Entanglement entropy of coupled harmonic oscillators: an approach in Fock space

Maxime Jonker

August 2, 2016

Master's Thesis

Supervisor:
Prof. Stefan Vandoren

Institute for Theoretical Physics

Utrecht University

Abstract

It has been known for decades that black holes behave as thermodynamic objects and, as such, have an entropy, which was acquired in exact form as the Bekenstein-Hawking entropy. However, the origin of this entropy, and in particular its proportionality to the area of the horizon, remained unexplained. Motivated by this mystery, several authors examined the possibility of entanglement entropy as a source of black hole entropy, by considering a scalar field in the ground state and tracing out the degrees of freedom inside an imaginary sphere, analogous to the interior of the black hole. The resulting entanglement entropy between the two regions turned out to scale with the area of their mutual boundary. In the simplest model the scalar field is represented by a system of coupled harmonic oscillators. After an introduction to the phenomenon of quantum entanglement and the associated entanglement entropy, we will review the problem of two coupled oscillators in the ground state and derive the entanglement entropy using an approach in Fock space, as opposed to the standard method involving integrals in positon space. This will also allow us to look at some excited states of the system. Subsequently we will try to extend this approach to a system of N coupled harmonic oscillators and derive the entanglement entropy between an inner and outer region of oscillators.

Contents

1 Introduction

1.1 Background and motivation

The starting point of the project presented in this thesis was a famous paper by Srednicki from 1993 [1], in which the so-called area law was derived. This paper was motivated by the desire to comprehend the form and origin of the entropy of a black hole. It had already been recognised that black holes behave to exterior observers as thermodynamic objects, and, as such, also have an entropy. This entropy, called the Bekenstein-Hawking entropy and denoted by S_{BH}, was in the 1970's found to be proportional to the area of the black hole horizon [2].

Classically, however, the entropy of a system is an extensive quantity, meaning that it scales with the system's volume. Besides, it is not obvious how to interpretate S_{BH} from the perspective of statistical mechanics, where the entropy S is usually related to the number of accessible microstates of the system, or, in the case of a quantum system, the number of available quantum states. It is, however, unknown how many quantum state configurations the black hole interior can have for a given macrostate and whether this number is even finite.

Srednicki [1], and a few years earlier Bombelli *et al.* [3], presumed that the black hole entropy could have a special quantum mechanical origin, namely that it could result from the quantum entanglement between the degrees of freedom interior and exterior to the horizon. Entanglement is a purely quantum mechanical phenomenon which will be explained below in Section 1.2. Associated with this phenomenon, is the notion of entanglement entropy.

In [1] and [3] the black hole and its surroundings were modelled by a scalar quantum field in the ground state, upon which the degrees of freedom inside an imaginary sphere, representing the black hole, were integrated out. The resulting reduced system represented the surroundings of the black hole, reflecting the fact that the interior of the horizon is inaccessible to exterior observers. The entanglement entropy resulting from the correlations between the degrees of freedom in the two regions, turned out to be proportional to the area of the boundary between the regions, hence the name area law, with this boundary representing the black hole horizon.

As a first approximation, the authors considered a system of coupled harmonic oscillators which was then extended to a bosonic scalar field. When integrating out a part of these oscillators and evaluating the corresponding entanglement entropy, they used integrals of wave functions in position space. In general, numerous accounts of entanglement entropy in systems consisting of coupled harmonic oscillators have been provided in the literature, but the problem is either approached from a position space basis, e.g. in [4] and [5], or the entanglement entropy is examined in terms of other quantities such as the logartihmic negativity, as in [6] and [7].

In this thesis we take a different approach: we will derive the entanglement entropy between coupled harmonic oscillators by using a basis in Fock space. The aim is to provide more insight into results obtained by other authors, but also to be able to extend these results to excited states of the system. From a broader perspective, we presume that an approach in Fock space could help in gaining a better understanding of entanglement entropy in quantum field theories. Only in

the case of $2d$ conformal field theories has entanglement entropy been thoroughly described and understood [8], where it is related to holographic entanglement entropy, which by the AdS/CFT correspondence has in turn provided new insight into black hole entropy [9]. This topic, however, is well beyond the scope of the project presented here.

We will now proceed by explaining the phenomenon of quantum entanglement and the resulting entanglement entropy in Section 1.2. Then we will discuss the simplest problem of two coupled harmonic oscillators in Chapter 2, where we will start by reviewing the derivation of the entanglement entropy for the system's ground state in position space and subsequently derive the same results from our Fock space approach. We will then show how to extend this to some particular excited states of the system. In Chapter 3, we will consider the problem of N coupled oscillators, again reviewing how to find the entanglement entropy from a basis in position space and subsequently examining the same system in the language of Fock space. At last, in Chapter 4, we will conclude our work and present an outlook.

1.2 Entanglement entropy in the quantum mechanical framework

In this section we are going to give a description of quantum entanglement within the mathematical framework of quantum mechanics and show how the notion of entropy is extended to entanglement entropy, which can be interpreted as a measure of quantum entanglement [10]. In order to do so, we will make a distinction between two different kinds of quantum states, namely pure states and mixed states, and describe both of them in terms of density operators. Density operators, also called density matrices, will prove to be a crucial tool for expressing the entropy associated to either a mixed quantum state or a pure, entangled quantum state.

1.2.1 Pure states

When the quantum state of a system is fully known, i.e. when there is full access to all the information in the system, we can express the state of the system as a pure state, say $|\Psi\rangle$. This state $|\Psi\rangle$ can still be a superposition of different quantum states, for example a superposition of different eigenstate of the Hamiltonian operator corresponding to the system. In this sense one might think there is no complete information about the state of the system, since one cannot tell what the exact energy of the system is until one performs a measurement and the system's wave function collapses into one of the Hamiltonian eigenstates. However, this kind of uncertainty is intrinsic to quantum mechanics and could therefore never be removed. Hence, it does not reflect any incompleteness with respect to our knowledge, but rather is an inherent feature of nature.

Let us now consider a system that can be divided in two subsystems, say A and B. The total Hilbert space in which the state vector of the system lives, can correspondingly be divided into two subspaces, i.e.:

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B. \tag{1.1}$$

Let us denote a basis of state vectors in $\mathcal{H}_A$ by $|\psi_n\rangle_A$ and a basis of state vectors in $\mathcal{H}_B$ by

$|\phi_n\rangle$. The state $|\Psi\rangle$ of the total system can generally be expressed as a superposition of tensor products between these basis vectors:

$$|\Psi\rangle \;=\; \sum_{n,m} C_{nm}\, |\psi_n\rangle_A \otimes |\phi_m\rangle_B \,. \tag{1.2}$$

In general it is not possible to describe the states of the two subsystems independently of each other, but in the case that this is possible, we speak of a separable state or product state. Mathematically this means that we can write each element of the coefficient matrix C_{nm} in the following way:

$$C_{nm} \;=\; c_{A,n}\, c_{B,m}, \text{ for all } n, m \,, \tag{1.3}$$

where the $c_{A,n}$ and $c_{B,m}$ are sets of coefficients satisfying

$$\sum_n |c_{A,n}|^2 \;=\; \sum_m |c_{B,m}|^2 \;=\; 1. \tag{1.4}$$

The state of the composite system can then be written as

$$|\Psi\rangle \;=\; \sum_n c_{A,n}\, |\psi_n\rangle_A \otimes \sum_m c_{B,m}\, |\phi_m\rangle_B \,. \tag{1.5}$$

As is clear from Eq.(1.5), the state $|\Psi\rangle$ can now be expressed as a tensor product between two pure states, each of which describes one of the subsystems and is restricted to the corresponding subspace of the total Hilbert space. When the composite system is in such a separable state, there is no quantum entanglement between subsystem A and subsystem B. Indeed, in terms of the quantum mechanical formalism we can define quantum entanglement as the phenomenon where the state of one system cannot be described independently of the state of another system. Consequently, we speak of an entangled state whenever the condition in Eq.(1.3) does not hold.

In order to understand quantum entanglement on a mathematically more rigorous level, let us introduce the density operator ρ, given by

$$\rho \;=\; |\Psi\rangle \langle\Psi| \;, \tag{1.6}$$

for any pure quantum state $|\Psi\rangle$. The density operator is a projetion operator that can be very useful when calculating quantum mechanical probabilities, which will become more apparent in due course, when we consider mixed states. The expectation value of an operator A in the state $|\Psi\rangle$ can be expressed by means of the density operator as

$$\langle A\rangle_\Psi \;=\; \mathrm{Tr}(A\rho) \,. \tag{1.7}$$

This can be verified by expanding the state $|\Psi\rangle$ in the complete and orthonormal set of eigenstates

$|\alpha_i\rangle$, with eigenvalues a_i, of the operator A, i.e.

$$|\Psi\rangle \;=\; \sum_i c_i\,|\alpha_i\rangle\;, \tag{1.8}$$

such that

$$\mathrm{Tr}(A\rho) \;=\; \sum_{i,j} c_i c_j^*\,\mathrm{Tr}(A\,|\alpha_i\rangle\,\langle\alpha_j| \;=\; \sum_{i,j} c_i c_j^* \sum_k \langle\alpha_k|\,A\,|\alpha_i\rangle\,\langle\alpha_j|\alpha_k\rangle \tag{1.9}$$

$$= \sum_{i,j} a_i c_i c_j^* \sum_k \langle\alpha_k|\alpha_i\rangle\,\langle\alpha_j|\alpha_k\rangle \;=\; \sum_i a_i |c_i|^2 = \langle A\rangle_\Psi\;, \tag{1.10}$$

where we used the orthonormality condition $\langle\alpha_i|\alpha_j\rangle = \delta_{ij}$ and where $|c_i|^2$ is interpreted in the standard way as the probability that a measurement of the observable represented by A yields outcome a_i.

Let us consider the density matrix for a state that has the form of Eq.(1.2), hence describing a system consisting of subsystems A and B. By Eq.(1.6), the density matrix can be written as

$$\rho = \sum_{n,m}\sum_{k,l} C_{nm}C_{kl}^*\,|\psi_n\rangle_A\langle\psi_k| \otimes |\phi_m\rangle_B\langle\phi_l|. \tag{1.11}$$

Although we cannot, in general, describe the state of either subsystem separately due to quantum entanglement, we can take the density matrix and trace over the degrees of freedom residing in one of the two subsystems, resulting in the reduced density matrix of the other subsystem, i.e.

$$\rho_A = \mathrm{Tr}_B\,\rho\,; \quad \rho_B = \mathrm{Tr}_A\,\rho\,. \tag{1.12}$$

Starting from Eq.(1.11) we find that the reduced density matrix ρ_A for subsystem A reads

$$\rho_A \;=\; \sum_{n,m}\sum_{k,l} C_{nm}C_{kl}^*\,|\psi_n\rangle_A\langle\psi_k| \sum_j {}_B\langle\phi_j|\phi_m\rangle_B\langle\phi_l|\phi_j\rangle_B \tag{1.13}$$

$$= \sum_{n,m,k} C_{nm}C_{km}^*\,|\psi_n\rangle_A\langle\psi_k| \;=\; \sum_{n,k}(CC^\dagger)_{nk}\,|\psi_n\rangle_A\langle\psi_k|, \tag{1.14}$$

where, in going from Eq.(1.13) to Eq.(1.14), we used again the orthonormality of the states $|\phi_i\rangle$, that is $\langle\phi_i|\phi_j\rangle = \delta_{ij}$. We see that the reduced density matrix ρ_A in the basis of $|\psi_n\rangle$ is given by $CC^\dagger$. The reduced density matrix thus satifies the general requirement for density matrices that the trace be equal to 1:

$$\mathrm{Tr}\rho_A = \mathrm{Tr}(CC^\dagger) = \sum_{n,m} |C_{nm}|^2 = 1\,. \tag{1.15}$$

Before proceeding with a definition of entanglement entropy in terms of reduced density matrices, it is useful to have a look at mixed states and the kind of density matrices they give rise to.

1.2.2 Mixed states

As explained above, pure states can be assigned to systems when one has all available knowledge with respect to the state of the system. However, often the obsever does not have full access to all the information about the system, for instance in the case of a statistical ensemble. The closest one can get in this case is a probability distribution over a large number of states. In this situation we speak of a mixed state.

Density matrices form a particularly useful way of describing systems like these, when one does not know in which exact state the system is, but one does know the probabilities for the different states the system could be in. If we denote the different possible states by $|\Psi_n\rangle$ and the corresponding probabilities by p_n, the density matrix corresponding to this mixed state takes the form

$$\rho = \sum_n p_n \rho_n \;=\; \sum_n p_n \left|\Psi_n\right\rangle \left\langle\Psi_n\right| \,, \tag{1.16}$$

where ρ_n is the density matrix corresponding to a pure state $|\Psi_n\rangle$. Note that the set of states $|\Psi_n\rangle$ does by no means have to form an orthonormal basis of the system's Hilbert space. Eq.(1.7) can be extended to mixed states such that the ensemble average $\langle A\rangle$ is given by

$$\langle A\rangle \;=\; \mathrm{Tr}(A\rho)\,. \tag{1.17}$$

The trace condition, i.e. the condition that the trace of the density matrix be equal to 1, still holds as well, which can be seen when expanding the states $|\Psi_n\rangle$ in an orthonormal set of states $|\psi_i\rangle$ spanning the Hilbert space:

$$|\Psi_n\rangle = \sum_i c_{n,i} \left|\psi_i\right\rangle \,, \tag{1.18}$$

leading to

$$\begin{aligned} \mathrm{Tr}\rho &= \sum_n p_n \mathrm{Tr}\rho_n && (1.19)\\ &= \sum_n p_n \sum_{i,j} c_{n,i} c^*_{n,j} \sum_k \left\langle\psi_k|\psi_i\right\rangle \left\langle\psi_j|\psi_k\right\rangle && (1.20)\\ &= \sum_{i,n} p_n |c_{n,i}|^2 \;=\; 1\,, && (1.21) \end{aligned}$$

since $\sum_n p_n = 1$ by definition.

A well known and often encountered example of a mixed state is the thermal mixture where the probability distribution is given by the Boltzmann distribution:

$$p_n = \frac{e^{-\beta\epsilon_n}}{\sum_n e^{-\beta\epsilon_n}} = \frac{e^{-\beta\epsilon_n}}{Z}\,, \tag{1.22}$$

with the ϵ_n denoting the energy eigenvalues and Z the partition function. The density operator in the basis of energy eigenstates $|n\rangle$ then takes the form

$$\rho = \sum_n \frac{e^{-\beta\epsilon_n}}{Z} |n\rangle \langle n| \,, \tag{1.23}$$

which can be written in basis independent form as

$$\rho = \frac{e^{-\beta H}}{\mathrm{Tr}\,(e^{-\beta H})} \,, \tag{1.24}$$

where H is the Hamiltonian operator.

Thermal mixtures and other statistical ensembles are the subject of study in the field of statistical mechanics, where relevant (classical) thermodynamic quantities are derived from the partition function of a system. One such quantity is the entropy S, which can be interpreted as a measure of the amount of disorder in the system. In the language of statistical physics this translates to the degree of spread in the probability distribution over the possible (classical) states of the system, for some fixed macroscopic quantities such as temperature. Hence, if the probability for the system to be in one specific state is high and the probabilities for the other states are low, the entropy is low, since one can predict with significant certainty what state the system is in. If, on the other hand, the distribution over all possible states shows a large spread, the system shows more disorder and the uncertainty is larger, resulting in a high entropy. The definition of entropy that explicitly takes these probabilities into account is the one for the Gibbs entropy [11], given by

$$S = -k_B \sum_i p_i \log p_i \,, \tag{1.25}$$

where p_i is the probability to be in state i and k_B is the Boltzmann constant.

A way to extend the notion of entropy from a classical quantity to a quantum mechanical one, is by interpreting the entropy as a measure of the degree of mixing of a quantum mechanical system. This should intuitively be clear, for the more mixed a system is, the larger the spread in the probability distribution and hence, the higher the entropy. Accordingly, there is no such entropy associated to pure states, as there is no uncertainty with respect to which state the system is in, when it is in a pure state. In the case of a mixture, the probabilities corresponding to the different quantum states are nothing but the eigenvalues of the density matrix that describes the mixed state, as follows from Eq.(1.16). Therefore,we can extend Eq.(1.25) to the so-called von Neumann entropy S_{vN}, which reads

$$S_{vN} = -\mathrm{Tr}(\rho \log \rho) \,. \tag{1.26}$$

The von Neumann entropy can be considered the quantum mechanical extension of the Gibbs entropy, since it describes the entropy associated with quantum mechanical mixtures.

The idea that the entropy is larger when the spread in the probability distribution over available states is larger, naturally applies in the quantum mechanical picture as well. Suppose there are N possible states, then the probability distribution is maximally spread when the probability for each state equals $1/N$. Quantum mechanically this situation corresponds to a mixed state in an N-dimensional Hilbert space where one can choose a basis of states such that the probability corresponding to each of these basis states equals $1/N$. This is expressed by an $N \times N$ density matrix of the form

$$\rho = \begin{pmatrix} 1/N & 0 & \cdots & 0 \\ 0 & 1/N & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/N \end{pmatrix} . \tag{1.27}$$

States of this form are called maximally mixed states and they consequently have the highest entropy. The expression for this maximum value of the von Neumann entropy follows from Eq.(1.26):

$$S = -N \left(\frac{1}{N} \log \left(\frac{1}{N} \right) \right) = \log N . \tag{1.28}$$

Now that we have related entropy to mixed quantum states, we can examine the kind of entropy related to the phenomenon of quantum entanglement: the entanglement entropy.

