lagrangian $\mathcal{L}_2$. However, instead of directly writing the whole expression as an expectation value, we define

$$F_B(x_A) := \int dy \int_{x_B(0)=y}^{x_B(\beta)=y} [\mathcal{D}x_B]\;\; \mathcal{L}_2(x_A, x_B)\, e^{-I_1[x_A,x_B]}\,. \tag{6.42}$$

Then the first order term of the partition function is given by

$$Z^{(1)}(\beta) = -\int_0^\beta d\tau \int dx \int_{x_A(0)=x}^{x_A(\beta)=x} F_B(x_A)\, e^{-I_1[x_A]}\,. \tag{6.43}$$

The choice of defining $F_B(x_A)$ is motivated by the fact that in $Z_2(\beta)$ we will still have these traces over particle B, but not over particle A. The same happened in the zeroth order when we were analysing the product of propagators: in $Z(\beta)^2$ we had $\Delta_A(x,\, 0; x,\, \beta)^2$, but in $Z_2(\beta)$ it was $\Delta_A(x_1,\, 0; x_2,\, \beta)\, \Delta_A(x_2,\, 0; x_1,\, \beta)$.

In equation 6.14, we have the first order approximation of $Z_2(\beta)$,

$$\begin{aligned} Z_2(\beta) = \int dx_1 \int dx_2 \int dy_1 \int dy_2 \\ \times \int_{x_A(0)=x_1}^{x_A(\beta)=x_2} \int_{x_B(0)=y_1}^{x_B(\beta)=y_1} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\,(1 - g\, I_2[x_A, x_B])\;\, e^{-I_1[x_A]-I_1[x_B]} \\ \times \int_{x_A(0)=x_2}^{x_A(\beta)=x_1} \int_{x_B(0)=y_2}^{x_B(\beta)=y_2} [\mathcal{D}x_A]\,[\mathcal{D}x_B]\,(1 - g\, I_2[x_A, x_B])\;\, e^{-I_1[x_A]-I_1[x_B]}\,. \end{aligned} \tag{6.44}$$

Collecting the first order terms, we find that

$$
\begin{aligned}
Z_2^{(1)}(\beta) = &- \left[\int dy\, \Delta_B(y,\, 0;\, y,\, \beta)\right] \int dx_1 \int dx_2 \\
&\times \Bigg[\int dy_1 \int_{x_A(0)=x_1}^{x_A(\beta)=x_2} \int_{x_B(0)=y_1}^{x_B(\beta)=y_1} [\mathcal{D}x_A]\,[\mathcal{D}x_B] \\
&\qquad \times I_2[x_A, x_B]\, e^{-I_1[x_A]-I_1[x_B]}\, \Delta_A(x_2,\, 0;\, x_1,\, \beta) \\
&+ \int dy_2 \int_{x_A(0)=x_2}^{x_A(\beta)=x_1} \int_{x_B(0)=y_2}^{x_B(\beta)=y_2} [\mathcal{D}x_A]\,[\mathcal{D}x_B] \\
&\qquad \times I_2[x_A, x_B]\, e^{-I_1[x_A]-I_1[x_B]}\, \Delta_A(x_1,\, 0;\, x_2,\, \beta) \Bigg].
\end{aligned}
\tag{6.45}
$$

After we insert the Euclidean Lagrangian $\mathcal{L}_2(x_A, x_B)$, and take the trace over particle B, we find that this term is

$$
\begin{aligned}
Z_2^{(1)}(\beta) = &- \left[\int dy\, \Delta_B(y,\, 0;\, y,\, \beta)\right] \int_0^\beta d\tau \int dx_1 \int dx_2 \\
&\times \Bigg[\int_{x_A(0)=x_1}^{x_A(\beta)=x_2} [\mathcal{D}x_A]\; F_B(x_A)\, e^{-I_1[x_A]}\, \Delta_A(x_2,\, 0;\, x_1,\, \beta) \\
&+ \int_{x_A(0)=x_2}^{x_A(\beta)=x_1} [\mathcal{D}x_A]\; F_B(x_A)\, e^{-I_1[x_A]}\, \Delta_A(x_1,\, 0;\, x_2,\, \beta) \Bigg].
\end{aligned}
\tag{6.46}
$$

This expression indicates that we have integrals of the matrix elements of $\hat{F}_B(x_A)$. We emphasize that the evolution from the initial to the final states indicated in the path integrals of both A and B are with respect to the evolution under the single-particle Lagrangian $\mathcal{L}_1$. Then, we define the matrix elements to be

$$
M_{AB}(x, x') := \int_{x_A(0)=x}^{x_A(\beta)=x'} [\mathcal{D}x_A]\; F_B(x_A)\, e^{-I_1[x_A]}\,. \tag{6.47}
$$

For the partition function, we actually take the mean value of $\mathcal{L}_2(x_A, x_B)$ with respect to particles A and B.