1.2.3 Entanglement entropy

Before we define entanglement entropy, we recall that the density matrix corresponding to a composite system consisting of subsystems A and B, can be traced over with respect to one of the subsystems, resulting in the reduced denity matrix of the other subsystem. Whereas the total density matrix describes a pure state, the reduced density matrix of either subsystem will, in the case that the two subsystems are entangled, be equivalent to the density matrix of a mixed state.

We will illustrate this by looking at a paradigm example of an entangled state: the spin singlet. This state describes two particles with spin $\frac{1}{2}$, call them spin_1 and spin_2, living in subspaces $\mathcal{H}_1$ and $\mathcal{H}_2$ of the total Hilbert space. In terms of the eigenstates, denoted by $|\uparrow\rangle$ and $|\downarrow\rangle$, of the spin operators corresponding to spin_1 and spin_2 along any fixed direction, the state reads

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_1 \otimes |\downarrow\rangle_2 - |\downarrow\rangle_1 \otimes |\uparrow\rangle_2 \right) . \tag{1.29}$$

Comparing this to Eq.(1.2) we can identify the matrix C as

$$C = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & 0 \end{pmatrix} . \tag{1.30}$$

Forming the density matrix ρ according to Eq.(1.11) and tracing out spin_2, we find the reduced density matrix ρ_1 of spin_1, the elements of which are, in the basis of eigenstates corresponding to spin_1, given by the elements of the matrix $CC^\dagger$. This gives

$$\rho_1 = CC^\dagger = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} , \tag{1.31}$$

or, equivalently,

$$\rho_1 = \frac{1}{2} \left|\uparrow\right\rangle_1 \left\langle\uparrow\right| + \frac{1}{2} \left|\downarrow\right\rangle_1 \left\langle\downarrow\right| . \tag{1.32}$$

A density matrix of this form could never correspond to a pure quantum state, but it could definitely describe a mixture of two pure states, both with probability $\frac{1}{2}$. One could even argue that tracing out one of the subsystems actually produces a mixed state. The incompleteness of information inherent to mixed states, is in this case not the result of a lack of knowledge about the state of the whole system, but of the fact that, due to the very nature of quantum entanglement, part of the information about subsystem A resides in the degrees of freedom of subsystem B which were traced out and are, therefore, no longer accessible.

In the same way that we could associate an entropy with the uncertainty carried by regular mixed states, we can define an entropy related to the mixed form of the reduced density matrix resulting from the quantum entanglement between different subsystems. This is what we call the entanglement entropy and it is defined in the same way as the von Neumann entropy in Eq.(1.26), but with the regular density matrix replaced by the reduced one. When a system in a pure state can be divided into two subsystems A and B that are entangled, the entanglement entropy can be expressed both in terms of ρ_A and ρ_B and is given by

$$S = -\text{Tr}(\rho_A \log \rho_A) \; = \; -\text{Tr}(\rho_B \log \rho_B) \, . \tag{1.33}$$

The equivalence of the two expressions in Eq.(1.33) can be proven by means of the Schmidt decomposition theorem [12]. In short this theorem says that there can always be found a basis such that the reduced density matrices of both subsystems are diagonal in this basis and have the same eigenvalues. The entanglement entropy in terms of these eigenvalues p_n simply reads

$$S = -\sum_n p_n \log p_n \, . \tag{1.34}$$

Returning to the spin singlet, we see that the reduced density matrix ρ_1 in Eq.(1.31) is of the form of the density matrix in Eq.(1.27), corresponding to a maximally mixed state. It follows that the entanglement entropy of singlet state is $S = \log 2$ and we say that this is an example of a maximally entangled state [5]. In general we can say that the entanglement entropy is measure for the amount of entanglement between two systems.

Now that we have given an account of quantum entanglement and entanglement entropy within the quantum mechanical framework. we will proceed in the next chapter with a derivation of the entanglement entropy corresponding to a system of two coupled harmonic oscillators.

2 Two coupled harmonic oscillators

As the harmonic oscillator could be considered the elementary building block of physical models, it is hardy surprising that it is a good starting point for studying the entanglement entropy of more complex systems and eventually quantum field theories, especially since a quantum field is essentially formed by an infinite set of harmonic oscillators. In this chapter we will restrict ourselves to the simplest system of harmonic oscillators that exhibits entanglement, namely the system of two equal, coupled harmonic oscillators.

In Section 2.1 we will follow [1] in finding the ground state of the system in position space, and deriving the corresponding entanglement entropy. In Section 2.2 we obtain the same results in Fock space using methods involving ladder operators. In Section 2.3 we will use the latter aproach to extend some of the results to excited states.

2.1 Ground state and entanglement entropy in position space

2.1.1 Diagonalising the Hamiltonian

Like any physical system, the system of two coupled harmonic oscillators can be described by a Hamiltonian. We suppose that the two oscillators are equal, in the sense that they have equal masses, which we set to 1, and equal frequencies when uncoupled. The Hamiltonian H is then, in general form, given by

$$H = \frac{1}{2}\left[p_1^2 + p_2^2 + k_0(x_1^2 + x_2^2) + k_1(x_1 - x_2)^2\right] , \tag{2.1}$$

where p_1 and p_2 are the momenta of the two oscillators and x_1 and x_2 their position coordinates, i.e. the coordinates desribing the displacement of the oscillators from their equilibrium positions. Furhtermore, $k_0^{1/2}$ is the frequency of both oscillators when they are uncoupled, while k_1 represents the coupling between them. The Hamiltonian can be cast into the form

$$H = \frac{1}{2}\sum_{i=1}^{2} p_i^2 + \frac{1}{2}\sum_{i,j=1}^{2} x_i K_{ij} x_j \, , \tag{2.2}$$

with K given by

$$K = \begin{pmatrix} k_0 + k_1 & -k_1 \\ -k_1 & k_0 + k_1 \end{pmatrix} . \tag{2.3}$$

In order to find an expression for the ground state of the system, we would like to diagonalise the matrix K by a unitary transformation, such that the Hamiltonian can be put into a decoupled form. Denoting the transformation matrix by U, a straightforward diagonalisation of Eq.(2.3) yields that

$$U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} , \tag{2.4}$$

such that the diagonal form K_D of K is given by

$$K_D = UK_DU^T = \begin{pmatrix} k_0 & 0 \\ 0 & k_0 + 2k_1 \end{pmatrix} . \tag{2.5}$$

We define new coordinates according to

$$\begin{pmatrix} x_+ \\ x_- \end{pmatrix} \equiv U \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \frac{x_1+x_2}{\sqrt{2}} \\ \frac{x_1-x_2}{\sqrt{2}} \end{pmatrix} ; \qquad \begin{pmatrix} p_+ \\ p_- \end{pmatrix} \equiv U \begin{pmatrix} p_1 \\ p_2 \end{pmatrix} , \tag{2.6}$$

in terms of which the Hamiltonian reads

$$H = \frac{1}{2} \left[p_+^2 + p_-^2 + \omega_+^2 x_+^2 + \omega_-^2 x_-^2 \right] , \tag{2.7}$$

where ω_+ and ω_- are the eigenvalues of Ω, thus the eigenfequencies of the system, given by

$$\omega_+ = k_0^{1/2} ; \qquad \omega_- = (k_0 + 2k_1)^{1/2} . \tag{2.8}$$

Eq.(2.7) shows precisely the decoupled form we aimed to obtain. It describes two uncoupled oscillators, one with frequency ω_+ and the other with frequency ω_-. The ground state wave function ψ_0 is then simply the product of the ground state wave functions corresponding to these oscillators, hence is given by

$$\psi_0(x_+, x_-) = \left(\frac{\omega_+}{\pi}\right)^{1/4} \exp\left[-\frac{1}{2}\omega_+ x_+^2\right] \times \left(\frac{\omega_-}{\pi}\right)^{1/4} \exp\left[-\frac{1}{2}\omega_- x_-^2\right] , \tag{2.9}$$

where we set $\hbar$ to 1, which will be maintained throughout this thesis. Eq.(2.9) can be rewritten in terms of the original coordinates as

$$\psi_0(x_1, x_2) = \frac{(\omega_+\omega_-)^{\frac{1}{4}}}{\sqrt{\pi}} \exp\left[-\frac{1}{2}\left(\frac{\omega_+ + \omega_-}{2}(x_1^2 + x_2^2) + (\omega_+ - \omega_-)x_1 x_2\right)\right] . \tag{2.10}$$

2.1.2 Deriving the entanglement entropy

Since we are eventually interested in the entanglement entropy between the oscillators, let us explicitly decompose the Hilbert space as

$$\mathcal{H}_1 \otimes \mathcal{H}_2 , \tag{2.11}$$

where $\mathcal{H}_1$ is the subspace corresponding to the oscillator with position x_1 and momentum p_1 and $\mathcal{H}_2$ is the subspace where the oscillator described by x_2 and p_2 lives. Now that we have obtained an expression for the ground state wave function in Eq.(2.10), we can form the density matrix and integrate out one of the two oscillators to arrive at the reduced density matrix, which will

eventually lead us to the entanglement entropy.

Because we are working in position space, the density matrix is given by

$$\rho(x_1, x_1'; x_2, x_2') = \langle x_1, x_2 | \, \rho \, | x_1', x_2' \rangle = \langle x_1, x_2 | \psi_0 \rangle \, \langle \psi_0 | x_1', x_2' \rangle = \psi_0(x_1, x_2) \psi_0^*(x_1', x_2') \, . \tag{2.12}$$

We now decide to integrate out the degrees of freedom corresponding to the second oscillator, which means that we have to integrate the density matrix over the variable x_2. This gives the reduced density matrix ρ_1 :

$$\rho_1(x_1, x_1') = \int_{-\infty}^{+\infty} dx_2 \, \psi_0(x_1, x_2) \psi_0^*(x_1, x_2') \, . \tag{2.13}$$

Substituting Eq.(2.10) into Eq.(2.13) and evaluating the gaussian integral by completing the square, we obtain

$$\rho_1(x_1, x_1') = \pi^{-\frac{1}{2}} \left(\frac{2\omega_+ \omega_-}{\omega_+ + \omega_-} \right)^{\frac{1}{2}} \exp \left[- \frac{(\omega_+ + \omega_-)^2 + 2\omega_+ \omega_-}{4(\omega_+ + \omega_-)} \, \frac{x_1^2 + x_1'^2}{2} + \frac{(\omega_+ - \omega_-)^2}{4(\omega_+ + \omega_-)} \, x_1 x_1' \right] . \tag{2.14}$$

In order to calculate the entanglement entropy S, we want to know the eigenvalues of $\rho_1(x_1, x_1')$ since S can be obtained straighforwardly from them, according to Eq.(1.34). Hence, we need to solve the eigenvalue equation

$$\int_{-\infty}^{+\infty} dx' \rho_1(x, x') f_i(x') = p_n f_n(x) \, . \tag{2.15}$$

The eigenfunctions $f_n(x)$ turn out to be equivalent to the eigenfuntions of a harmonic oscillator with frequency $\omega = (\omega_- \omega_+)^{1/2}$, such that

$$f_n(x) = H_n(\omega^{\frac{1}{2}} x) \exp(-\omega x^2/2) \, . \tag{2.16}$$

The eigenvalues p_n are given by

$$p_n = (1 - \xi^2) \xi^{2n} \, , \tag{2.17}$$

where the parameter ξ is defined by

$$\xi = \frac{\omega_-^{1/2} - \omega_+^{1/2}}{\omega_-^{1/2} + \omega_+^{1/2}} \, . \tag{2.18}$$

Note that this expression for ξ entails, by Eq.(2.8), that $0 < \xi < 1$, which is necessary in order for the p_n in Eq.(2.17) form a well defined probability distribution. The entanglement entropy

as a function of ξ is then given by

$$S(\xi) = -\sum_{n=0}^{\infty} p_n \log p_n \; = -\log(1-\xi^2) - \frac{\xi^2}{1-\xi^2}\log \xi^2. \tag{2.19}$$

2.2 Ground state and entanglement entropy in Fock space

In this section we are going to reproduce the result in Eq.(2.19) by taking an aproach to the problem in the language of Fock space instead of working with integrals in position space. Our aim in doing so is not merely to reproduce something we already know, but to gain more insight into the form of the ground state and density matrix when expressed in a basis that explicitly incorporates and illustrates the distinction between the two subspaces corresponding to the two oscillators. Moreover, we hope that this will enable us to extend our results more easily to excited states of the system.

2.2.1 Finding the ground state

To obtain an expression for the ground state in terms of ladder operators acting on states in Fock space, we start by introducing the annihilation and creation and operators corresponding to the $x_\pm$ and $p_\pm$ in Eq.(2.6):

$$a_\pm = \sqrt{\frac{\omega_\pm}{2}}(x_\pm + \frac{i}{\omega_\pm}p_\pm)\,; \qquad a_\pm^\dagger = \sqrt{\frac{\omega_\pm}{2}}(x_\pm - \frac{i}{\omega_\pm}p_\pm)\,, \tag{2.20}$$

satisfying the standard bosonic commutation relations:

$$[a_-, a_-^\dagger] = [a_+, a_+^\dagger] = 1\,. \tag{2.21}$$

Because the Hamiltonian is decoupled in this basis, we can write it in terms of the ladder operators as

$$H = \omega_+ a_+^\dagger a_+ + \omega_- a_-^\dagger a_- + \frac{1}{2}(\omega_+ + \omega_-)\,, \tag{2.22}$$

where the first terms are number operators, corresponding to the new uncoupled oscillators, and the third term represents the ground state energy. Due to the decoupled form of Eq.(2.22), any eigenstate of H can be written as a product of the single oscillator eigenstates of the operators $a_-^\dagger a_-$ and $a_+^\dagger a_+$. Hence, the ground state is written in this basis as

$$|0\rangle = |0\rangle_- \otimes |0\rangle_+ \,. \tag{2.23}$$

Clearly $|0\rangle$ is annihilated by both annihilation operators:

$$a_\pm |0\rangle = 0\,. \tag{2.24}$$

Although we have obtained an expression for the ground state, in the form of Eq.(2.22), it does not allow us to calculate the entanglement entropy between the two original oscillators. The reason is that the $\pm$-basis corresponds to a different decomposition of the Hilbert space than the one we have supposed, given by Eq.(2.11) .Therefore we cannot integrate out the degrees of freedom in either of our chosen subspaces from a state expressed in this $\pm$-basis. This is also evident from the fact that $a_\pm$ and $a_\pm^\dagger$ depend on the position and momentum of both original oscillators as a result of the transformation in Eq.(2.6).

Hence, we want to express $|0\rangle$ in terms of ladder operators that are confined to either $\mathcal{H}_1$ or $\mathcal{H}_2$, which is equivalent to saying that we want to find and expression of the form

$$|0\rangle = \sum_{n,m} C_{nm} |n\rangle_1 \otimes |m\rangle_2 \,, \tag{2.25}$$

where the $|n\rangle_1$ constitute a basis in $\mathcal{H}_1$ and the $|m\rangle_2$ in $\mathcal{H}_2$. The first step towards finding the ladder operators corresponding to this desired basis, that is, the ladder operators raising and lowering the states $|n\rangle_1$ and $|m\rangle_2$ in Eq.(2.25), is to realise and utilise the fact that linear combinations of a_+ ad a_- also annihilate $|0\rangle$. By anticipation and trial and error, the following particular combination turns out to be fruitful:

$$a = \frac{1}{\sqrt{2}}(a_+ + a_-)\,; \qquad b = \frac{1}{\sqrt{2}}(a_+ - a_-)\,, \tag{2.26}$$

where a and b are in fact new annihilation operators rotated by an angle $\pi/4$ with rspect to a_+ and a_-. Following Eqs.(2.6) and (2.20), we can write a and b in terms of the original position and momentum operators, which, upon some reordering, yields

$$a = \frac{1}{\sqrt{1-\xi^2}} \left(\sqrt{\frac{\omega}{2}} \left(x_1 + \frac{i}{\omega} p_1 \right) - \xi \sqrt{\frac{\omega}{2}} \left(x_2 - \frac{i}{\omega} p_2 \right) \right) \,; \tag{2.27}$$

$$b = a\,(x_1 \leftrightarrow x_2,\, p_1 \leftrightarrow p_2)\,, \tag{2.28}$$

where, just like in section 2.1, ω and ξ are, given by

$$\omega = (\omega_- \omega_+)^{1/2}\,; \qquad \xi = \frac{\omega_-^{1/2} - \omega_+^{1/2}}{\omega_-^{1/2} + \omega_+^{1/2}}\,. \tag{2.29}$$

In the expression for a given by Eq.(2.27) we can recognise two ladder operators of the form that we are looking for, one of them living exclusively in $\mathcal{H}_I$, the other in $\mathcal{H}_{II}$. More precisely, if we let

$$\alpha = \sqrt{\frac{\omega}{2}} \left(x_1 + \frac{i}{\omega} p_1 \right) \,; \qquad \beta = \sqrt{\frac{\omega}{2}} \left(x_2 + \frac{i}{\omega} p_2 \right) \,, \tag{2.30}$$

we can write a and b as

$$a = \frac{1}{\sqrt{1-\xi^2}}\left(\alpha - \xi\beta^\dagger\right) \; ; \qquad b = \frac{1}{\sqrt{1-\xi^2}}\left(\beta - \xi\alpha^\dagger\right) \; . \tag{2.31}$$

Note that α, despite depending only on x_1 and p_1, does not really correspond to the original oscillator with coordinates x_1 and p_1, nor does β correspond to the original oscillator described by x_2 and p_2 in the Hamiltonian in Eq.(2.1). These original oscillators both had frequency $k_0^{1/2} = \omega_+$ and were, from a classical point of view, coupled by a spring constant k_1, whereas α and β correspond to oscillators with frequency $\omega = (\omega_-\omega_+)^{1/2}$ that result from a rotation among the system's eigenstates.