Finally, using the notation with matrix elements and expectation values, we

find that the first order terms of the partition function and of $Z_2(\beta)$ are

$$Z^{(1)}(\beta) = -\int_0^\beta d\tau \int dx\, M_{AB}(x,x)\,, \tag{6.48}$$

$$\begin{aligned} Z_2^{(1)}(\beta) = &-\left[\int dy\, \Delta_B(y,\,0;\,y,\,\beta)\right] \int_0^\beta d\tau \int dx_1 \int dx_2 \\ &\times \left[\, M_{AB}(x_1,x_2)\, \Delta_A(x_2,\,0;\,x_1,\,\beta) + M_{AB}(x_2,x_1)\, \Delta_A(x_1,\,0;\,x_2,\,\beta)\right]\,. \end{aligned} \tag{6.49}$$

Then together with the zeroth order terms obtained last section and 6.21, we obtain for the partition function,

$$Z(\beta) = \int dx\, \Delta_A(x,\,0;\,x,\,\beta) \int dy\, \Delta_B(y,\,0;\,y,\,\beta) - g \int_0^\beta d\tau \int dx\, M_{AB}(x,x)\,. \tag{6.50}$$

This already illustrates our main point: we have expressed the partition function in terms of expectation values. The same is true for $Z_2(\beta)$, which is given by

$$\begin{aligned} Z_2(\beta) = &\int dx_1 \int dx_2\, \Delta_A(x_1,\,0;\,x_2,\,\beta)\Delta_A(x_2,\,0;\,x_1,\,\beta) \left[\int dy\, \Delta_B(y,\,0;\,y,\,\beta)\right]^2 \\ &- g \left[\int dy\, \Delta_B(y,\,0;\,y,\,\beta)\right] \int_0^\beta d\tau \int dx_1 \int dx_2 \\ &\times \left[\, M_{AB}(x_1,x_2)\, \Delta_A(x_2,\,0;\,x_1,\,\beta) + M_{AB}(x_2,x_1)\, \Delta_A(x_1,\,0;\,x_2,\,\beta)\right]\,. \end{aligned} \tag{6.51}$$

For a specific Lagrangian, we need to compute all these terms, then replace each one in equation 6.38 to obtain the first order approximation of $\mathrm{Tr}_A(\rho_A^2)$. Basically, we are saying that one can compute the trace relevant for entanglement by computing two kinds of objects: the propagators under evolution with the Lagrangian $\mathcal{L}_1$, and the matrix elements the interaction Lagrangian $\mathcal{L}_2$.

Such calculations can be challenging, but they are rather common in thermal field theory, and many different analytical methods have been developed to compute them. However, our point is that when the quantities $F_B(x_A)$, $M_{AB}(x,x')$ and the propagators cannot be computed analytically, which is the common situation, they can be computed numerically using standard techniques developed for complicated problems in quantum field theory, as the Monte Carlo method or

stochastic quantization. This is out of the scope of this dissertation, but the message is clear: once one can identify a parameter responsible for the entanglement we are interested in, and if the strength of the entanglement is weak, one can use the formalism just developed.

Once we have computed all the zeroth and first order terms, which are theory-dependent, we can replace them in 6.38, take the limit $\beta \to \infty$, and then obtain the $\mathrm{Tr}_A(\rho_A^2)$. Afterwards, we are able to compute the linear entropy, which defined as $S_L(\rho_A) := 1 - \mathrm{Tr}_A(\rho_A^2)$. In the first order approximation, we have

$$S_L(\rho_A) = 1 - \lim_{\beta\to\infty} \left[\frac{Z_2^{(0)}(\beta)}{Z^{(0)}(\beta)^2} + g\, \frac{Z_2^{(1)}(\beta)}{Z^{(0)}(\beta)^2} - g\, \frac{2\, Z_2^{(0)}(\beta)\, Z^{(1)}(\beta)}{Z^{(0)}(\beta)^3} \right] . \tag{6.52}$$

In the last section, we have argued that the zeroth order approximation of the trace $\mathrm{Tr}_A(\rho_A^2)$ gives unity. Therefore, we can cancel this term with the unity in the definition to find

$$S_L(\rho_A) = g \lim_{\beta\to\infty} \left[\frac{2\, Z_2^{(0)}(\beta)\, Z^{(1)}(\beta)}{Z^{(0)}(\beta)^3} - \frac{Z_2^{(1)}(\beta)}{Z^{(0)}(\beta)^2} \right] . \tag{6.53}$$