Since a and b annihilate the ground state, it follows from Eq.(2.31) that

$$(\alpha - \xi\beta^\dagger)\,|0\rangle \; = \; (\beta - \xi\alpha^\dagger)\,|0\rangle = 0\,, . \tag{2.32}$$

hence

$$\alpha\,|0\rangle = \xi\beta^\dagger\,|0\rangle \; ; \tag{2.33}$$

$$\beta\,|0\rangle = \xi\alpha^\dagger\,|0\rangle \; . \tag{2.34}$$

Writing the ground state in the form of Eq.(2.25) and acting on it with α gives

$$\alpha\,|0\rangle = \sum_{n,m=0}^{\infty} C_{nm}\sqrt{n}\,|n-1\rangle_1 \otimes |m\rangle_2 = \sum_{n,m=0}^{\infty} C_{(n+1)m}\sqrt{n+1}\,|n\rangle_1 \otimes |m\rangle_2 \; , \tag{2.35}$$

where we used that the $\alpha^{(\dagger)}$ act on $|n\rangle_1$ as standard ladder operators, i.e.

$$\alpha\,|n\rangle_1 = \sqrt{n}\,|n-1\rangle_1 \; ; \qquad \alpha^\dagger\,|n\rangle_1 = \sqrt{n+1}\,|n+1\rangle_1 \; . \tag{2.36}$$

Meanwhile, the right hand side of Eq.(2.33) can be worked out to give

$$\xi\beta^\dagger\,|0\rangle = \sum_{n,m=0}^{\infty} \xi C_{nm}\sqrt{m+1}\,|n\rangle_1 \otimes |m+1\rangle_2 = \sum_{n,m=0}^{\infty} \xi C_{n(m-1)}\sqrt{m}\,|n\rangle_1 \otimes |m\rangle_2 \; . \tag{2.37}$$

Equating Eqs.(2.35) and (2.37) it follows that their coefficients have to be equal, i.e.

$$C_{(n+1)m}\sqrt{n+1} = \xi C_{n(m-1)}\sqrt{m}\,. \tag{2.38}$$

Working out Eq.(2.34) in the same way yields a similar relation, viz.

$$C_{n(m+1)}\sqrt{m+1} = \xi C_{(n-1)m}\sqrt{n}. \tag{2.39}$$

Subsequently, Eq.(2.38) can be rewritten as

$$C_{nm} = \xi C_{(n-m)(m-1)} \sqrt{\frac{m}{n}} \,, \tag{2.40}$$

while from Eq.(2.39) it follows that

$$C_{nm} = \xi C_{(n-1)(m-1)} \sqrt{\frac{n}{m}} \,. \tag{2.41}$$

Eqs.(2.40) and (2.41) can only be consistent under the condition that $C_{nm} \propto \xi^n \delta_{nm}$. To find the right proportionality factor, we just have to make sure the ground state is normalised, which, according to Eq.(2.25), implies that $\sum_{n,m} |C_{nm}|^2 = 1$. It is then easily derived that

$$C_{nm} = \sqrt{1-\xi^2}\xi^n \delta_{nm} \,, \tag{2.42}$$

as, by definition, $0 < \xi < 1$. The ground state, at last, takes the form

$$|0\rangle = \sqrt{1-\xi^2} \sum_{n=0}^{\infty} \xi^n \, |n\rangle_1 \otimes |n\rangle_2 \,, \tag{2.43}$$

which, in terms of ladder operators, can be expressed as

$$|0\rangle = \sqrt{1-\xi^2} \sum_{n=0}^{\infty} \xi^n \, \frac{(\alpha^\dagger)^n}{\sqrt{n!}} \, \frac{(\beta^\dagger)^n}{\sqrt{n!}} \, |0\rangle_1 \otimes |0\rangle_2 \tag{2.44}$$

$$= \sqrt{1-\xi^2} \, \mathrm{e}^{\xi \alpha^\dagger \beta^\dagger} \, |0\rangle_1 \otimes |0\rangle_2 \,. \tag{2.45}$$

This result is in agreement with [3] and [5], however these authors did not give the relation between the operators we denote by α and β and the position and momentum operators x_1, p_1 and x_2, p_2. In other words, they did not show how to arrive at the new ladder operators $\alpha^{(\dagger)}$ and $\beta^{(\dagger)}$ starting from the system's two original oscillators. Nor did they give an expression for the parameter we named ξ in terms of the system's initial parameters, e.g. its eigenfrequencies. Here we have shown precisely how the basis used to express $|0\rangle$ in Eq.(2.45) is obtained from the basis of the system's eigenstates and the position and momentum operators corresponding to the two original oscillators.

2.2.2 Deriving the entanglement entopy

Having obtained an expression for the ground state in a basis that adopts the decompostion into $\mathcal{H}_I$ and $\mathcal{H}_{II}$, we are able to trace out either of the two subspaces. We first form the total density

matrix ρ from Eq.(2.43):

$$\rho = |0\rangle\langle 0| = (1-\xi^2)\sum_{n,n} \xi^{n+m}|n\rangle_1\langle m| \otimes |n\rangle_2\langle m| \,. \tag{2.46}$$

We subsequently trace over that part of ρ living in $\mathcal{H}_2$, forming the reduced density matrix ρ_1:

$$\rho_1 = \mathrm{Tr}_2\rho = (1-\xi^2)\sum_{n,m} \xi^{n+m}|n\rangle_1\langle m| \otimes \sum_k {}_2\langle k|n\rangle_2\langle m|k\rangle_2 \tag{2.47}$$

$$= (1-\xi^2)\sum_n \xi^{2n}|n\rangle_1\langle n| \,, \tag{2.48}$$

where we used the orthonormality of the basis, i.e. ${}_2\langle m|k\rangle_2 = \delta_{mk}$. Casting ρ_1 into the form

$$\rho_1 = \sum_n p_n |n\rangle_1\langle n| \,, \tag{2.49}$$

it is clear that its eigenstates are just the eigenstates $|n\rangle$ of an oscillator with frequency ω and its eigenvalues p_n are equal to $(1-\xi^2)\xi^{2n}$. This is in agreement with our discussion in Section 2.1, in particular Eqs.(2.16) and (2.17), and therefore perhaps not so surprising. However, the Fock space approach we took here probably provides more insight into the origin and derivation of this result.

We explained in Section 1.2 that reduced density matrices are often equivalent to density matrices describing mixtures. As also pointed out by Srednicki, the reduced density matrix we obtained in Eq.(2.48) can in fact be associated with a thermal mixture. We recall that a thermal mixture is given by a density matrix of the form

$$\rho_{th} = \frac{1}{Z} e^{-\beta H} \,, \tag{2.50}$$

which, in the basis of eigenstates of H, for a quantum harmonic oscillator becomes

$$\rho_{th} = \sum_n \frac{e^{-\beta n\omega}}{1-e^{-\beta\omega}} \, |n\rangle\langle n| \,. \tag{2.51}$$

Comparing this with Eq.(2.48), we see that both expressions are indeed equivalent if

$$p_n = \frac{e^{-\beta n\omega}}{1-e^{-\beta\omega}} = (1-\xi^2)\xi^{2n} \,, \tag{2.52}$$

which holds if we define the temperaure T of the mixture as

$$T = \beta^{-1} = \frac{\omega}{\log(\xi^{-2})} \,. \tag{2.53}$$

One should keep in mind, however, that this is just a way to interpret the form of ρ_1, which

is *not* the same as saying that the reduced system has a temperature T given by Eq.(2.53). The effect of tracing out one of the two oscillators is just that the resulting reduced system can mathematically be described as if it were a thermal mixture.

Since the entanglement entrop S only depends on the eigenvalues of ρ_1, we arrive at the same expression for S as in Eq.(2.19), i.e.

$$S(\xi) = -\sum_{n=0}^{\infty} p_n \log p_n \; = -\log(1-\xi^2) - \frac{\xi^2}{1-\xi^2}\log \xi^2 \,. \tag{2.54}$$

We note that we would obtain the same result if we decided instead to take the trace with respect to $\mathcal{H}_1$, which is easy to see from Eq.(2.47). The reduced density matrix would in this case read

$$\rho_2 = (1-\xi^2)\sum_n \xi^{2n} |n\rangle_2 \langle n| \,, \tag{2.55}$$

which shows that ρ_1 has the same eigenvalues as ρ_2 and consequently leads to the same entanglement entropy.

So far we have restricted our considerations and derivations to the ground state of the system. In the following section we will try to extend the methods we employed in this section to include some excited states as well.

2.3 Entanglement entropy of excited states

Another advantage of deriving an expression for the ground state in Fock space, besides putting the reduced density matrix in a more illuminating form, is that it allows us to straightforwardly act on it with creation operators and form excited states.

2.3.1 Excited states

Let us consider in particular the creation operators $a^\dagger$ and $b^\dagger$, obtained by taking the hermitian conjugate of Eq.(2.31). Acting with $a^\dagger$ on the ground state, given by Eq.(2.45), yields

$$a^\dagger |0\rangle = \sqrt{1-\xi^2} a^\dagger e^{\xi \alpha^\dagger \beta^\dagger} |0\rangle_1 \otimes |0\rangle_2 \tag{2.56}$$

$$= \sqrt{1-\xi^2} \left(e^{\xi \alpha^\dagger \beta^\dagger} a^\dagger + \left[a^\dagger, e^{\xi \alpha^\dagger \beta^\dagger} \right] \right) |0\rangle_1 \otimes |0\rangle_2 \,. \tag{2.57}$$

Substituting $a^\dagger = \frac{1}{\sqrt{1-\xi^2}}(\alpha^\dagger - \xi\beta)$ and using that $\beta |0\rangle_2 = 0$, we get

$$a^\dagger |0\rangle = \left(e^{\xi \alpha^\dagger \beta^\dagger} \alpha^\dagger - \xi \left[b, e^{\xi \alpha^\dagger \beta^\dagger} \right] \right) |0\rangle_1 \otimes |0\rangle_2 \,. \tag{2.58}$$

To work out the commutator we first expand the exponential and then use the following identity:

$$[A, B^n] = nB^{n-1}[A,B] \quad \text{iff } [[A,B],B] = 0 \,, \tag{2.59}$$

which is proven in the Appendix (see A.1). This leads to

$$\left[b, e^{\xi\alpha^\dagger\beta^\dagger}\right] = \sum_{n=0}^{\infty} \frac{\xi^n}{n!}(\alpha^\dagger)^n[\beta, (\beta^\dagger)^n] \tag{2.60}$$

$$= \sum_{n=0}^{\infty} \frac{\xi^n}{n!}(\alpha^\dagger)^n\, n\, (\beta^\dagger)^{n-1} \tag{2.61}$$

$$= \xi \sum_{n=1}^{\infty} \frac{\xi^{n-1}}{(n-1)!}(\alpha^\dagger)^{n-1}(\beta^\dagger)^{n-1}\alpha^\dagger \tag{2.62}$$

$$= \xi \sum_{n=0}^{\infty} \frac{\xi^n}{n!}(\alpha^\dagger)^n(\beta^\dagger)^n\alpha^\dagger = e^{\xi\alpha^\dagger\beta^\dagger}\alpha^\dagger\,, \tag{2.63}$$

where we used that the $n = 0$ term in the sum in Eq.(2.61) does not contribute so we might as well let n start at 1. Substituting this result into Eq.(2.58), we arrive at

$$a^\dagger |0\rangle = (1-\xi^2)\, e^{\xi\alpha^\dagger\beta^\dagger}\alpha^\dagger |0\rangle_1 \otimes |0\rangle_2\,. \tag{2.64}$$

We see that acting with $a^\dagger$ on $|0\rangle$ results in an excitation of the oscillator corresponding to $\alpha^{(\dagger)}$. This result can be easily extended to acting n times with $a^\dagger$, yielding

$$(a^\dagger)^n |0\rangle = \left(\sqrt{1-\xi^2}\right)^{n+1} e^{\xi\alpha^\dagger\beta^\dagger}(\alpha^\dagger)^n |0\rangle_1 \otimes |0\rangle_2 \tag{2.65}$$

$$= \left(\sqrt{1-\xi^2}\right)^{n+1} e^{\xi\alpha^\dagger\beta^\dagger}\sqrt{n!}\, |n\rangle_1 \otimes |0\rangle_2\,, \tag{2.66}$$

where the factor $\sqrt{n!}$ arises because $\alpha^\dagger$ acts on $|0\rangle_1$ according to Eq.(2.36)

The state in Eq.(2.66) is, however, not properly normalised yet. Indeed, when calculating its norm, we find

$$|(a^\dagger)^n |0\rangle|^2 = \left(1-\xi^2\right)^{n+1} n! \left| \sum_{j=0}^{\infty} \frac{\xi^j}{j!}\sqrt{\frac{(n+j)!}{n!}}\sqrt{j!}\, |n+j\rangle_1 \otimes |j\rangle_2 \right|^2 \tag{2.67}$$

$$= \left(1-\xi^2\right)^{n+1} \sum_{j=0}^{\infty} \xi^{2j}\frac{(n+j)!}{j!} = n!\,. \tag{2.68}$$

We can now define normalised excited states, $|n_\alpha\rangle$, by

$$|n_\alpha\rangle \equiv \frac{1}{\sqrt{n!}}(\alpha^\dagger)^n |0\rangle = \left(\sqrt{1-\xi^2}\right)^{n+1} e^{\xi\alpha^\dagger\beta^\dagger} |n\rangle_1 \otimes |0\rangle_2\,. \tag{2.69}$$

The above discussion applies equally if, instead of $\alpha^\dagger$, we would act n times with $\beta^\dagger$, resulting

in an excited state $|n_\beta\rangle$, defined by

$$|n_\beta\rangle \equiv \frac{1}{\sqrt{n!}}\,(\beta^\dagger)^n\,|0\rangle \;=\; \left(\sqrt{1-\xi^2}\right)^{n+1}\; e^{\xi\alpha^\dagger\beta^\dagger}\,|0\rangle_1 \otimes |n\rangle_2\;. \tag{2.70}$$

2.3.2 Entanglement entropy

We can now evaluate the entanglement entropy between the two subsystems in the excited states defined above. To that end, we first have to obtain the reduced density matrix by tracing out one of the two subsystems. We will consider the state $|n_\alpha\rangle$, defined in Eq.(2.69), which has a density matrix given by

$$\rho = |n_\alpha\rangle\,\langle n_\alpha| = \frac{1}{n!}\left(1-\xi^2\right)^{n+1}\sum_{j,k=0}^{\infty}\xi^{j+k}\sqrt{\frac{(n+j)!\,(n+k)!}{j!\,k!}}\,|n+j\rangle_1\langle n+k|\otimes|j\rangle_2\langle k|\,. \tag{2.71}$$

We form the reduced density matrix ρ_1 in the usual way, by tracing over the basis $|m\rangle_2$, yielding

$$\rho_1 = (1-\xi^2)^{n+1}\sum_{j=0}^{\infty}\xi^{2j}\,\frac{(n+j)!}{n!\,j!}\,|n+j\rangle_1\langle n+j|\,. \tag{2.72}$$

From Eq.(2.72) we can read off the eigenvalues p_j of ρ_1. The entanglement entropy S follows in the usual way according to $S = -\sum_j p_j \log p_j$, which gives

$$S = -\sum_j (1-\xi^2)^{n+1}\,\xi^{2j}\,\frac{(n+j)!}{n!\,j!}\log\left[(1-\xi^2)^{n+1}\xi^{2j}\,\frac{(n+j)!}{n!\,j!}\right]\,. \tag{2.73}$$

Writing the logarithmic term as $\log(1-\xi^2)^{n+1} + \log\xi^{2j} + \log\frac{(n+j)!}{n!\,j!}$ and simpifying the resulting first term of S gives

$$-\,(1-\xi^2)^{n+1}\log(1-\xi^2)^{n+1}\sum_j \xi^{2j}\,\frac{(n+j)!}{n!\,j!} \;=\; -(n+1)\log(1-\xi^2)\,, \tag{2.74}$$

where we recognised $\sum_j \xi^{2j}\frac{(n+j)!}{n!\,j!}$ as the infinte Taylor series of $f(\xi^2) = (1-\xi^2)^{-n-1}$ around $\xi^2 = 0$. The second term of S can, by some lines of algebraic manipulation, be cast into the form

$$-\,(1-\xi^2)^{n+1}\sum_j \xi^{2j}\,\frac{(n+j)!}{n!\,j!}\log\xi^{2j} \;=\; -(n+1)\frac{\xi^2}{1-\xi^2}\log\xi^2\,. \tag{2.75}$$

Combining it all, we find the following expression for S:

$$S \;=\; -(n+1)\log(1-\xi^2) - (n+1)\frac{\xi^2}{1-\xi^2}\log\xi^2 - (1-\xi^2)^{n+1}\sum_j \xi^{2j}\,\frac{(n+j)!}{n!\,j!}\log\frac{(n+j)!}{n!\,j!}\,. \tag{2.76}$$

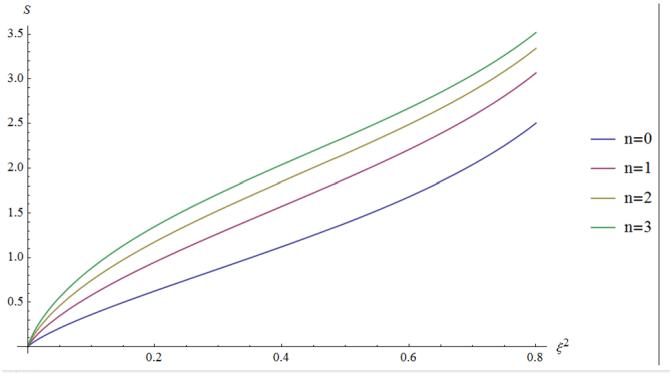

Figure 1: Entanglement entropy for excited states.