Furthermore, for the second Rényi entropy, defined as $S_2(\rho_A) := -\log\left[\mathrm{Tr}_A(\rho_A^2)\right]$, we have to make a series expansion in the log to find how this entanglement measure depends on g. A Taylor series expansion of $\log(a + bx)$ around $x = 0$ gives $\log(a) + \frac{b}{a}\, x$, which we can use in equation 6.38 for the trace to write

$$\begin{aligned} \log\left[\mathrm{Tr}_A(\rho_A^2)\right] = & \lim_{\beta\to\infty} \log\left[\frac{Z_2^{(0)}(\beta)}{Z^{(0)}(\beta)^2} \right] \\ & + g \lim_{\beta\to\infty} \left[\frac{Z_2^{(1)}(\beta)}{Z^{(0)}(\beta)^2} - \frac{2\, Z_2^{(0)}(\beta)\, Z^{(1)}(\beta)}{Z^{(0)}(\beta)^3} \right] \left[\frac{Z^{(0)}(\beta)^2}{Z_2^{(0)}(\beta)} \right] . \end{aligned} \tag{6.54}$$

Then we use the results obtained in the zeroth order, i.e. that $Z_2^{(0)}(\beta)/Z^{(0)}(\beta)^2$ is unit, and finally find that the second Rényi entropy is

$$S_2(\rho_A) = g \lim_{\beta\to\infty} \left[\frac{2\, Z_2^{(0)}(\beta)\, Z^{(1)}(\beta)}{Z^{(0)}(\beta)^3} - \frac{Z_2^{(1)}(\beta)}{Z^{(0)}(\beta)^2} \right] . \tag{6.55}$$

Note that in this approximation, we obtain the same expression for the linear entropy and the second Rényi entropy. This is natural to expect because in the

weak entanglement limit the trace $\mathrm{Tr}_A(\rho_A^2)$ is close to unity, which allow us to expand the logarithm

$$\log\left[\mathrm{Tr}_A(\rho_A^2)\right] = \log\left\{1 - \left[1 - \mathrm{Tr}_A(\rho_A^2)\right]\right\} \tag{6.56}$$

$$\approx -\left[1 - \mathrm{Tr}_A(\rho_A^2)\right] . \tag{6.57}$$

Then we identify the linear entropy in the parenthesis on the RHS, and minus the second Rényi entropy in the LHS. Thus, in the weak entanglement they are approximately the same

$$S_2(\rho_A) \approx S_L(\rho_A) . \tag{6.58}$$

When computing these entanglement measures, we also have to keep in mind that both the second Rényi entropy and the linear entropy are non-negative measures. This statement constraints the first order approximation to always satisfy the following inequality

$$\lim_{\beta\to\infty}\left[\frac{2\,Z_2^{(0)}(\beta)\,Z^{(1)}(\beta)}{Z^{(0)}(\beta)^3} - \frac{Z_2^{(1)}(\beta)}{Z^{(0)}(\beta)^2}\right] \geq 0 . \tag{6.59}$$

For the system of coupled harmonic oscillators that we have been using, the first order correction vanishes due to the form of the interaction part of the action,

$$I_2[x_A, x_B] = \int_0^\beta d\tau\, \frac{1}{2}\left[x_A(\tau) - x_B(\tau)\right]^2 . \tag{6.60}$$

In any case, we will explicitly compute the zeroth and first order terms that appear in the trace, which are given in equations 6.50 and 6.51. The other parts of the Euclidean Lagrangian, which appear in equations 6.24 and 6.25, describe two simple harmonic oscillators, for particles A and B, of frequency $\omega_+ = \sqrt{k}$. These details are just to remind us that the propagators, mean values and matrix elements are computed with the simple harmonic oscillator.

When we discussed the zeroth order, we used equation 6.23, which is the simple harmonic oscillator. Although in this expression the propagator carries the subindice A, it is exactly equal to the propagator for particle B. This is the case

because, as we have already mentioned, the non-interacting part of the action I_1 is the same for both particles.

The zeroth order of the coupled harmonic oscillator partition function has already been partially calculated in equation 6.28, except for the B part. Since the Δ_B propagator is the same as Δ_A, the zeroth order of the partition function simplifies to

$$Z^{(0)}(\beta) = \left[\int dx\, \Delta_A(x,\, 0;\, x,\, \beta)\right]^2 \tag{6.61}$$

$$= \frac{1}{4}\,\mathrm{csch}\left(\frac{\omega_+\beta}{2}\right)^2 . \tag{6.62}$$

Similarly, we can use the fact that the propagators are the same to complete equation 6.30, which gives part of the zeroth order of $Z_2(\beta)$. As a result, we find

$$Z_2^{(0)}(\beta) = \frac{1}{8}\,\mathrm{csch}\left(\frac{\omega_+\beta}{2}\right)^2 \mathrm{csch}(\omega_+\beta)\,. \tag{6.63}$$

Now we have to compute the first order terms $Z^{(1)}(\beta)$ and $Z_2^{(1)}(\beta)$. Before we specify the calculations, we will fix what is the precise form of the matrix elements $M_{AB}(x, x')$. The matrix elements are defined in equation 6.47 as a function of $F_B(x_A)$, which are mean values of the interaction Euclidean Lagrangian with respect to the B particles.

For these reasons, we start the calculations by the mean values $F(\beta)$, which are defined in equation 6.42. Another way to write the mean values is

$$F_B(x_A) = \int dy\, \langle y,\, \beta|\, \mathcal{L}_2(x_A, x_B)\, |y,\, 0\rangle\,, \tag{6.64}$$

and such expression only makes sense if we consider the B part inside $\mathcal{L}_2(x_A, x_B)$ as operators. For the coupled harmonic oscillator, we have

$$\mathcal{L}_2(x_A, x_B) = \frac{1}{2}\,x_A^2(\tau) + \frac{1}{2}\,\hat{x}_B^2(\tau) - \,x_A(\tau)\hat{x}_B(\tau)\,. \tag{6.65}$$

Therefore, with the exception of the first term, we need to insert an identity at the position occupied by particle B at time τ. This will allow us to extract the

eigenvalue of the position operator $\hat{x}_B$,

$$\begin{aligned} F_B(x_A) &= \frac{1}{2}\, x_A^2(\tau) \int dy\, \Delta_B(y,\, 0;\, y,\, \beta) \\ &\quad + \frac{1}{2} \int dy \int dq\, \langle y,\, \beta|\, \left[\hat{x}_B^2 - x_A(\tau)\, \hat{x}_B(\tau)\right] |q,\, \tau\rangle\, \langle q,\, \tau|y,\, 0\rangle \qquad (6.66) \\ &= \frac{1}{2}\, x_A^2(\tau) \int dy\, \Delta_B(y,\, 0;\, y,\, \beta) \\ &\quad + \frac{1}{2} \int dy \int dq\, \left[q^2 - x_A(\tau)\, q\right] \Delta_B(y,\, 0;\, q,\, \tau)\Delta_B(q,\, \tau; y,\, \beta)\,. \qquad (6.67) \end{aligned}$$

After performing the integral over y, we obtain

$$\begin{aligned} F_B(x_A) &= \frac{1}{4}\, \operatorname{csch}\left(\frac{\omega_+\beta}{2}\right) x_A^2(\tau) \\ &\quad + \frac{\sqrt{\omega_+\, \operatorname{csch}(\beta\omega)}}{2\sqrt{2\pi}} \int dq\, \left[q^2 - x_A(\tau)\, q\right]\, e^{-q^2\omega \tanh\left(\frac{\beta\omega}{2}\right)}\,. \qquad (6.68) \end{aligned}$$

Since the function $q \exp\left(-q^2\right)$ is odd, the integral of this part vanishes. Then the mean value of the interaction Lagrangian with respect to particle B is

$$F_B(x_A) = \frac{1}{4}\, \operatorname{csch}\left(\frac{\omega_+\beta}{2}\right) x_A^2(\tau) + \frac{1}{8\,\omega_+}\, \coth\left(\frac{\omega_+\beta}{2}\right) \operatorname{csch}\left(\frac{\omega_+\beta}{2}\right). \qquad (6.69)$$

Now we can compute the matrix elements of $F_B(x_A)$. We can write equation 6.47, which defines $M_{AB}(x, x')$, in the following form

$$M_{AB}(x, x') = \langle x',\, \beta|\, F_B(x_A)\, |x,\, 0\rangle\ , \qquad (6.70)$$

as long as we consider the x_A inside F_B as operators. Once again, we have to insert an identity at the intermediate time τ in order to obtain the eigenvalue of the operator $\hat{x}_A^2(\tau)$,