The reader can check that upon setting $n = 0$, i.e. going back to the ground state, the expression in Eq.(2.54) is retrieved.

Since Eq.(2.76) might not be very illuminating, we numerically evaluate S for the first three excited levels, i.e. $n = 1$ up to $n = 3$. A plot of the result is shown in Fig.1, where we also included the ground state and where S is displayed as a function of ξ^2. We see that S increases for each level, whereas the shape of the graph showing the dependence of S on ξ^2, remains roughly the same. We also see that S increases for increasing ξ^2, in each of the levels. This can be explained by recalling the expression for ξ, given by Eq.(2.18), and noting that ξ is small when $\omega_+ \approx \omega_-$. As follows from Eq.(2.8), this is the case when $k_1 \approx 0$, hence when the coupling between the two original oscillators is small. This should intuitively make sense, since there is simply no entanglement between decoupled systems.

We remark that the particular excited states we have been considering here are not the eigenstates of the system's Hamiltonian. After all, these eigenstates are formed by acting with the operators $a_\pm^\dagger$ on the ground state in the $\pm$-basis, as is evident from Eq.(2.23). Instead, the creation operators $a^\dagger$ and $b^\dagger$ that we used to excite $|0\rangle$ are linear combinations of $a_\pm^\dagger$, following from Eq.(2.26). Consequently, the states $|n_\alpha\rangle$ and $|n_\beta\rangle$ are linear combinations of the eigenstates of H. The reason we chose to consider these states rather than the actual eigenstates, is because they allowed for a better analytical derivation and a more elegant result. Further work could examine the form of the entanglement entropy in the excited eigenstates.

Now that we have worked through the problem of two coupled oscillators and derived the entanglement entropy between them, not only in the ground state but in some particular excited states as well, it is time to consider the more general and more complicated problem consisting of N coupled oscillators, where N can be any positive integer. This will be the topic of the next chapter.

3 N coupled harmonic oscillators

In this chapter we are, as announced, going to look at a system consisting of a general number of N coupled harmonic oscillators. We are interested in this generalisation not only for the obvious reason that results obtained for this general case will be more informative, but, moreover, because this system forms the most simple model of a scalar quantum field and as such constitutes the first step towards an approach in quantum field theory. As before, we aim to obtain the entanglement entropy between two subsystems. Therefore, we will divide our composite system into two subsystems consisting, respectively, of the first n oscillators and the remaining $N-n$ oscillators, where we assume that $n < N-n$. We we will solely focus on the ground state of the composite system, and derive the entanglement entropy in this ground state. Following the structure of the previous chapter, we will first give a derivation of the ground state and subsequently the entanglement entropy by working in position space, in line with [1] and [3]. This is done is Section 3.1. After that, in Section 3.2, we will attempt to generalise our approach from Section 2.2 in deriving a convenient expression for the ground state in Fock space that enables us to calculate the entanglement entopy between the two subsystems.

3.1 Ground state and entanglement entropy in position space

3.1.1 Diagonalising the Hamiltonian

As always we start from the Hamiltonian of the system, which is just a generalisation of the Hamiltionian in Eq.(2.2), and therefore takes the form

$$H = \frac{1}{2}\sum_{A=1}^{N} p_A^2 + \frac{1}{2}\sum_{A,B=1}^{N} x_A K_{AB} x_B \,. \tag{3.1}$$

The matrix K describes the coupling between each of the oscillators and can be diagonalised by a unitary transformation U. We define the matrix Ω as the square root of K, i.e. $\Omega \equiv K^{1/2}$, which means that it can be diagonalised by the same unitary transformation, viz.

$$\Omega \;=\; U^T \Omega_D \, U \;=\; U^T K_D^{1/2} \, U \,, \tag{3.2}$$

where Ω_D denotes the diagonal form of Ω and K_D denotes the diagonal form of K. By employing the unitarity of U one can easily check from Eq.(3.2) that $\Omega \cdot \Omega = K$. The eigenvalues ω_A of Ω are the square roots of the eigenvalues of K and form the eigenfrequencies of the system, like ω_+ and ω_- did in the case of two oscillators. In terms of them, the ground state wave function $\psi_0(x_1, \ldots, x_N)$ is a product of single oscillator ground states, each corresponding to one of the eigenfrequencies, i.e.

$$\psi_0(x_1, \ldots, x_N) = \prod_A \left(\frac{\omega_A}{\pi}\right)^{1/4} \exp\left[-\frac{1}{2}\omega_A \tilde{x}_A^2\right] \,, \tag{3.3}$$

where $\tilde{x}_A \equiv \sum_B U_{AB} x_B$. Eq.(3.3) can be written in terms of the original variables x_A as

$$\psi_0(x_1, \ldots, x_N) = \left(\det\left(\frac{\Omega}{\pi}\right)\right)^{1/4} \exp\left[-\frac{1}{2}\,\boldsymbol{x}\cdot\Omega\cdot\boldsymbol{x}\right], \tag{3.4}$$

where $\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_N \end{pmatrix}$. The density matrix $\rho(\boldsymbol{x}, \boldsymbol{x'})$ corresponding to the ground state is then given by

$$\rho(\boldsymbol{x}, \boldsymbol{x'}) = \psi_0(\boldsymbol{x})\psi_0^*(\boldsymbol{x'}) = \left(\det\left(\frac{\Omega}{\pi}\right)\right)^{1/2} \exp\left[-\frac{1}{2}\boldsymbol{x}\cdot\Omega\cdot\boldsymbol{x} - \frac{1}{2}\boldsymbol{x'}\cdot\Omega\cdot\boldsymbol{x'}\right]. \tag{3.5}$$

3.1.2 Reduced density matrix

We will now decompose the Hilbert space $\mathcal{H}$ into two subspaces, in accordance with the division of the composite system into two subssystems, such that

$$\mathcal{H} \;=\; \mathcal{H}_I \otimes \mathcal{H}_{II}\,, \tag{3.6}$$

with the first n oscillators living in $\mathcal{H}_I$ and the remaining $N-n$ oscillators living in $\mathcal{H}_{II}$. From now on, we will label operators and variables restricted to $\mathcal{H}_I$ by indices a, b, etc., and those restricted to $\mathcal{H}_{II}$ by i, j, etc. Consequently, a runs from 1 to n whereas i runs from $n+1$ to N. When we do not restrict ourselves to either subspace but refer to the complete system, we will keep using capital indices A, B, etc. Accordingly we decompose Ω into four sectors:

$$\Omega_{AB} = \begin{pmatrix} (\Omega_1)_{ab} & (\Omega_2)_{aj} \\ (\Omega_2^T)_{ib} & (\Omega_3)_{ij} \end{pmatrix}. \tag{3.7}$$

For later use, we also define its inverse to be

$$O_{AB} \equiv (\Omega^{-1})_{AB} = \begin{pmatrix} (O_1)_{ab} & (O_2)_{aj} \\ (O_2^T)_{ib} & (O_3)_{ij} \end{pmatrix}. \tag{3.8}$$

We will now form the reduced density matrix ρ_I corresponding to the subsystem made up of the first n oscillators, which means we will have to integrate over the variables corresponding to the other $N-n$ oscillators. Indeed, we integrate $\rho(\boldsymbol{x}, \boldsymbol{x'})$ in Eq.(3.5) over the variables x_i to

obtain an expression for ρ_I, which, using Eq.(3.7), can be written as

$$\rho_I(\{x_a\},\{x'_a\}) = \left(\prod_i \int dx_i\right) \rho(\{x_a\},\{x_j\};\{x'_a\},\{x_j\}) \tag{3.9}$$

$$= \left(\det\left(\frac{\Omega}{\pi}\right)\right)^{1/2} \exp\left[-\frac{1}{2}x_a(\Omega_1)_{ab}x_b - \frac{1}{2}x'_a(\Omega_1)_{ab}x'_b\right]$$
$$\times \left(\prod_i \int dx_i\right) \exp\left[-(x_a + x'_a)(\Omega_2)_{aj}x_j - x_i(\Omega_3)_{ij}x_j\right] . \tag{3.10}$$

In the above expression summation over repeated indices is implied, as will be the case from now on unless indicated otherwise. The integral in Eq.(3.10) can be evaluated by completing the square, yielding

$$\left(\frac{\pi^{N-n}}{\det\Omega_3}\right)^{1/2} \exp\left[\frac{1}{4}(x_a + x'_a)\Omega_{2\,aj}\left(\Omega_3^{-1}\right)_{jk}\left(\Omega_2^T\right)_{kb}(x_b + x'_b)\right] .$$

Substituting this expression into Eq.(3.10) and reordering the terms, we obtain

$$\rho_I(\{x_a\},\{x'_a\}) = \left(\det\left(\frac{O_1^{-1}}{\pi}\right)\right)^{1/2} \exp\left[-\frac{1}{2}(x_a\Gamma_{ab}x_b + x'_a\Gamma_{ab}x'_b) + x'_a\Delta_{ab}x_b\right] , \tag{3.11}$$

with the matrices Γ and Δ defined as

$$\Delta \equiv \frac{1}{2}\Omega_2 \cdot \Omega_3^{-1} \cdot \Omega_2^T \quad \text{and} \quad \Gamma \equiv \Omega_1 - \Delta\,. \tag{3.12}$$

We also used that $\det\Omega = \det\Omega_3 \det(O_1^{-1})$, as pointed out by [3]. Furthermore, we note for later reference that

$$O_1^{-1} = \Omega_1 - \Omega_2\Omega_3^{-1}\Omega_2^T\,, \tag{3.13}$$

which we will prove in the Appendix (see A.10) and is also demonstrated in [3].

In order to diagonalise ρ_I, and find its eigenvalues, we have to carry out two subsequent transformations. The first one is a coordinate transformation, transforming x_a into new coordinates y_a, defined by

$$y_a = \Gamma_{D\;ab}^{1/2}V_{bc}x_c\,, \tag{3.14}$$

where V is an orthogonal matrix that brings Γ into diagional form, such that

$$\Gamma = V^T\Gamma_D V\,. \tag{3.15}$$

However, when performing a coordinate transormation we should take into account that the normalisation of the reduced density matrix has to be preserved, since its trace must always be

equal to 1, i.e.

$$\int \prod_a dx_a \, \rho_{red}(\{x_a\}, \{x_a\}) = 1 \, . \tag{3.16}$$

We know that a transformation of the integration variable in general contributes a jacobian factor, such that, if $\boldsymbol{y} = A\boldsymbol{x}$,

$$\int d\boldsymbol{x} \, \rho(A \cdot \boldsymbol{x}) = \frac{1}{\det A} \int d\boldsymbol{y} \, \rho(\boldsymbol{y}). \tag{3.17}$$

In our particular case we have that $A = \Gamma_D^{1/2} V$, hence $\det A = \det \Gamma_D^{1/2} = (\det \Gamma)^{1/2}$, due to the orthogonality of V. Plugging this into Eq.(3.11), we find that

$$\rho_{red}(\{y_a\}, \{y'_a\}) = (\det(\pi O_1 \Gamma))^{-1/2} \exp\left[-\frac{1}{2}(y_a^2 + y_a'^2) + y'_a \Lambda_{ab} y_b \right] , \tag{3.18}$$

where $\Lambda \equiv \Gamma_D^{-1/2} V \Delta V^T \Gamma_D^{-1/2}$. In order to diagonalise Λ, a second transformation is required, hence we introduce $z_a = S_{ab} y_b$, where S is again an orthogonal matrix and $\Lambda = S^T \Lambda_D S$. Implementing this in Eq.(3.18), we obtain ρ_I in diagonal form as

$$\rho_I(\{z_a\}, \{z'_a\}) = (\det(\pi O_1 \Gamma))^{-1/2} \prod_{a=1}^{n} \exp\left[-\frac{1}{2}(z_a^2 + z'^2_a) + \lambda_a z_a z'_a \right] , \tag{3.19}$$

where this time there is no implicit summation over a in the exponent. The λ_a denote the eigenvalues of Λ which are, by definition of Λ, also the eigenvalues of the matrix $\Gamma^{-1}\Delta$.

Let us now explicitly work out this result for the case of two coupled oscillators and compare with the reduced density matrix we derived for this case in Chapter 2, Paragraph 2.1.2. The matrix Ω and its inverse O are given by

$$\Omega = \frac{1}{2} \begin{pmatrix} \omega_+ + \omega_- & \omega_+ - \omega_- \\ \omega_+ - \omega_- & \omega_+ + \omega_- \end{pmatrix} \; ; \quad O = \frac{1}{2} \begin{pmatrix} \frac{1}{\omega_+} + \frac{1}{\omega_-} & \frac{1}{\omega_+} - \frac{1}{\omega_-} \\ \frac{1}{\omega_+} - \frac{1}{\omega_-} & \frac{1}{\omega_+} + \frac{1}{\omega_-} \end{pmatrix} . \tag{3.20}$$

From this it follows, in combination with Eq.(3.12), that

$$\Delta = \frac{(2\omega_+ - \omega_-)^2}{4(\omega_+ + \omega_-)} \, ; \tag{3.21}$$

$$\Gamma = \frac{1}{2}(\omega_+ + \omega_-) - \Delta \; = \; \frac{(\omega_+ + \omega_-)^2 + 2\omega_+\omega_-}{4(\omega_+ + \omega_-)} \, ; \tag{3.22}$$

$$O_1^{-1} = \frac{\omega_+ \omega_-}{\omega_+ + \omega_-} \, . \tag{3.23}$$

Comparing with Eq.(2.14), we see that we can indeed write the reduced density matrix as

$$\rho_1(x_1, x'_1) = \left(\frac{O_1^{-1}}{\pi} \right)^{1/2} \exp\left[-\frac{1}{2}\Gamma(x_1^2 + x_1'^2) + \Delta x_1 x'_1 \right] , \tag{3.24}$$

in agreement with Eq.(3.11). Because Γ and Δ are just scalars in this case, the transformation in Eq.(3.14) takes the simple form

$$y_1 = \Gamma^{1/2} x_1 \,, \tag{3.25}$$

which leads to

$$\rho_1(z_1, z_1') = \left(\frac{O_1^{-1}}{\pi\Gamma}\right)^{-1/2} \exp\left[-\frac{1}{2}(y_1^2 + y_1'^2) + \lambda y_1 y_1'\right] \,, \tag{3.26}$$

where $\lambda = \frac{\Delta}{\Gamma}$. A second transformation is not necessary, or would be just the identity, i.e. $z_1 = y_1$. Furthermore, λ is related to the parameter ξ, given in Eq.(2.18), by

$$\xi^2 = \frac{\lambda}{1 + \sqrt{1 - \lambda^2}} \,. \tag{3.27}$$

Comparing Eq.(3.19) with Eq.(3.26), we see that ρ_I is just a tensorial product of reduced density matrices corresponding to systems of two coupled oscillators. Hence, we can write

$$\rho_{\rm I}(\{z_a\}, \{z_a'\}) = \rho_{\rm red}(z_1, z_1', \lambda_1) \otimes \rho_{\rm red}(z_2, z_2', \lambda_2) \otimes \cdots \otimes \rho_{\rm red}(z_n, z_n', \lambda_n) \,. \tag{3.28}$$

Now that we have derived the above expression for the reduced density matrix ρ_I, we will employ it to find the associated entanglement entropy.

3.1.3 Deriving the entanglement entropy

Obtaining an expression for the entanglement entropy is quite straightforward once one has managed to find the eigenvalues of the reduced density matrix, for the entanglement entropy S in terms of these eigenvalues is simply given by Eq.(1.34). What will be very helpful now, is the fact that ρ_I turns out te be a product of reduced density matrices of which we already know the eigenvalues and thus the associated entanglement entropy, namely the one given by Eq.(2.19). A a consequence of the form of ρ_I, the entanglement entropy S will just be the sum of these separate entanglement entropies corresponding to each of the reduced density matrices in the product in Eq.(3.28) . Indeed, denoting the eigenvalues of ρ_I by p_m, we have

$$S = -\sum_m p_m \log p_m = \sum_{\{m_a\}} p_{m_1} p_{m_2} \cdots p_{m_n} \log(p_{m_1} p_{m_2} \cdots p_{m_n}) \tag{3.29}$$

$$= \sum_{\{m_a\}} p_{m_1} p_{m_2} \cdots p_{m_n} \left(\log p_{m_1} + \log p_{m_2} + \cdots + \log p_{m_n}\right) \tag{3.30}$$

$$= \sum_{a=1}^{n} \sum_{m_a=0}^{\infty} p_{m_a} \log p_{m_a} = \sum_{a=1}^{n} S_a \,. \tag{3.31}$$

Here S_a is the entanglement entropy corresponding to the reduced density matrix $\rho_{\text{red}}(z_a, z'_a, \lambda_a)$, hence, from Eq.(2.19),

$$S_a = S(\xi_a) = -\log(1-\xi_a^2) - \frac{\xi_a^2}{1-\xi_a^2}\log\xi_a^2\,, \tag{3.32}$$

where

$$\xi_a^2 = \frac{\lambda_a}{1+\sqrt{1-\lambda_a^2}}\,, \tag{3.33}$$

as follows from Eq.(3.27). For completeness, we point out that in Eqs.(3.32) and (3.33) there is no summation over the index a. At last, we conclude that the total entanglement entropy S is then given by

$$S = \sum_a S(\xi_a)\,. \tag{3.34}$$

.