$$\begin{aligned} M_{AB}(x, x') &= \frac{1}{4}\, \operatorname{csch}\left(\frac{\omega_+\beta}{2}\right)^2 \int dq\, \langle x',\, \beta|\, \hat{x}_A^2\, |q,\, \tau\rangle\, \langle q,\, \tau|x,\, 0\rangle \\ &\quad + \frac{1}{8\,\omega_+} \coth\left(\frac{\omega_+\beta}{2}\right) \operatorname{csch}\left(\frac{\omega_+\beta}{2}\right) \langle x',\, \beta|x,\, 0\rangle \qquad (6.71) \\ &= \frac{1}{4}\, \operatorname{csch}\left(\frac{\omega_+\beta}{2}\right)^2 \int dq\, q^2\, \Delta_A(x,\, 0;\, q,\, \tau)\Delta_A(q,\, \tau;\, x',\, \beta) \\ &\quad + \frac{1}{8\,\omega_+} \coth\left(\frac{\omega_+\beta}{2}\right) \operatorname{csch}\left(\frac{\omega_+\beta}{2}\right) \Delta_A(x,\, 0;\, x',\, \beta)\,. \qquad (6.72) \end{aligned}$$

The integral over q gives the expression bellow, which depends on τ,

$$\frac{\omega_+}{b_1(\tau,\beta)}\left[x\,\mathrm{csch}(\omega_+\tau)+x'\,\mathrm{csch}(\omega_+(\beta-\tau))\right]^2\times\,\Delta_A(x,\,0;\,x',\,\beta)$$
$$+\,\frac{b_0(\tau,\beta)}{b_1(\tau,\beta)}\times\Delta_A(x,\,0;\,x',\,\beta)\,, \tag{6.73}$$

where the functions $b_0(\tau,\beta)$ and $b_1(\tau,\beta)$ are defined as

$$b_0(\tau,\beta)\coloneqq\coth\left[\omega_+(\beta-\tau)\right]+\coth(\tau\omega_+)\,, \tag{6.74}$$
$$b_1(\tau,\beta)\coloneqq\omega_+\left[\coth(\omega_+(\beta-\tau))+\coth(\omega_+\tau)\right]^{5/2}$$
$$\times\sqrt{\mathrm{csch}(\omega_+\beta)\sinh(\omega_+\tau)\sinh\left[\omega_+(\beta-\tau)\right]}\,. \tag{6.75}$$

With the result of the integral over q, we can write the full expression for the matrix elements,

$$M_{AB}(x,x')=\,\Delta_A(x,\,0;\,x',\,\beta)$$
$$\times\left\{\frac{\omega_+}{4}\,\mathrm{csch}\left(\frac{\omega_+\beta}{2}\right)\frac{\left[x\,\mathrm{csch}(\omega_+\tau)+x'\,\mathrm{csch}(\omega_+(\beta-\tau))\right]^2}{b_1(\tau,\beta)}\right.$$
$$\left.+\,\frac{1}{4}\,\mathrm{csch}\left(\frac{\omega_+\beta}{2}\right)\frac{b_0(\tau,\beta)}{b_1(\tau,\beta)}+\frac{1}{8\,\omega_+}\coth\left(\frac{\omega_+\beta}{2}\right)\mathrm{csch}\left(\frac{\omega_+\beta}{2}\right)\right\}. \tag{6.76}$$

Finally, we can compute the first order corrections of $Z(\beta)$ and $Z_2(\beta)$, given in equations 6.48 and 6.49. After the integration over x, the first order correction of the partition function becomes

$$Z^{(1)}(\beta)=-\,\frac{1}{\omega_+}\,(1+e^{\,\omega_+\beta})^4\int_0^\beta d\tau$$
$$\times\left\{\frac{e^{4\,\omega_+\tau}\sqrt{\mathrm{csch}(\omega_+\beta)\,\mathrm{csch}[\omega_+(\beta-\tau)]\,\mathrm{csch}(\omega_+\tau)}}{(e^{2\,\omega_+\beta}-e^{2\,\omega_+\tau})^2(e^{2\,\omega_+\tau}-1)^2[\coth[\omega_+(\beta-\tau)]+\coth(\omega_+\tau)]^{\frac{5}{2}}}\right\}. \tag{6.77}$$

Then integrating the functions over τ from 0 to β, we obtain

$$Z^{(1)}(\beta)=\,-\,\frac{\beta}{16\,\omega_+}\,\mathrm{csch}\left(\frac{\omega_+\beta}{2}\right)^4\sinh(\omega_+\beta)\,. \tag{6.78}$$

For the factor $Z_2(\beta)$, after the integrals over x_1 and x_2 in equation 6.49, we obtain an expression that does not depend on τ. Therefore, after all integrations we find

$$Z_2^{(1)}(\beta) = -\frac{\beta}{16\,\omega_+}\left[1+2\,\cosh(\omega_+\beta)\right]\operatorname{csch}\left(\frac{\omega_+\beta}{2}\right)^2\operatorname{csch}(\omega_+\beta)^2\,. \tag{6.79}$$