3.2 Ground state and entanglement entropy in Fock space

Analogously to what we did in the case of two coupled oscillators, we will now try to obtain an expression for the ground state of N coupled oscillators, using the language of creation and annihilation operators acting on states in Fock space. In order to calculate the entanglement entropy between the two subsystems, this expression will have to be of such a form that it allows us to trace out the degrees of freedom residing in one of the two subsystems. In other words, we need to find the ground state of the composite system in a particular basis in Fock space that manifestly incorporates the decomposition of the Hilbert space into the two subspaces, $\mathcal{H}_I$ and $\mathcal{H}_{II}$, corresponding to the subsystems.

3.2.1 Diagonalising the Hamiltonian

Like before, we start from the Hamiltonian descibing the system of N coupled oscillators given by Eq.(3.1). As described above, this system can be diagonlised by performing a unitary transformation on the position coordinates and conjugate momenta in the form of the matrix U. Let us denote the new position operators again by $\tilde{x}_A$ and likewise for the momenta, such that

$$\tilde{x}_A = U_{AB}x_B\,; \qquad \tilde{p}_A = U_{AB}p_B\,. \tag{3.35}$$

Using the fact that this particular transformation diagonalises Ω, given in Eq.(3.2), we can define creation and annihilation operators in the usual way:

$$\tilde{a}_A = \frac{1}{\sqrt{2}}\left(\sqrt{\omega_{\boldsymbol{A}}}\,\tilde{x}_A + \frac{i}{\sqrt{\omega_{\boldsymbol{A}}}}\tilde{p}_A\right)\,; \qquad \tilde{a}_A^\dagger = \frac{1}{\sqrt{2}}\left(\sqrt{\omega_{\boldsymbol{A}}}\,\tilde{x}_A - \frac{i}{\sqrt{\omega_{\boldsymbol{A}}}}\tilde{p}_A\right)\,, \tag{3.36}$$

where the ω_A are the eigenvalues of Ω and we introduced the convention that a bold index indicates that it is not to be summed over. In terms of these operators the Hamiltonian takes the following decoupled form:

$$H = \sum_A \omega_A (\tilde{a}_A^\dagger \tilde{a}_A + \frac{1}{2}) \,. \tag{3.37}$$

The ground state $|0\rangle$ of the system can now be expressed as a product of ground states in this basis:

$$|0\rangle = |\tilde{0}\rangle_1 \otimes |\tilde{0}\rangle_2 \otimes \cdots \otimes |\tilde{0}\rangle_N \,. \tag{3.38}$$

Obviously the ground state is annihilated by all the $\tilde{a}_A$, i.e. $\tilde{a}_A |0\rangle = 0$. Since the ground state is a simple product state in this basis, there is no entanglement between the corresponding oscillators, by which we mean the oscillators corresponding to the $\tilde{a}_A$ and $\tilde{a}_A^\dagger$ operators. However, we are interested in the entanglement between the original oscillators, in particular between the first n and remaining $N-n$ oscillators. In order to find it, we will need to express the ground state in a way that allows us to trace over the degrees of freedom corresponding to either of the subsystems. Analogously to the problem of two coupled oscillators, we want to express the ground state in terms of ladder operators that live in either of the two subspaces corresponding to the two subsystems.

As before, we label operators living in subspace $\mathcal{H}_I$, corresponding to the first n oscillators, by indices $a, b, \ldots$ and operators living in $\mathcal{H}_{II}$, corresponding to the remaining $N-n$ oscillators, by indices $i, j, \ldots$ When we consider the whole system and do not explicitly distinguish between the two subsystems, we will use capital indices $A, B, \ldots$ We now look for annihilation operators α_a and β_i, and their hermitian conjugates, such that the α_a depend only on the position operators x_a and momentum operators p_a, whereas the β_i depend only on the operators x_i and p_i. In this way the $\alpha_a^{(\dagger)}$ are indeed restricted to $\mathcal{H}_I$ and the $\beta_i^{(\dagger)}$ to $\mathcal{H}_{II}$. Note that each of the α_a can depend on a linear combination of the x_a, and their conjugate momenta, i.e. a linear combination of $x_1, \ldots, x_n$ and consequently a linear combination of $p_1, \ldots, p_n$. Likewse, each of the β_i can depend on a linear combination of the x_i and their conjugate momenta. The new annihilation operators are generalisations of the operators α and β in Eq.(2.30).

3.2.2 A Bogoliubov transformation

In order to be able to express the ground state of the composite system in terms of these new operators we have to relate them to the $\tilde{a}_A$ and $\tilde{a}_A^\dagger$, since it is only in the basis of the latter that the ground state has been - implicitly - solved for. Rotating a set of pairs of creation and annihilation operators into another set, which is our aim, is done by performing a Bogoliubov transformation. Usually a Bogoliubov transformation is carried out in order to diagonalise the Hamiltonian of a quantum many-body system [13]. Its aim is then to yield those ladder operators in terms of which the Hamiltonian takes a decoupled form and ideally consists only of number

operators. However, we already know these operators: they are the $\tilde{a}_A$ and $\tilde{a}_A^\dagger$ in terms of which the Hamiltonian is given by Eq.(3.37). What we want to do is to rotate these operators back to sets of operators, the $\alpha_a^{(\dagger)}$ and $\beta_i^{(\dagger)}$, living in $\mathcal{H}_I$ and $\mathcal{H}_{II}$, respectively. The Hamiltonian will no longer be decoupled in this new basis but that is no concern to us. It is, after all, the coupling between the two subsystems, in the form of the entanglement entropy, that we are interested in.

Denoting the transformation matrix by T, the Bogoliubov transformation has the folowing form

$$\begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \\ \beta_{n+1} \\ \vdots \\ \beta_N \\ \alpha_1^\dagger \\ \vdots \\ \alpha_n^\dagger \\ \beta_{n+1}^\dagger \\ \vdots \\ \beta_N^\dagger \end{pmatrix} = T \cdot \begin{pmatrix} \tilde{a}_1 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \tilde{a}_N \\ \tilde{a}_1^\dagger \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \tilde{a}_N^\dagger \end{pmatrix}, \tag{3.39}$$

where T is a square matrix of size $2N \times 2N$. In order to make the division into the two subspaces more apparent, we decompose the matrix T into several submatrices:

$$T = \begin{pmatrix} V_{aA} & W_{aB} \\ R_{iA} & S_{iB} \\ W_{bA} & V_{bB} \\ S_{jA} & R_{jB} \end{pmatrix}. \tag{3.40}$$

Here we assume, mainly for simplicity, that T is real, but this will not impose any restriction on the solution in the end. Apart from this, the form of T as given in Eq.(3.40) is still completely general. Note that the matrices V and W are of size $n \times N$ whereas R and S are of size $N-n \times n$. The transformation can now be expressed in a somewhat more insightful way as

$$\begin{pmatrix} \alpha_a \\ \beta_i \\ \alpha_b^\dagger \\ \beta_j^\dagger \end{pmatrix} = \begin{pmatrix} V_{aA}\tilde{a}_A + W_{aB}\tilde{a}_B^\dagger \\ R_{iA}\tilde{a}_A + S_{iB}\tilde{a}_B^\dagger \\ W_{bA}\tilde{a}_A + V_{bB}\tilde{a}_B^\dagger \\ S_{jA}\tilde{a}_A + R_{jB}\tilde{a}_B^\dagger \end{pmatrix}, \tag{3.41}$$

with summation over repeated indices implied as before. For this transformation to be a well defined Bogoliubov transormation, T needs to satisfy certain constraints. These follow from the requirement that the standard commutation relations be conserved, i.e.

$$[\alpha_a, \alpha_b^\dagger] = \delta_{ab}\,; \qquad [\beta_i, \beta_j^\dagger] = \delta_{ij}\,, \tag{3.42}$$

with all other commutators vanishing. Upon imposing these relations on Eq.(3.41) we find the following constraints for the submatrices of T:

$$V \cdot V^T - W \cdot W^T = \mathbb{1}_{n\times n}\,; \tag{3.43}$$
$$R \cdot R^T - S \cdot S^T = \mathbb{1}_{N-n\times N-n}\,; \tag{3.44}$$
$$V \cdot R^T - W \cdot S^T = V \cdot S^T - W \cdot R^T = 0\,; \tag{3.45}$$
$$V \cdot W^T - W \cdot V^T = R \cdot S^T - S \cdot R^T = 0\,. \tag{3.46}$$

These constraints also allow us to construct the inverse of T, giving

$$T^{-1} = \begin{pmatrix} V_{Aa}^T & R_{Ai}^T & -W_{Ab}^T & -S_{Aj}^T \\ -W_{Ba}^T & -S_{Bi}^T & V_{Bb}^T & R_{Bj}^T \end{pmatrix}. \tag{3.47}$$

One can easily check that this is indeed the inverse of T by multiplying Eq.(3.40) with Eq.(3.47) and employing the relations in Eqs.(3.43)-(3.46). The expression for T^{-1} enables us to express the operators $\tilde{a}_A$ and $\tilde{a}_A^\dagger$ in terms of our new operators, $\alpha_a^{(\dagger)}$ and $\beta_i^{(\dagger)}$, yielding

$$\begin{pmatrix} \tilde{a}_A \\ \tilde{a}_B^\dagger \end{pmatrix} = \begin{pmatrix} V_{Aa}^T\alpha_a + R_{Ai}^T\beta_i - W_{Ab}^T\alpha_b^\dagger - S_{Aj}^T\beta_j^\dagger \\ -W_{Ba}^T\alpha_a - S_{Bi}^T\beta_i + V_{Bb}^T\alpha_b^\dagger + R_{Bj}^T\beta_j^\dagger \end{pmatrix}. \tag{3.48}$$

Hence, so far we have supposed two sets of ladder operators, the $\alpha_a^{(\dagger)}$ and $\beta_i^{(\dagger)}$ that are related to the $\tilde{a}_A$ and $\tilde{a}_A^\dagger$ by a Bogoliubov transformation, where $\tilde{a}_A$ and $\tilde{a}_A^\dagger$ are the ladder operators that diagonlise the Hamiltonian and thus decouple the system. Furthermore, the distinction between the $\alpha_a^{(\dagger)}$ and $\beta_i^{(\dagger)}$ operators corresponds to the way we have divided the system into two subsystems, such that the $\alpha_a^{(\dagger)}$ live in the subspace of the first n oscillators and the $\beta_i^{(\dagger)}$ live in the subspace of the remaining $N-n$ oscillators. It is important to note that these ladder

operators do not in general correspond to the original oscillators asscociated with the positions x_A and momenta p_A. For instance, the pair of ladder operators α_1 and $\alpha_1^\dagger$ does not, in general, correspond to the oscillator with position x_1 and momentum p_1. Instead, it corresponds to an oscillator that was not manifestly present from the beginning but results from a rotation among the x_a and p_a. Likewise, each pair of β_i and $\beta_i^\dagger$ corresponds to an oscillator resulting from a rotation among the x_i and p_i.

Subsequently we have decomposed the the matrix T that transforms the $\tilde{a}_A$ and $\tilde{a}_A^\dagger$ into the new ladder operators, into the four matrices V, W, S and R, in such a way that V and W are linked to the first subspace and R and S to the second subspace. The four matrices themselves are still unspecified, but have to satisfy the constraints in Eqs.(3.43)-(3.46), from which the inverse transformation matrix T^{-1} follows.

Note that everything we have done so far is completely general as we have not imposed any restrictions on the system or subsystems. However, we would like to obtain more explicit expressions for the transformation matrices, in order to eventually relate them to the original parameters of the system, i.e. the degrees of freedom residing in the matrix Ω, and to calculate the entanglement entropy in terms of these parameters. In proceeding along this path, we will give up to a certain extent the generality that we have maintained up to this point, which will be demonstrated below.

3.2.3 An ansatz

The form of the inverse transformation T^{-1}, i.e. the rotation transforming the $\alpha_a^{(\dagger)}$ and $\beta_i^{(\dagger)}$ into the $\tilde{a}_A$ and $\tilde{a}_A^\dagger$, is relevant when we want to find more explicit expressions for the submatrices of T. To see this, note that we can exploit the fact that all the $\tilde{a}_A$ annihilate the ground state, i.e.

$$\tilde{a}_A \left|0\right\rangle = 0\,. \tag{3.49}$$

Substituting Eq.(3.48) into Eq.(3.49) would yield a set of new equations for the matrices V, R, W and S, if we knew how all the ladder operators act on the ground state. Therefore, at this point, we decide to suppose an ansatz for the ground state, which will enable us to act on it with the ladder operators and work out the equations following from Eq.(3.49).

Since the problem at hand is nothing but a generalisation of the problem of two coupled oscillators, we assume that the ground state of the N oscillator problem can be expressed in a way analogous to that of the two oscillator problem. Generalising Eq.(2.45), we therefore suppose the following ansatz for the ground state $\left|0\right\rangle$:

$$\left|0\right\rangle \propto e^{X_{ai}\alpha_a^\dagger\beta_i^\dagger}\left|0\right\rangle_\alpha \otimes \left|0\right\rangle_\beta\,, \tag{3.50}$$

where X is an $n \times N-n$ matrix and the $\left|0\right\rangle_\alpha$ and $\left|0\right\rangle_\beta$ are actually products of the states

annihilated by the α_a and β_i, respectively, i.e.

$$|0\rangle_\alpha \equiv \prod_a \otimes |0\rangle_{\alpha_a} \; ; \qquad |0\rangle_\beta \equiv \prod_i \otimes |0\rangle_{\beta_i} \; . \tag{3.51}$$

Hence, each of the $|0\rangle_{\alpha_a}$ and $|0\rangle_{\beta_i}$ is a single oscillator ground state by itself and, as such, reacts in the standard way when acted on by the corresponding ladder operators, viz.

$$\alpha_a |0\rangle_{\alpha_a} = 0 \, ; \qquad (\alpha_a^\dagger)^n |0\rangle_{\alpha_a} = \sqrt{n!}\, |n\rangle_{\alpha_a} \; ; \tag{3.52}$$

$$\beta_i |0\rangle_{\beta_i} = 0 \, ; \qquad (\beta_i^\dagger)^n |0\rangle_{\beta_i} = \sqrt{n!}\, |n\rangle_{\beta_i} \; . \tag{3.53}$$

Using Eq.(3.48) and the ansatz in Eq.(3.50), we can expand Eq.(3.49) to give

$$\left(V^T_{Aa} \alpha_a + R^T_{Ai} \beta_i - W^T_{Ab} \alpha_b^\dagger - S^T_{Aj} \beta_j^\dagger \right) \; e^{X_{ck} \alpha_c^\dagger \beta_k^\dagger} |0\rangle_\alpha \otimes |0\rangle_\beta \; = \; 0 \, . \tag{3.54}$$

Considering each of the four terms separately, we will proceed by working out the first one:

$$\begin{aligned}
& V^T_{Aa} \alpha_a e^{X_{ck} \alpha_c^\dagger \beta_k^\dagger} |0\rangle_\alpha \otimes |0\rangle_\beta \\
= \; & V^T_{Aa} \left[\alpha_a, e^{X_{ck} \alpha_c^\dagger \beta_k^\dagger} \right] |0\rangle_\alpha \otimes |0\rangle_\beta \\
= \; & V^T_{Aa} \left[\alpha_a, \sum_{n=0}^{\infty} \frac{\left(X_{ck} \, \alpha_c^\dagger \beta_k^\dagger \right)^n}{n!} \right] |0\rangle_\alpha \otimes |0\rangle_\beta \; = \; V^T_{Aa} \sum_{n=1}^{\infty} \frac{1}{n!} \left[\alpha_a, \left(X_{ck} \, \alpha_c^\dagger \beta_k^\dagger \right)^n \right] |0\rangle_\alpha \otimes |0\rangle_\beta \; ,
\end{aligned} \tag{3.55}$$

where in going from the first to the second line, we use that $\alpha_a |0\rangle_\alpha = 0$ and we subsequently expanded the exponential. In order to work out the commutator we use again the identity given in Eq.(2.59), which leads to

$$\begin{aligned}
\left[\alpha_a, \left(X_{ck} \, \alpha_c^\dagger \beta_k^\dagger \right)^n \right] &= n \left(X_{ck} \, \alpha_c^\dagger \beta_k^\dagger \right)^{n-1} \left[\alpha_a, X_{bj} \, \alpha_b^\dagger \beta_j^\dagger \right] \\
&= n \left(X_{ck} \, \alpha_c^\dagger \beta_k^\dagger \right)^{n-1} X_{aj} \beta_j^\dagger \, ,
\end{aligned} \tag{3.56}$$

where we also employed the standard commutation relations given by Eq.(3.42). Substituting this result into Eq.(3.55), we arrive at

$$\begin{aligned}
& V^T_{Aa} \alpha_a e^{X_{ck} \alpha_c^\dagger \beta_k^\dagger} |0\rangle_\alpha \otimes |0\rangle_\beta \\
= \; & V^T_{Aa} \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left(X_{ck} \, \alpha_c^\dagger \beta_k^\dagger \right)^{n-1} X_{aj} \beta_j^\dagger |0\rangle_\alpha \otimes |0\rangle_\beta \\
= \; & e^{X_{ck} \, \alpha_c^\dagger \beta_k^\dagger} \left(V^T X \right)_{Aj} \beta_j^\dagger |0\rangle_\alpha \otimes |0\rangle_\beta \; .
\end{aligned} \tag{3.57}$$

In a similar way we can work out the second term in Eq.(3.54), yielding

$$\begin{aligned} & R^T_{Ai}\beta_i \, e^{X_{ck}\alpha^\dagger_c\beta^\dagger_k} \, |0\rangle_\alpha \otimes |0\rangle_\beta \\ &= e^{X_{ck}\,\alpha^\dagger_c\beta^\dagger_k} \, \left(R^T X^T\right)_{Ab} \alpha^\dagger_b \, |0\rangle_\alpha \otimes |0\rangle_\beta \, . \end{aligned} \tag{3.58}$$

The third and fourth term do not require too much effort since they can be commuted through the exponent straight away. Putting everyting together, we can rewrite Eq.(3.54) as

$$e^{X_{ck}\alpha^\dagger_c\beta^\dagger_k} \left[\left(V^T X\right)_{Aj} \beta^\dagger_j + \left(R^T X^T\right)_{Ab} \alpha^\dagger_b - W^T_{Ab}\alpha^\dagger_b - S^T_{Aj}\beta^\dagger_j \right] |0\rangle_\alpha \otimes |0\rangle_\beta \, = \, 0 \, , \tag{3.59}$$

from which it follows straightforwardly that

$$\left(V^T X\right)_{Aj} = S^T_{Aj} \, ; \qquad \left(R^T X^T\right)_{Ab} = W^T_{Ab} \, , \tag{3.60}$$

hence

$$S_{iA} = \left(X^T V\right)_{iA} \, ; \qquad W_{aA} = \left(X \, R\right)_{aA} \, . \tag{3.61}$$

In addition to the conditions given by Eqs.(3.43)-(3.46), we now have those in Eq.(3.61) following from the ansatz, further specifying the relations between the matrices V, W, R and S. However, since the matrix X is still unspecified, this does not reduce the number of unknown variables sufficiently to find an explicit form of the transformation matrices. Therefore, we will refine our ansatz to a more restrictive form, enabling us to obtain more specified expressions for these matrices.

3.2.4 A more restrictive ansatz

Once again generalising the solution to the problem of two oscillators, we suppose that the matrix X has the following form:

$$X_{ai} = \xi_{\boldsymbol{a}} \tilde{\delta}_{ai} = \begin{pmatrix} \xi_1 & 0 & \cdots & 0 & \cdots & 0 \\ 0 & \xi_2 & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \cdots & 0 \\ 0 & 0 & \cdots & \xi_n & \cdots & 0 \end{pmatrix}_{n \times N-n} \, , \tag{3.62}$$

where each of the ξ_a is a parameter yet to be related to the parameters already present in the system. The bold index in $\xi_{\boldsymbol{a}}$ in Eq.(3.62) indicates, as before, that it is not being summed over and the tilde above the delta serves to distinguish it from the standard delta function, since δ_{ai} would be equal to zero by definition. In matrix form, $\tilde{\delta}_{ai}$ is defined by

$$\tilde{\delta}_{ai} \equiv \begin{pmatrix} \mathbb{1}_{n\times n} & \emptyset_{n \times N-2n} \end{pmatrix} \, . \tag{3.63}$$

The ansatz we assumed in Eq.(3.50), will then take the following form:

$$|0\rangle \;\propto\; e^{\xi_{\boldsymbol{a}}\tilde{\delta}_{ai}\alpha_a^\dagger\beta_i^\dagger}\,|0\rangle_\alpha \otimes |0\rangle_\beta\,. \tag{3.64}$$

A look at Eq.(3.64) shows that each of the $\alpha_a^\dagger$ is now coupled, so to say, to one of the $\beta_i^\dagger$, which allows the state to be written as a product state of pairs, as we will see later on. Indeed, it is precisely this decomposition into pairs of oscillators that forms the motivation for the assumption of this particular ansatz.

We will now implement the ansatz for X_{ai} as given by Eq.(3.62) into the previously found relations for the transformation matrices, in order to obtain new expressions solely in terms the parameters ξ_a. We start by modifying the expressions for S and S^T in Eqs.(3.60) and (3.61) in accordance with Eq.(3.62) and substitute the result into Eq.(3.44), yielding

$$\left(R\,R^T\right)_{ij} - \tilde{\delta}_{ia}\xi_{\boldsymbol{a}}\left(V\,V^T\right)_{ab}\xi_{\boldsymbol{b}}\tilde{\delta}_{bj} \;=\; \delta_{ij}\,, \tag{3.65}$$

which can be written equivalently as

$$\left(R\,R^T\right)_{ij} \;=\; \delta_{ij} + \tilde{\delta}_{ia}\xi_{\boldsymbol{a}}\left(V\,V^T\right)_{ab}\xi_{\boldsymbol{b}}\tilde{\delta}_{bj}\,. \tag{3.66}$$

Following the same steps for W, W^T and substituting into (3.43), yields

$$\left(V\,V^T\right)_{ab} - \xi_{\boldsymbol{a}}\tilde{\delta}_{ai}\left(R\,R^T\right)_{ij}\tilde{\delta}_{jb}\xi_{\boldsymbol{b}} \;=\; \delta_{ab}\,. \tag{3.67}$$

Now we can substitute the expression for $\left(R\,R^T\right)_{ij}$ given by Eq.(3.66), into Eq.(3.67), which eventually leads to

$$\left(V\,V^T\right)_{ab} \;=\; \frac{1}{1-\xi_{\boldsymbol{a}}^2}\delta_{ab}\,. \tag{3.68}$$

Combining this result with Eq.(3.66) gives a similar expression for $\left(R\,R^T\right)_{ij}$, namely

$$\left(R\,R^T\right)_{ij} \;=\; \delta_{ij} + \tilde{\delta}_{ia}\frac{\xi_{\boldsymbol{a}}^2}{1-\xi_{\boldsymbol{a}}^2}\tilde{\delta}_{aj}\,. \tag{3.69}$$

With the results in Eqs.(3.68) and (3.69), we only have to rewrite Eqs.(3.60) and (3.61) to find two more similar results for the remaining two matrices, viz.

$$\left(W\,W^T\right)_{ab} \;=\; \frac{\xi_{\boldsymbol{a}}^2}{1-\xi_{\boldsymbol{a}}^2}\delta_{ab}\,; \tag{3.70}$$

$$\left(S\,S^T\right)_{ij} \;=\; \tilde{\delta}_{ia}\frac{\xi_{\boldsymbol{a}}^2}{1-\xi_{\boldsymbol{a}}^2}\tilde{\delta}_{aj}\,. \tag{3.71}$$

At this point we have found some simple expressions for the quadratic products of transformations matrices in terms of the parameters ξ_a, but we do not know how these ξ_a are related to the parameters initially present in the system. Furthermore, we have supposed an ansatz for

the ground state in terms of the same ξ_a and two sets of ladder operators, $\alpha_a^{(\dagger)}$ and $\beta_i^{(\dagger)}$, living in subspaces $\mathcal{H}_I$ and $\mathcal{H}_{II}$, respectively. As stated above, the $\alpha_a^{(\dagger)}$ can therefore only depend on the x_a and p_a, while the $\beta_i^{(\dagger)}$ can only depend on the x_i and p_i. We will now examine what the precise relation is between these new sets of ladder operators and the original position and momentum operators of the system, thereby attempting to establish more explicitly how the supposed ansatz depends on the initial parameters.

Let us recall that $\alpha_a^{(\dagger)}$ and $\beta_i^{(\dagger)}$ are related to the ladder operators $\tilde{a}_A^{(\dagger)}$ by the transformation in Eq.(3.41), and that we do know how the $\tilde{a}_A^{(\dagger)}$ depend on the initial coordinates of the system, as is apparent from Eqs.(3.35) and (3.36). Making this dependency explicit, we have

$$\tilde{a}_A = \frac{1}{\sqrt{2}}\left(\sqrt{\omega_{\boldsymbol{A}}}U_{AB}x_B + \frac{i}{\sqrt{\omega_{\boldsymbol{A}}}}U_{AB}p_B\right); \tag{3.72}$$

$$\tilde{a}_A^\dagger = \frac{1}{\sqrt{2}}\left(\sqrt{\omega_{\boldsymbol{A}}}U_{AB}x_B - \frac{i}{\sqrt{\omega_{\boldsymbol{A}}}}U_{AB}p_B\right). \tag{3.73}$$

Plugging this into Eq.(3.41) yields expressions for $\alpha_a^{(\dagger)}$ and $\beta_i^{(\dagger)}$ in terms of the transformation matrices and the orginal position and momentum operators, viz.

$$\alpha_a = \frac{1}{\sqrt{2}}(V+W)_{aA}\sqrt{\omega_{\boldsymbol{A}}}\,U_{AB}x_B + \frac{i}{\sqrt{2}}(V-W)_{aA}\frac{1}{\sqrt{\omega_{\boldsymbol{A}}}}U_{AB}p_B\,; \tag{3.74}$$

$$\alpha_a^\dagger = \frac{1}{\sqrt{2}}(V+W)_{aA}\sqrt{\omega_{\boldsymbol{A}}}\,U_{AB}x_B - \frac{i}{\sqrt{2}}(V-W)_{aA}\frac{1}{\sqrt{\omega_{\boldsymbol{A}}}}U_{AB}p_B\,, \tag{3.75}$$

and

$$\beta_i = \frac{1}{\sqrt{2}}(R+S)_{iA}\sqrt{\omega_{\boldsymbol{A}}}\,U_{AB}x_B + \frac{i}{\sqrt{2}}(R-S)_{iA}\frac{1}{\sqrt{\omega_{\boldsymbol{A}}}}U_{AB}p_B\,; \tag{3.76}$$

$$\beta_i^\dagger = \frac{1}{\sqrt{2}}(R+S)_{iA}\sqrt{\omega_{\boldsymbol{A}}}\,U_{AB}x_B - \frac{i}{\sqrt{2}}(R-S)_{iA}\frac{1}{\sqrt{\omega_{\boldsymbol{A}}}}U_{AB}p_B\,. \tag{3.77}$$

Subsequently we use the fact that $\alpha_a^{(\dagger)}$ can only depend on the x_a and p_a, and $\beta_i^{(\dagger)}$ only on x_i and p_i, to infer certain restrictions on the form of the matrix products on the right hand sides of Eqs.(3.74)-(3.75). Considering first the terms in Eqs.(3.74) and (3.75), we see that

$$(V+W)\cdot\Omega^{1/2}\cdot U = \begin{pmatrix} A_{n\times n} & \emptyset_{n\times N-n}\end{pmatrix}: \tag{3.78}$$

$$(V-W)\cdot\Omega^{-1/2}\cdot U = \begin{pmatrix} B_{n\times n} & \emptyset_{n\times N-n}\end{pmatrix}, \tag{3.79}$$

where A and B are matrices living in $\mathcal{H}_I$ that are yet to be specified. The first step in doing so, is to plug them back into Eq.(3.74), yielding

$$\alpha_a = \frac{1}{\sqrt{2}}A_{ab}x_b + \frac{i}{\sqrt{2}}B_{ab}p_b\,. \tag{3.80}$$

Since we want each α_a to be a well defined annihilation operator corresponding to a harmonic oscillator that emerges from the transformation, we should be able to associate a position and momentum operator to each of these new oscillators, as well as a frequency. Denoting these position and momentum operators by $\bar{x}_a$ and $\bar{p}_a$ and the frequencies by $\bar{\omega}_a$, we define them as

$$\bar{\omega}_{\boldsymbol{a}}^{1/2}\,\bar{x}_a \;\equiv\; A_{ab}x_b\,; \qquad \bar{\omega}_{\boldsymbol{a}}^{-1/2}\,\bar{p}_a \;\equiv\; B_{ab}p_b\,, \tag{3.81}$$

so that α_a takes the familiar form

$$\alpha_a \;=\; \frac{1}{\sqrt{2}}\left(\sqrt{\bar{\omega}_{\boldsymbol{a}}}\,\bar{x}_a \;+\; \frac{i}{\sqrt{\bar{\omega}_{\boldsymbol{a}}}}\,\bar{p}_a\right)\,. \tag{3.82}$$

Naturally, $\alpha_a^\dagger$ can be written as

$$\alpha_a^\dagger \;=\; \frac{1}{\sqrt{2}}\left(\sqrt{\bar{\omega}_{\boldsymbol{a}}}\,\bar{x}_a \;-\; \frac{i}{\sqrt{\bar{\omega}_{\boldsymbol{a}}}}\,\bar{p}_a\right)\,. \tag{3.83}$$

Note that the $\bar{\omega}_a$ are generalisations of the frequency $\omega = \sqrt{\omega_+\omega_-}$ associated with the oscillator corresponding to the $\alpha^{(\dagger)}$ in Section 2.2. Meanwhile, for the $\bar{x}_a$ and $\bar{p}_a$ to be well defined position and momentum operators, they must satisfy the canonical commutation relation, i.e.

$$[\bar{x}_a, \bar{p}_b] = \delta_{ab}[x\,,\,p_x]\,, \tag{3.84}$$

where by $[x\,,\,p_x]$ we mean the commutator of any position operator x and its conjugate momentum p_x. Imposing this on the definitions in Eq.(3.81) gives

$$\delta_{ab}\,[x\,,\,p_x] \;=\; \sqrt{\frac{\bar{\omega}_{\boldsymbol{a}}}{\bar{\omega}_{\boldsymbol{b}}}}\,[\bar{x}_a\,,\,\bar{p}_b] \;=\; A_{ac}B_{bd}\,[x_c\,,\,p_d] \;= A_{ac}B_{bd}\delta_{cd}[x\,,\,p_x] \;=\; A_{ac}B_{bc}\,[x\,,\,p_x]\,, \tag{3.85}$$

from which we derive that $\left(A\,B^T\right)_{ab} = \delta_{ab}$, hence $B = \left(A^{-1}\right)^T$.

The steps we have taken above, starting from Eqs.(3.74) and (3.75), can be carried out in a similar way when starting from Eqs.(3.76) and (3.77), leading this time to

$$(R+S)\cdot\Omega^{1/2}\cdot U = \begin{pmatrix}\emptyset_{N-n\times n} & C_{N-n\times N-n}\end{pmatrix}\,; \tag{3.86}$$

$$(R-S)\cdot\Omega^{-1/2}\cdot U = \begin{pmatrix}\emptyset_{N-n\times n} & D_{N-n\times N-n}\end{pmatrix}\,, \tag{3.87}$$

where $D = \left(C^{-1}\right)^T$, which follows from the same argument as the relation between A and B above.

Our next step will be to obtain expressions for the four transformation matrices V, W, R and S, in terms of A, B and Ω. To this end, we multiply Eq.(3.78) from the right with $U^T\cdot\Omega^{-1/2}$

and (3.79) with $U^T \cdot \Omega^{1/2}$. Adding the two resulting equations gives

$$V_{aA} = \frac{1}{2}\left(A_{ab}\, U^T_{bA}\omega_{\boldsymbol{A}}^{-1/2} \,+\, \left(A^{-1}\right)^T_{ab}\, U^T_{bA}\omega_{\boldsymbol{A}}^{1/2}\right), \tag{3.88}$$

while subtracting yields

$$W_{aA} = \frac{1}{2}\left(A_{ab}\, U^T_{bA}\omega_{\boldsymbol{A}}^{-1/2} \,-\, \left(A^{-1}\right)^T_{ab}\, U^T_{bA}\omega_{\boldsymbol{A}}^{1/2}\right). \tag{3.89}$$

Likewise, from Eqs.(3.86) and (3.87) we arrive at

$$R_{iA} = \frac{1}{2}\left(C_{ij}\, U^T_{jA}\omega_{\boldsymbol{A}}^{-1/2} \,+\, \left(C^{-1}\right)^T_{ij}\, U^T_{jA}\omega_{\boldsymbol{A}}^{1/2}\right); \tag{3.90}$$

$$S_{iA} = \frac{1}{2}\left(C_{ij}\, U^T_{jA}\omega_{\boldsymbol{A}}^{-1/2} \,-\, \left(C^{-1}\right)^T_{ij}\, U^T_{jA}\omega_{\boldsymbol{A}}^{1/2}\right). \tag{3.91}$$

The reader may check that the expressions in Eqs.(3.88)-(3.91) are consistent with the constraints in Eqs.(3.43)-(3.46). We have now managed to express the four transformation matrices in terms of the system's initial paramters, contained in the matrix Ω, and the matrices A and C. However, we still want to find the relation between Ω and the ξ_a, as the latter are the still unspecified parameters in terms of which the ansatz for the ground state was established.

3.2.5 Relating the ansatz to the system's initial parameters

In order to achieve a better understanding of the way in which the ξ_a depend on the system's degrees of freedom, we will have to exploit all the information contained in the relations that followed from our ansatz. We start by employing once more the relations in Eq.(3.61), multiplying the first by X from the left, subsequently adding them and then substituting Eqs.(3.89)-(3.92), which gives

$$\xi_{\boldsymbol{a}}\tilde{\delta}_{ai}C_{ij}U^T_{jA}\omega_{\boldsymbol{A}}^{-1/2} \,=\, \frac{1}{2}(\xi_{\boldsymbol{a}}^2+1)A_{ab}U^T_{bA}\omega_{\boldsymbol{A}}^{-1/2} \,+\, \frac{1}{2}(\xi_{\boldsymbol{a}}^2-1)\left(A^{-1}\right)^T_{ab}U^T_{bA}\omega_{\boldsymbol{A}}^{1/2}. \tag{3.92}$$

Multiplying by $\omega_{\boldsymbol{A}}^{1/2}U_{Ak}$ from the right, the first term on the right hand side vanishes due to the orthogonality of U and after relabeling indices we get

$$\xi_{\boldsymbol{a}}\tilde{\delta}_{ai}C_{ij} \,=\, \frac{1}{2}(\xi_{\boldsymbol{a}}^2-1)\left(A^{-1}\right)^T_{ab}U^T_{bA}\omega_{\boldsymbol{A}}U_{Aj}\,. \tag{3.93}$$

Recalling our decoposition of Ω and its inverse O into different sectors, as given by Eqs.(3.7) and (3.8), we see that we can write Eq.(3.93) as

$$\tilde{\delta}_{ai}C_{ij} \,=\, \frac{\xi_{\boldsymbol{a}}^2-1}{2\xi_{\boldsymbol{a}}}\left(A^{-1}\right)^T_{ab}\left(\Omega_2\right)_{bj}\,. \tag{3.94}$$

.