After computing the zeroth and first order corrections of both $Z(\beta)$ and $Z_2(\beta)$, we are able to write the trace $\mathrm{Tr}_A(\rho_A^2)$ by replacing the different order corrections in equation 6.38,

$$\mathrm{Tr}_A(\rho_A^2) = \lim_{\beta\to\infty}\left[\tanh\left(\frac{\omega_+\beta}{2}\right) - g\,\frac{1}{2\,\omega_+}\,\frac{\beta}{\left[1+\cosh(\omega_+\beta)\right]}\right]. \tag{6.80}$$

The limit of the first term gives unity, as we have already calculated previously, while the second vanishes. Therefore, for this specific interaction, the results are trivial: as a first order approximations, both linear entropy and second Rényi entropy vanish. In the next section we discuss how one can compute higher order terms, but we will not perform these calculations for the coupled harmonic oscillators.

6.4 Higher orders

The higher order corrections in the perturbative expansion of the exponential $\exp[-g\,I_2[x_A,x_B]]$ around $g=0$ require that we compute some extra integrals over time. The nth term in the series expansion of the exponential is

$$g^n\,\frac{(-1)^n}{n!}\,I_2[x_A,x_B]^n\,, \tag{6.81}$$

or, in terms of the Euclidean-Lagrangian $\mathcal{L}_2$,

$$g^n\,\frac{(-1)^n}{n!}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_n\,\mathcal{L}_2(x_A(\tau_1),x_B(\tau_1))\,\ldots\,\mathcal{L}_2(x_A(\tau_n),x_B(\tau_n))\,. \tag{6.82}$$

The density matrix without approximations is given by equation 6.1, and we see that in the reduced density matrix, given by equation 6.1, there will be mean

values over the degrees of freedom of particle B. Therefore, it is useful to define the following nth order mean values

$$F_B^{(n)}[\{x_A(\tau_i)\}] := \int dy \int_{x_B(0)=y}^{x_B(\beta)=y} [\mathcal{D}x_B] \; \frac{(-1)^n}{n!} \prod_{i=1}^{n} \mathcal{L}_2(x_A(\tau_i), x_B(\tau_i)) \, e^{-I_1[x_B]} \,, \tag{6.83}$$

when $n = 0$ we have only the integral of the B propagator, i.e. the zeroth order of previous sections. The reduced density matrix, using this notation, is given by

$$\begin{aligned} \rho_A(x, x') = \lim_{\beta\to\infty} \frac{1}{Z(\beta)} \int_{x_A(0)=x}^{x_A(\beta)=x'} [\mathcal{D}x_A] \\ \times \left(F_B^{(0)} + g \int_0^\beta d\tau \, F_B^{(1)} + \cdots + g^n \prod_{i=1}^{n} \int_0^\beta d\tau_i \, F_B^{(n)} \right) e^{-I_1[x_A]} \,, \end{aligned} \tag{6.84}$$

and the partition function is

$$\begin{aligned} Z(\beta) = \int dx \int_{x_A(0)=x}^{x_A(\beta)=x} [\mathcal{D}x_A] \\ \times \left(F_B^{(0)} + g \int_0^\beta d\tau \, F_B^{(1)} + \cdots + g^n \prod_{i=1}^{n} \int_0^\beta d\tau_i \, F_B^{(n)} \right) e^{-I_1[x_A]} \,. \end{aligned} \tag{6.85}$$

In the expression for the partition function we have expectation values of the Euclidean Lagrangian $\mathcal{L}_2(x_A, x_B)$, with respect to both particles A and B. On the other hand, in $Z_2(\beta)$, we will have integrals over matrix elements. For this reason, we define

$$M_{AB}^{(n)}(x, x') = \int_{x_A(0)=x}^{x_A(\beta)=x'} [\mathcal{D}x_A] \; F_B^{(n)} \, e^{-I_1[x_A]} \,. \tag{6.86}$$

In terms of the matrix elements the partition function becomes

$$Z(\beta) = \int dx \left[M_{AB}^{(0)}(x, x) + \cdots + g^n \prod_{i=1}^{n} \int_0^\beta d\tau_i \, M_{AB}^{(n)}(x, x) \right] \,, \tag{6.87}$$

while the factor $Z_2(\beta)$ is

$$\begin{aligned} Z_2(\beta) = \int dx_1 \int dx_2 \left[M_{AB}^{(0)}(x_1, x_2) + \cdots + g^n \prod_{i=1}^{n} \int_0^\beta d\tau_i \, M_{AB}^{(n)}(x_1, x_2) \right] \\ \times \left[M_{AB}^{(0)}(x_2, x_1) + \cdots + g^n \prod_{i=1}^{n} \int_0^\beta d\tau_i \, M_{AB}^{(n)}(x_2, x_1) \right] \,. \end{aligned} \tag{6.88}$$

Then we collect the terms of same order to write $Z(\beta)$ and $Z_2(\beta)$ as

$$Z(\beta) = Z^{(0)}(\beta) + g\, Z^{(1)}(\beta) + \cdots + g^n\, Z^{(n)}(\beta), \tag{6.89}$$

$$Z_2(\beta) = Z_2^{(0)}(\beta) + g\, Z_2^{(1)}(\beta) + \cdots + g^n\, Z_2^{(n)}(\beta), \tag{6.90}$$

where the nth term of each is given by

$$Z^{(n)}(\beta) = \prod_{i=1}^{n} \int_0^\beta d\tau_i \int dx\, M_{AB}^{(n)}(x,x)\,, \tag{6.91}$$

$$Z_2^{(n)}(\beta) = \sum_{k=0}^{n} \int dx_1 \int dx_2 \prod_{i=1}^{n} \int_0^\beta d\tau_i\, M_{AB}^{(n)}(x_1,x_2) \prod_{j=1}^{n-k} \int_0^\beta d\tau_j\, M_{AB}^{(n-k)}(x_2,x_1)\,. \tag{6.92}$$

Therefore, in order to obtain the nth order correction of the trace $\mathrm{Tr}_A(\rho^2)$, we basically have to find the generic form of the matrix elements $M_{AB}(x,x')$ and perform several integrations involving them. When we calculate up to nth order, the trace becomes

$$\mathrm{Tr}_A(\rho_A^2) = \frac{\sum_{j=0}^{n} g^j\, Z_2^{(j)}(\beta)}{\left[\sum_{k=0}^{n} g^k\, Z^{(k)}(\beta)\right]^2}\,. \tag{6.93}$$

Afterwards, we make a series expansion of the denominator $Z(\beta)^2$ to find the form of $\mathrm{Tr}_A(\rho_A^2)$ as a power series in g. Higher order corrections can be demanding to compute analytically, but in our expressions the relevant quantities are given in a form that can be translated for use in numerical methods. Finally, one can use the results in $\mathrm{Tr}_A(\rho_A^2)$ to compute the approximation up to nth order of the linear entropy $S_L(\rho_A) = 1 - \mathrm{Tr}_A(\rho_A^2)$, and the second Rényi entropy $S_2(\rho_A) = -\log[\mathrm{Tr}_A(\rho_A^2)]$.

In summary, in this chapter, we have presented a practical method to compute the second Rényi entropy and the linear entropy. The basic idea is to write the density matrix as thermal distribution using the formalism described in chapter 5, and then make a perturbative expansion of $\exp(-g\, I_2[x_A, x_B])$ in powers of g, where $g\, I_2[x_A, x_B]$ corresponds to the entangling part of the full action of the problem. The method is limited to weak entanglement, but has the advantage that

well-established numerical techniques [10, 11] become applicable to compute entanglement measures. Stochastic quantization, in particular, can be quite useful. Although the tecnique is essentially a numerical method, analytical calculations are also possible within the approach known as noise perturbatiuon theory, recently used in different contexts [21, 22, 23, 24, 25]. Despite the limitation to weak entanglement, we recall that, in practice, entanglement is very fragile, for instance in macroscopic or not fully isolated systems. As such, perturbative approaches offer a very attractive possibility to quantify entanglement in many-body systems.

Chapter 7

Outlook

Our primary goal in this dissertation was to review methods to quantify entanglement in a quantum bipartite system. In quantum many-body physics, it is often hard to find an exact expression for the wave function due to the large size of the Hilbert space. Therefore, in these cases full diagonalization of the reduced density matrix is almost impossible, and we need to find other approaches to compute entanglement measures. We have discussed methods that are based on the Feynman path integrals, and we have provided ways to compute two entanglement measures for bipartite systems, namely the second Rényi entropy and the linear entropy. These measures are defined in terms of the trace of square of the reduced density matrix of one of the parts of the bipartite system, $\mathrm{Tr}_A(\rho_A^2)$. Our second goal was to formulate a practical method to compute entanglement measures in terms of expectation values and matrix elements of the dynamical variables of the system. We have used a system of two coupled harmonic oscillators to exemplify the application of the different methods. This system consists in a good pedagogical example because it allows us to compute analytically the entanglement entropies, including the path integrals.