Instead of adding, we can also subtract the two equations that follow from working out the two relations in Eq.(3.61), and subsequently multiply by $\omega_{\boldsymbol{A}}^{-1/2} U_{Aj}$, which leads to

$$\tilde{\delta}_{ai} \left(C^{-1}\right)^T_{ij} \;=\; \frac{1-\xi_{\boldsymbol{a}}^2}{2\xi_{\boldsymbol{a}}} A_{ab} (O_2)_{bj} \,. \tag{3.95}$$

Meanwhile, writing $S = X^T \cdot V$ explicitly, gives

$$C_{ij} U^T_{jA} \omega_{\boldsymbol{A}}^{-1/2} \;-\; \left(C^{-1}\right)^T_{ij} U^T_{jA} \omega_{\boldsymbol{A}}^{1/2} \;=\; \tilde{\delta}_{ia} \left(A_{ab} U^T_{bA} \omega_{\boldsymbol{A}}^{-1/2} \;+\; \left(A^{-1}\right)^T_{ab} U^T_{bA} \omega_{\boldsymbol{A}}^{1/2} \right) . \tag{3.96}$$

Multiplying by $\omega_{\boldsymbol{A}}^{1/2} U_{Ac}$ from the right and relabeling yields

$$-\left(C^{-1}\right)^T_{ij} (\Omega_2)^T_{jb} \;=\; \tilde{\delta}_{ia} \xi_{\boldsymbol{a}} \left(A_{ab} + \left(A^{-1}\right)^T_{ac} (\Omega_1)_{cb} \right) , \tag{3.97}$$

where we used again that $U^T_{jA} U_{Ac} = \delta_{jc} = 0$. Taking the transpose of Eq.(3.94) and multiplying this from the left by $(C^{-1})^T_{ij}$ and from the right by $\frac{2\xi_{\boldsymbol{a}}}{\xi_{\boldsymbol{a}}^2 - 1} A_{ab}$ gives

$$\tilde{\delta}_{ia} \frac{2\xi_{\boldsymbol{a}}}{\xi_{\boldsymbol{a}}^2 - 1} A_{ab} \;=\; \left(C^{-1}\right)^T_{ij} (\Omega_2)^T_{jb} \,. \tag{3.98}$$

Substituting this result into the left hand side of Eq.(3.97) and rewriting the resulting expression eventually leads to

$$(A^{-1})^T_{ab} (\Omega_1)_{bc} (A^{-1})_{cd} \;=\; \frac{1+\xi_{\boldsymbol{a}}^2}{1-\xi_{\boldsymbol{a}}^2} \delta_{ad} \,. \tag{3.99}$$

This result seems to be quite useful as it directly relates the ξ_a to Ω_1. In particular, it tells us that the transformation by A^{-1} and its transpose puts Ω_1 into a diagonal form, with the diagonal elements given by the right hand side of Eq.(3.99). We will later return to the implications of this, but not before we show how to derive similar results for the other sectors of Ω and its inverse O.

Going back to Eq.(3.96), we now multiply by $\omega_{\boldsymbol{A}}^{-1/2} U_{Ac}$ from the right, which gives

$$C_{ij} (O_2)^T_{jb} \;=\; \tilde{\delta}_{ia} \xi_{\boldsymbol{a}} \left(A_{ac} (O_1)_{cb} \;+\; \left(A^{-1}\right)^T_{ab} \right) . \tag{3.100}$$

Similarly to what we did above with Eq.(3.94), we take the transpose of Eq.(3.95) and multiply from the left by C_{ij} and from the right by $\frac{2\xi_{\boldsymbol{a}}}{1-\xi_{\boldsymbol{a}}^2} (A^{-1})^T_{ab}$, obtaining

$$\tilde{\delta}_{ia} \frac{2\xi_{\boldsymbol{a}}}{1-\xi_{\boldsymbol{a}}^2} \left(A^{-1}\right)^T_{ab} \;=\; C_{ij} \left(O_2\right)^T_{jb} \,. \tag{3.101}$$

Upon substituting Eq.(3.101) into the left hand side of Eq.(3.100) and rewriting, we arrive at

$$A_{ab} (O_1)_{bc} A^T_{cd} \;=\; \frac{1+\xi_{\boldsymbol{a}}^2}{1-\xi_{\boldsymbol{a}}^2} \delta_{ad} \,. \tag{3.102}$$

It is obvious that Eq.(3.102) shows a strong similarity in form to Eq.(3.99) and both relate the ξ_a to parameters corresponding to the interactions within $\mathcal{H}_I$.

In order to find the analogous relations for the sector descibing the degrees of freedom within $\mathcal{H}_{II}$, we start again from Eq.(3.96), but now we multiply from the right by either $\omega_{\boldsymbol{A}}^{1/2}U_{Ak}$ or $\omega_{\boldsymbol{A}}^{-1/2}U_{Ak}$. Note that this time we pick different sectors of U compared to when we derived Eqs.(3.97) and (3.100). The first of these options, i.e. multiplying by $\omega_{\boldsymbol{A}}^{1/2}U_{Ak}$, leads to

$$C_{ik} - \left(C^{-1}\right)^T_{\ ij}\,(\Omega_3)_{jk} \;=\; \tilde{\delta}_{ia}\xi_{\boldsymbol{a}}\left(A^{-1}\right)^T_{\ ab}\,(\Omega_2)_{bk}\,. \tag{3.103}$$

Now we repeat the same trick as before, that is, we modify Eq.(3.94) in such a way that it takes a convenient form. This time it is straightforward to see that we can rewrite it to

$$\tilde{\delta}_{ia}\frac{2\xi_{\boldsymbol{a}}^2}{\xi_{\boldsymbol{a}}^2-1}\tilde{\delta}_{aj}C_{jk} \;=\; \tilde{\delta}_{ia}\xi_{\boldsymbol{a}}\left(A^{-1}\right)^T_{\ ab}\,(\Omega_2)_{bk}\,. \tag{3.104}$$

Now we can equate the left hand sides of Eqs.(3.103) and (3.104), which, after some reordering, leads to

$$\left(C^{-1}\right)^T_{\ ik}\,(\Omega_3)_{kl}\left(C^{-1}\right)_{lj} \;=\; \tilde{\delta}_{ia}\frac{2\xi_{\boldsymbol{a}}^2}{1-\xi_{\boldsymbol{a}}^2}\tilde{\delta}_{aj} \;+\; \delta_{ij}\,. \tag{3.105}$$

At last we work out the multiplication of Eq.(3.96) by $\omega_{\boldsymbol{A}}^{-1/2}U_{Ak}$ from the right, to find

$$C_{ij}(O_3)_{jk} \;-\; \left(C^{-1}\right)^T_{\ ik} \;=\; \tilde{\delta}_{ia}\xi_{\boldsymbol{a}}A_{ab}(O_2)_{bk}\,, \tag{3.106}$$

and we rewrite Eq.(3.95) to

$$\tilde{\delta}_{ia}\frac{2\xi_{\boldsymbol{a}}^2}{1-\xi_{\boldsymbol{a}}^2}\tilde{\delta}_{aj}\left(C^{-1}\right)^T_{jk} \;=\; \tilde{\delta}_{ia}\xi_{\boldsymbol{a}}A_{ab}(O_2)_{bk}\,. \tag{3.107}$$

Equating the left hand sides of Eqs.(3.106) and (3.107) and reordering a little, we finally arrive, perhaps not surprisingly, at

$$C_{ik}(O_3)_{kl}C^T_{lj} \;=\tilde{\delta}_{ia}\frac{2\xi_{\boldsymbol{a}}^2}{1-\xi_{\boldsymbol{a}}^2}\tilde{\delta}_{aj} \;+\; \delta_{ij}\,. \tag{3.108}$$

As anticipated, we have obtained two more relations between the paramters ξ_a and the initial parameters of the system, this time the ones described by the matrices Ω_3 and O_3 that contain the degrees of freedom in $\mathcal{H}_{II}$. The form of Eqs.(3.105) and (3.108) is strikingly similar to that of Eqs.(3.99) and (3.102). To illustrate this a little more clearly, we can write the right hand side

of Eqs.(3.99) and (3.102) in matrix form as

$$\begin{pmatrix} \frac{1+\xi_1^2}{1-\xi_1^2} & 0 & \cdots & 0 \\ 0 & \frac{1+\xi_2^2}{1-\xi_2^2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1+\xi_n^2}{1-\xi_n^2} \end{pmatrix}, \tag{3.109}$$

and that of Eqs.(3.105) and (3.108) as

$$\begin{pmatrix} \begin{pmatrix} \frac{1+\xi_1^2}{1-\xi_1^2} & 0 & \cdots & 0 \\ 0 & \frac{1+\xi_2^2}{1-\xi_2^2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1+\xi_n^2}{1-\xi_n^2} \end{pmatrix} & \emptyset_{n\times N-2n} \\ \emptyset_{N-2n\times n} & \mathbb{1}_{N-2n\times N-2n} \end{pmatrix}. \tag{3.110}$$

We see that the matrix in (3.110) does not contain any more independent parameters than that in (3.109). In fact, we can say that the diagonal elements of the second matrix are equal to $\frac{1+\xi_i^2}{1-\xi_i 2}$ with the first n of these ξ_i equal to the ξ_a and the remaining $N-2n$ of these ξ_i equal to zero. The question now rises how to interpret these relations and this is what we will address in the following paragraph.

3.2.6 Determination of ξ_a

In finding an answer to the question raised above, let us consider for now just the relations concerning the first subspace, hence Eqs.(3.99) and (3.102). At first one might think that the matrix in (3.109) is the diagonal form of the matrices Ω_1 and O_1. However, this is not entirely correct. One way to see this is by realising that Ω_1 has dimensions of frequency, hence so do its eigenvalues, whereas the ξ_a are dimensionless parameters, as follows from the form of the ansatz in Eq.(3.64). Therefore, the diagonal elements in (3.109) cannot be the eigenvalues of Ω_1. Along the same line of reasoning, we realise they cannot be the eigenvalues of O_2 either, since those would have dimensions of inverse frequency. Another way to look at it, is by arguing that Eqs.(3.98) and (3.102) would ony describe well defined diagonalisation transformations if A were orthogonal such that $A^T = A^{-1}$. However, from the previous argument, as well as from Eq.(3.81), it follows that A, and thus A^T, have dimension of square root of frequency, while A^{-1} has the inverse dimension and therefore cannot be equal to A^T.

In accordance with Eq.(3.81), we can write A as $A_{ab} = \bar{\omega}_{\boldsymbol{a}}^{1/2} P_{ab}$, for some matrix P, such that

$$\left(A^{-1}\right)^T_{ab} = \bar{\omega}_{\boldsymbol{a}}^{-1/2} \left(P^{-1}\right)^T_{ab}, \tag{3.111}$$

leading to

$$\bar{x}_a \;=\; P_{ab}x_b\,; \qquad \bar{p}_a \;=\; \left(P^{-1}\right)^T_{ab} p_b\,. \tag{3.112}$$

We argue that the $\bar{\omega}_a$ are not fixed since any dimensionless factor can be absorbed by the $\bar{x}_a$ and $\bar{p}_a$ and therefore we can pick our $\bar{\omega}_a$ in a specific way. In particular, we choose them to be such that the matrix P becomes orthogonal, i.e. $P^T = P^{-1}$. Now Eq.(3.99) can be rewritten as

$$(\Omega_1)_{ab} \;=\; P^T_{ac}\,\bar{\omega}_{\boldsymbol{c}}^{1/2}\,\frac{1+\xi_{\boldsymbol{c}}^2}{1-\xi_{\boldsymbol{c}}^2}\delta_{cd}\,\bar{\omega}_{\boldsymbol{d}}^{1/2}\,P_{db} \;=\; (P^{-1})_{ac}\,\bar{\omega}_{\boldsymbol{c}}\,\frac{1+\xi_{\boldsymbol{c}}^2}{1-\xi_{\boldsymbol{c}}^2}\,P_{cb}\,. \tag{3.113}$$

This shows that Ω_1 is diagonalised by P and its eigenvalues are equal to $\bar{\omega}_{\boldsymbol{a}}\,\frac{1+\xi_{\boldsymbol{a}}^2}{1-\xi_{\boldsymbol{a}}^2}$. At first sight, this finally seems to entail the relation between the ξ_a and the parameters of the system that we have been looking for. However, we do not know the $\bar{\omega}_a$ and therefore diagonalising Ω_1 will not be sufficient to determine the ξ_a. Instead, we will have to make use of other information as well, in particular that contained in (3.102). Employing Eq.(3.111), it is straightforward to show that Eq.(3.102) is equivalent to

$$(O_1)_{ab} \;=\; \left(P^{-1}\right)_{ac}\frac{1}{\bar{\omega}_{\boldsymbol{c}}}\frac{1+\xi_{\boldsymbol{c}}^2}{1-\xi_{\boldsymbol{c}}^2}P_{cb}\,, \tag{3.114}$$

from which it follows that

$$\left(O_1^{-1}\right)_{ab} \;=\; \left(P^{-1}\right)_{ac}\bar{\omega}_{\boldsymbol{c}}\frac{1-\xi_{\boldsymbol{c}}^2}{1+\xi_{\boldsymbol{c}}^2}P_{cb}\,. \tag{3.115}$$

Clearly, diagonalising O or O^{-1} will leave us with the same problem: insufficient information to completely determine the ξ_a. However, when we combine Eqs.(3.113) and (3.115), we will be able to get around this issue. We will now illustrate this in a way that allows us at the same time to make the conncetion with Section 3.1, where we solved the problem in postion space. In the end, both methods should yield equivalent solutions.

Let us hereto recall the matrices Γ and Δ from Paragraph 3.1.2, given in Eq.(3.12). By employing the identity in Eq.(3.13), they can be written conveniently as

$$\Gamma_{ab} = \frac{1}{2}\left(\Omega_1 \,+\, O_1^{-1}\right)_{ab}\,; \tag{3.116}$$

$$\Delta_{ab} = \frac{1}{2}\left(\Omega_1 \,-\, O_1^{-1}\right)_{ab}\,. \tag{3.117}$$

Combining this with Eqs.(3.113) and (3.115), we can write Γ_{ab} as

$$\begin{aligned}\Gamma_{ab} \;&=\; \left(P^{-1}\right)_{ac}\frac{\bar{\omega}_{\boldsymbol{c}}}{2}\left(\frac{1+\xi_{\boldsymbol{c}}^2}{1-\xi_{\boldsymbol{c}}^2} \,+\, \frac{1-\xi_{\boldsymbol{c}}^2}{1+\xi_{\boldsymbol{c}}^2}\right)P_{cb}\\ &=\left(P^{-1}\right)_{ac}\bar{\omega}_{\boldsymbol{c}}\,\frac{1+\xi_{\boldsymbol{c}}^4}{1-\xi_{\boldsymbol{c}}^4}\,P_{cb}\,.\end{aligned} \tag{3.118}$$

Its inverse, Γ^{-1}, is then given by

$$\left(\Gamma^{-1}\right)_{ab} \;=\; \left(P^{-1}\right)_{ac} \frac{1}{\bar{\omega}_{\boldsymbol{c}}} \frac{1-\xi_{\boldsymbol{c}}^4}{1+\xi_{\boldsymbol{c}}^4} P_{cb}\,. \tag{3.119}$$

Likewise, Δ_{ab} can be written as

$$\Delta_{ab} \;=\; \left(P^{-1}\right)_{ac} \bar{\omega}_{\boldsymbol{c}} \frac{2\xi_{\boldsymbol{c}}^2}{1-\xi_{\boldsymbol{c}}^4} P_{cb}\,. \tag{3.120}$$

For reasons that will become clear in a moment, we now multiply the matrices Γ^{-1} and Δ, as given by Eqs.(3.119) and (3.120), to arrive at

$$\left(\Gamma^{-1}\Delta\right)_{ab} \;=\; \left(P^{-1}\right)_{ac} \frac{2\xi_{\boldsymbol{c}}^2}{1+\xi_{\boldsymbol{c}}^4} P_{cb}\,. \tag{3.121}$$

Finally we have obtained an expression that unambiguously describes the relation between the ξ_a and the system's initial parameters. Eq.(3.121) tells us what the eigenvalues of $(\Gamma^{-1}\Delta)_{ab}$ are in terms of the ξ_a, with Γ^{-1} and Δ fully defined in terms of Ω. More specifically, if we denote these eigenvalues by λ_a, we have that

$$\lambda_a \;=\; \frac{2\xi_{\boldsymbol{a}}^2}{1+\xi_{\boldsymbol{a}}^4}\,, \tag{3.122}$$

which can be inverted to give

$$\xi_{\boldsymbol{a}}^2 \;=\; \frac{\lambda_a}{1+\sqrt{1-\lambda_a^2}}\,. \tag{3.123}$$

A look at Eq.(3.33) reveals that our expression for ξ_a is equivalent to the one found for the ξ_a in Section 3.1, since in both cases the λ_a are the eigenvalus of the matrix $\left(\Gamma^{-1}\Delta\right)_{ab}$.