Chapters 2 and 3 review the very basic concepts in quantum information and path integrals, respectively. Chapter 4 deals with the path integral representation of the ground-state wave function. This method is very standard, and it can be found in some textbooks [18]. The idea was to represent the two particle ground state wavefunction $\Psi(x, y)$ as the path integral from an arbitrary point (c_A, c_B) at imaginary time $\tau \to -\infty$ to the point (x, y) at $\tau = 0$. Together with the conjugate, we could write the ground state density matrix as a product of two path integrals

with special boundary conditions. Then we have worked on the reduced density matrix and the trace of its powers $\mathrm{Tr}\,\rho_A^n$. In particular, for $n = 2$, the trace is a product of four path integrals with boundary conditions that do no match. We have applied this method to successfully compute the linear entropy and second Rényi entropy for a system of two coupled harmonic oscillators.

The drawbacks to this method are that we have to know how to compute the path integral for the Euclidean Lagrangian $\mathcal{L}_E(x_A, x_B)$, and that we have to choose the boundary conditions (c_A, c_B) that appear at the times $\tau = \pm\infty$. We could get rid of these boundary conditions by replacing them with integrals, but this would make the calculations more complicated. The choice has to be carefully made because $\Psi(c_A, c_B)$ must not vanish. This method applied for entanglement between regions in space allows a clever technique to join these path integrals into a single one. In the review article of Ref. [1], the author demonstrates that, when A and B are intervals in space, the product of path integrals in $\mathrm{Tr}_A(\rho_A^n)$ reduces to a single path integral performed in a different geometry. Then the author has shown how to compute the entanglement entropy for free fields by taking the limit $n \to 1$ in the replica trick. Other applications of this method can be found in Refs. [26, 27, 28, 29], in which the authors use an auxiliary space, and a Monte Carlo method, to compute $\mathrm{Tr}_A(\rho_A^2)$ as the expectation value of a non physical operator.

In the method reviewed in Chapter 5, the ground state density matrix is given as the zero temperature limit of the thermal distribution $\exp(-\beta H)$ of inverse temperature β. The density matrix has the form of an evolution operator in imaginary time and it was straightforward to write it as a path integral. This technique proved to be very useful as it decreased by half the number of path integrals that appear in all quantities. Just like the method of chapter 4, this one requires that we know how to compute the path integral with the Euclidean Lagrangian $\mathcal{L}_E(x_A, x_B)$.

Once again, we have applied the method of chapter 5 to obtain the second Rényi entropy and linear entropy for the system of two coupled harmonic os-

cillators. This system consists in a good pedagogical example because we can analytically compute the path integral. Furthermore, for very large Hilbert spaces or complicated interactions, one can discretize the system and apply numerical methods to find the path integral, some examples are the Monte Carlo method and stochastic quantization. In Refs. [8, 9], the authors use the same representation introduced in chapter 5 for the reduced density matrix. In these works, they use an approximation in the replica trick expression to calculate entanglement entropy in lattice gauge theories, which effectively corresponds to the calculation of $\mathrm{Tr}_A(\rho_A^2)$.

In chapter 6, we have used the method of chapter 5 to formulate a practical method to compute entanglement measures. The method is based on a perturbative expansion of $\exp\left(-g\, I_2[x_A, x_B]\right)$ in powers of g, where $I_2(x_A, x_B)$ is the interaction part of the action, which has strength measured by the entanglement parameter g. The validity of this method is limited to the weakly entangled systems. The method allowed us to express $\mathrm{Tr}_A(\rho_A^2)$, and therefore entanglement, in terms of propagators, expectation values, and matrix elements computed with the single particle Euclidean Lagrangian $\mathcal{L}_1$.

We have applied the perturbative expansion method to obtain explicit expressions for the linear entropy and second Rényi entropy to first order in the entangling coupling. For the coupled harmonic oscillator we have shown explicitly that in the zeroth order approximation $\mathrm{Tr}_A(\rho_A^2) = 1$, which characterizes a pure state. This is the correct result because $g = 0$ corresponds to the limit where the particles are not entangled at all, and for a pure state we have $\rho_A^2 = \rho_A$. Still for the case of the coupled harmonic oscillators, we have shown explicitly that the $\mathcal{O}(g)$ vanishes due to the form of the action of the problem. For a generic problem, the $\mathcal{O}(g)$ expression we derived will not be zero.

In a near future, we expect to apply the perturbative expansion introduced in chapter 6 to systems with more involved interactions. We are also looking forward to explore to apply this perturbative method in field theory models. For these problems, we strongly believe that the use of the stochastic quantization

method will be fruitful to obtain the necessary propagators, expectation values, and matrix elements that are required to obtain the entanglement measures.

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