In deriving this result we have restricted ourselves to the sectors corresponding to $\mathcal{H}_I$, that is, from the beginning of Paragraph 3.2.6 we have only used equations for Ω_1 and O_1. One might now wonder whether we would have obtained the same result, had we instead used Eqs.(3.105) and (3.106). The answer to this question is yes, which follows from the fact that all the arguments we used in the derivation in this paragraph have their analog in the other sector. For instance, the analog of Eq.(3.111) would be

$$C_{ij} \;=\; \bar{\omega}_{\boldsymbol{i}}^{1/2} Q_{ij}\,, \tag{3.124}$$

with Q an orthogonal matrix. Defining $\xi_i \equiv \tilde{\delta}_{ia}\xi_a$, we would, instead of Eqs.(3.113) and (3.115), obtain

$$(\Omega_3)_{ij} \;=\; \left(Q^{-1}\right)_{ik} \bar{\omega}_{\boldsymbol{k}} \frac{1+\xi_{\boldsymbol{k}}^2}{1-\xi_{\boldsymbol{k}}^2} Q_{kj}\,, \qquad \text{and} \qquad \left(O_3^{-1}\right)_{ij} \;=\; \left(Q^{-1}\right)_{ik} \bar{\omega}_{\boldsymbol{k}} \frac{1-\xi_{\boldsymbol{k}}^2}{1+\xi_{\boldsymbol{k}}^2} Q_{kj}\,. \tag{3.125}$$

Then defining $\tilde{\Gamma}_{ij} \equiv \frac{1}{2}\left(\Omega_3 + O_3^{-1}\right)$ and $\tilde{\Delta}_{ij} \equiv \frac{1}{2}\left(\Omega_3 - O_3^{-1}\right)$, we find that the eigenvalues λ_i of

$\Gamma^{-1}\Delta$ are given by

$$\lambda_i \;=\; \frac{2\xi_{\boldsymbol{i}}^2}{1+\xi_{\boldsymbol{i}}^4}\,, \tag{3.126}$$

showing equivalence to Eq.(3.122). The matrices $\tilde{\Gamma}$ and $\tilde{\Delta}$ would have shown up instead of Γ and Δ in the derivation in position space that we discussed in Section 3.1, if we had integrated over the x_a instead of x_i when calculating the reduced density matrix. Back there it was not so evident, but the derivation we just did thus explicitly shows that in either case, integrating out one or the other subsystem, one obtains the same entanglement entropy, confirming the general law.

We have found the relation between the parameters in our ansatz, ξ_a and the system's initial parameters, and shown that they are in fact the same ξ_a as the ones that emerged in section 3.1. The task that remains is to calculate the entanglement entropy following from our ansatz and show its equivalence to the entanglement entropy found in Paragraph 3.1.3.

3.2.7 Deriving the entanglement entropy

Let us now return to our ansatz in Eq.(3.64), that, including the correct normalisation factor, reads

$$|0\rangle \;=\; \prod_i \prod_a \otimes \left(\sqrt{1-\xi_{\boldsymbol{a}}^2}\, e^{\xi_{\boldsymbol{b}}\tilde{\delta}_{bj}\alpha_b^\dagger\beta_j^\dagger}\;|0\rangle_{\alpha_a}\otimes|0\rangle_{\beta_i}\right). \tag{3.127}$$

We mentioned before that in this form the state can be factorised into pairs across the $|0\rangle_\alpha$ and $|0\rangle_\beta$. Indeed, we can see how this works when writing Eq.(3.127) explicitly as

$$\begin{aligned}|0\rangle \;=\; \sqrt{1-\xi_1^2}\cdots\sqrt{1-\xi_n^2}\, e^{\xi_1\alpha_1^\dagger\beta_{n+1}^\dagger}\cdots e^{\xi_n\alpha_n^\dagger\beta_{2n}^\dagger}\;|0\rangle_{\alpha_1}\otimes|0\rangle_{\beta_{n+1}}\otimes\cdots\otimes|0\rangle_{\alpha_n}\otimes|0\rangle_{\beta_{2n}}\\ \otimes|0\rangle_{\beta_{2n+1}}\otimes\cdots\otimes|0\rangle_{\beta_N}\,,\end{aligned} \tag{3.128}$$

which can be grouped to give

$$\begin{aligned}|0\rangle \;=\; \sqrt{1-\xi_1^2}\, e^{\xi_1\alpha_1^\dagger\beta_{n+1}^\dagger}\;|0\rangle_{\alpha_1}\otimes|0\rangle_{\beta_{n+1}}\otimes\cdots\otimes\sqrt{1-\xi_n^2}\, e^{\xi_n\alpha_n^\dagger\beta_{2n}^\dagger}\;|0\rangle_{\alpha_n}\otimes|0\rangle_{\beta_{2n}}\\ \otimes|0\rangle_{\beta_{2n+1}}\otimes\cdots\otimes|0\rangle_{\beta_N}\,.\end{aligned} \tag{3.129}$$

This shows how each $\alpha_a^\dagger$ is paired with $\beta_{n+a}^\dagger$ by ξ_a and how each of the pairs represents as system of two coupled oscillators like the one we discussed in section 2.2. The fact that there are, by assumption, more α's than β's, results in a product of $N-2n$ single oscillator ground states corresponding to the β's that are left over, so to say. Recalling how we can expand each exponential and write each paired state in the form of Eq.(2.43), we can write the density matrix

ρ as

$$\rho = |0\rangle\langle 0| = \prod_a \otimes \left((1-\xi_{\boldsymbol{a}}^2) \sum_{r,s} \xi_{\boldsymbol{a}}^{r+s} |r\rangle_{\alpha_a} \langle s| \otimes |r\rangle_{\beta_{\alpha+n}} \langle s| \right) \otimes \ |0\rangle_{\beta_{2n+1}} \langle 0| \otimes \cdots \otimes |0\rangle_{\beta_N} \langle 0| \,. \tag{3.130}$$

Taking the trace over the oscillators living in $\mathcal{H}_{II}$, that is, the oscillators corresponding to the $\beta_i^{(\dagger)}$, we obtain the reduced density matrix ρ_I corresponding to the subsystem in $\mathcal{H}_I$, which is given by

$$\rho_I \ = \prod_a \otimes \left((1-\xi_{\boldsymbol{a}}^2) \sum_r \xi_{\boldsymbol{a}}^{2r} |r\rangle_{\alpha_a} \langle r| \right) . \tag{3.131}$$

As anticipated, ρ_I is a tensor product of reduced density matrices corresponding to systems consisting of two coupled oscillators, with each of these systems characterised by a paramter ξ_a. By the same argument as explained in Paragraph 3.1.3, it follows that the entanglement entropy S is just the sum of the entanglement entropies corresponding to each of these systems of two oscillators, that is

$$S \ = \sum_a S(\xi_a) \,. \tag{3.132}$$

We chose here to trace out the degrees of freedom in $\mathcal{H}_{II}$, leading to ρ_I, but we could have traced over the oscillators in $\mathcal{H}_I$ as well. This would yield the reduced density matrix ρ_{II}, given by

$$\rho_{II} \ = \ \prod_a \otimes \left((1-\xi_{\boldsymbol{a}}^2) \sum_r \xi_{\boldsymbol{a}}^{2r} |r\rangle_{\beta_{n+a}} \langle r| \right) \otimes |0\rangle_{\beta_{2n+1}} \langle 0| \otimes \cdots \otimes |0\rangle_{\beta_N} \langle 0| \,. \tag{3.133}$$

Clearly the only difference in form with ρ_I is the additional product of unpaired β ground states. However, this leaves the spectrum of eigenvalues the same, since the additional terms take the form of identity matrices in the tensor product. Therefore, the entanglement entropy resulting from ρ_{II} is equal to that following from ρ_I, like it should be.

4 Conclusion and outlook

In this thesis we have examined the entanglement entropy in a system of coupled harmonic oscillators. We reviewed and explained results from the literature that were derived in position space, by means of wave functions and integration over position coordinates. The point of the thesis was to take an approach in Fock space, which would not only allow us to rederive already know results in a different way, but also enhance our understanding of how these results come about. Moreover, taking a different approach to the problem would potentially enable us to generalise the results more easily to excited states.

After reviewing the phenomenon of quantum entanglement and the associated entanglement entropy within a quantum mechanical framework in Chapter 1, we dove into the problem of two coupled harmonic oscillators in Chapter 2. Following [1], we showed how the entanglement entropy between the oscillators in the ground state of the composite system could be derived by integrating the density matrix over the position coordinates of one of the oscillators and determining the eigenvalues of the resulting reduced density matrix. The entanglement entropy S was expressed as a function of the parameter ξ, which, in turn, solely depended on the ratio between the two eigenfrequencies of the system in such a way that it increased for larger coupling between the two original oscillators. We then considered the same system in Fock space, where we tried to find an expression for the ground state in a basis enabling us to trace over one of the subspaces. In doing so, we had to perform a rotation of the ladder operators corresponding to the eigenstates of Hamiltonian, to a new set of ladder operators, consisting of a pair living in one of the subpaces and another pair living in the other subspace. Upon finding the desired transformation, we could express the ground state in the basis corresponding to these new ladder operators. It was from there straightforward to obtain the reduced density matrix, which had a diagonal form in this basis. Therefore, as opposed to the case in postion space, the eigenvalues could now be read off immediately.

As anticipated, the obtained expression for the ground state was such that it could be acted on by creation operators to form excited states. We only considered particular excited states that were linear combinations of the Hamiltonian eigenstates, for these turned out to have an interesting and elegant form in the basis we were working in. More precisely, we acted with a creation operator that caused only the states forming the basis in one of the two subspaces, to be excited to the next level. The corresponding reduced density matrix could be evaluated analytically in diagonal form, from which we numerically evaluated S in the first three excited states. S turned out to increase with each level of excitation but its curve depicting the depence on ξ, hence on the coupling strength, remained of the same form. Further work could examine how S would behave for excited eigenstates.

We then moved on to the problem of N coupled oscillators. Decomposing the system into a subsystem consisting of the first n oscillators and its complement, consisting of the remaining $N - n$ oscillators, we started again by reviewing [1] on how to find the ground state, reduced

density matrix and entanglement entropy in position space. It was shown that the reduced density matrix could, in the right basis of position coordinates, be written as a product of reduced density matrices corresponding to systems of two coupled oscillators, each specified by a paramater ξ_a. Consequently, S turned out to be just the sum of the entanglement entropies $S(\xi_a)$.

When attempting to reproduce this result in Fock space, we had to find again the particular transformation leading to the set of ladder operators in terms of which we could express the ground state in a convenient form. We could obtain a very general form of what this transformation should look like, based on several constaints to guarantee that the new ladder operators would be well defined and satisfy the standard bosonic commutation relations. However, this was not enough to obtain an explicit solution.

Therefore, we supposed an ansatz based on our result for the two oscillator ground state. We then refined this ansatz by introducing the parameters ξ_a in such a way that the reduced density matrix would take a diagonal form and, moreover, be a tensor product of density matrices corresponding to systems of two coupled oscillators, with each pair coupled by one the ξ_a. Evidently this would lead to the correct form of the entanglement entropy as a sum of $S(\xi_a)$. However, since we introduced the ξ_a by hand, we still had to relate them to the system's initial parameters and show that they were in fact the same ξ_a as the ones obtained before. By employing all the information contained in all the constraints, we were eventually able to achieve this, hence showing that our ansatz was correct.

It is hardly debatable that the derivation of the entanglement entropy in position space seems to be less tedious than that in Fock space. In fact, we implicitly used the results from the method in position space in order to set up an ansatz for the ground state in Fock space, which we otherwise might have never found. On the other hand, this also shows that it is rather the convenient basis for the ground state, than the actual entanglement entropy, that was hard to obtain in Fock space. The underlying reason is that in position space, the reduced density matrix was obtained in nondiagonal form and had to be diagonalised afterwards, whereas our derivation in Fock space was all about finding the basis in which the reduced density matrix would be diaginal to begin with. Indeed, once the ground state was expressed in the desired basis, the reduced density matrix and entanglement entopy could be obtained very easily from it. Besides, once the ground state has been obtained in Fock space, it is easier to form excited states and find the corresponding entanglement entropy, as was explicitly shown for the case of two oscillators. Unfortunately there was no time for this project to examine excited states in the N oscillator system, which is therefore left for future work.

As mentioned before, the reason for studying a system of coupled harmonic oscillators, is that it forms the first approximation to a quantum scalar field. In fact, in [1], the area law for entanglement entropy of a scalar field in the ground state was derived by extending the results for the system of N coupled oscillators. However, in general, entanglement entropy in quantum field theories is not thoroughly understood or described yet. The presumption is that an approach in

Fock space could contribute to a better understanding of entanglement entropy in quantum field theories, not only in the ground state but also in excited states. One could, for instance, wonder whether the area law still holds in excited states, or what happens when we consider a fermionic field instead of, or together with, a bosonic one. When approaching these questions from a Fock space perspective, this thesis can hopefully serve as a first step towards finding an answer.

Appendix

In Section 2.3 we used an identiy, given by Eq.(2.59), wich we will prove here. Let A and B be two operators, then

$$\begin{aligned}
[A, B^n] =& AB^n - B^n A && \text{(A.1)}\\
=& ABB^{n-1} - BB^{n-1}A && \text{(A.2)}\\
=& ABB^{n-1} - BB^{n-1}A + BAB^{n-1} - BAB^{n-1} && \text{(A.3)}\\
=& (AB - BA)B^{n-1} + B(AB^{n-1} - B^{n-1}A) && \text{(A.4)}\\
=& [A, B]B^{n-1} + B[A, B^{n-1}]\,. && \text{(A.5)}
\end{aligned}$$

We have obtained a recursive relation, as the result in Eq.(A.5) can be substituted again into its second term and so on, yielding

$$\begin{aligned}
[A, B^n] =& [A, B]B^{n-1} + B[A, B^{n-1}] && \text{(A.6)}\\
=& [A, B]B^{n-1} + B\left([A, B]B^{n-2} + B[A, B^{n-2}]\right) && \text{(A.7)}\\
=& [A, B]B^{n-1} + B[A, B]B^{n-2} + B^2[A, B]B^{n-3} + \cdots + B^{n-1}[A, B]. && \text{(A.8)}
\end{aligned}$$

If B commutes with $[A, B]$, this simplifies to

$$[A, B^n] = nB^{n-1}[A, B], \tag{A.9}$$

hence proving the identity in Eq.(2.59).

We will now show the correctness of Eq.(3.13) in Section 3.1, where we will follow [3]. We want to prove that

$$O_1^{-1} = \Omega_1 - \Omega_2\Omega_3^{-1}\Omega_2^T\,, \tag{A.10}$$

which is most easily done by multiplying the right hand side with O_1 and showing that this yields the identity matrix. Using only the indices to indicate the different sectors of Ω and O , we have

$$O_1\left[\Omega_1 - \Omega_2)\Omega_3^{-1}\Omega_2^T\right] = O_{ab}\Omega_{bc} - O_{ab}\Omega_{bi}(\Omega_3^{-1})_{ij}\Omega_{jc}\,. \tag{A.11}$$

We can write $O_{ab}\Omega_{bc} = O_{aA}\Omega_{Ac} - O_{ai}\Omega_{ic}$ and, likewise, $O_{ab}\Omega_{bi} = O_{aA}\Omega_{Ai} - O_{ak}\Omega_{ki}$. Substituting this in (A.11) gives

$$O_{aA}\Omega_{Ac} - O_{ai}\Omega_{ic} - \left(O_{aA}\Omega_{Ai} - O_{ak}\Omega_{ki}\right)(\Omega_3^{-1})_{ij}\Omega_{jc}\,. \tag{A.12}$$

Using that $O_{aA}\Omega_{Ac} = \delta_{ac}$ and $O_{aA}\Omega_{Ai} = \delta_{ai} = 0$, we can simplify (A.12) to

$$\delta_{ab} - O_{ai}\Omega_{ic} + O_{ak}\Omega_{ki})(\Omega_3^{-1})_{ij}\Omega_{jc}\,. \tag{A.13}$$

Realising that $\Omega_{ki} = (\Omega_3)_{ki}$, (A.13) becomes

$$\delta_{ab} - O_{ai}\Omega_{ic} + O_{ak}\delta_{kj}\Omega_{jc} = \delta_{ab}. \tag{A.14}$$

Thus, we conclude that

$$(O_1)_{ac}\left[\Omega_1 - \Omega_2)\Omega_3^{-1}\Omega_2^T\right]_{cb} = \delta_{ab}\,, \tag{A.15}$$

which was to be proven.

References

[1] M. Srednicki. Entropy and area. *Physical Review Letters* **71.5**, 666 (1993).

[2] J.D. Bekenstein. Black holes and entropy. *Physical Review D* **7**, 2333 (1973).

[3] L. Bombelli, R. Koul and R.D. Sorkin. Quantum source of entropy for black holes. *Physical Review D* **34(2)**, 373 (1986).

[4] A. Jellal, F. Madouri and A. Merdaci. Entanglement in coupled harmonic oscillators studied using a unitary transformation. *Journal of Statistical Mechanics: Theory and Experiment*, **2011.09**, P09015 (2011).

[5] I. Peschel and V. Eisler. Reduced density matrices and entanglement entropy in free lattice models. *Journal of physics A: Mathematical and Theoretical* **42**, 504003 (2009).

[6] M.B. Plenio, J. Eisert, J. Dreissig and M. Cramer. Entropy, entanglement, and area: analytical results for harmonic lattice systems. *Physical review letters* **94**, 060503 (2005).

[7] K. Audenaert, J. Eisert, M.B. Plenio and R.F. Werner. Entanglement properties of the harmonic chain. *Physical Review A* **66**, 042327 (2002).

[8] P. Calabrese and J. Cardy. Entanglement entropy and quantum field theory. *Journal of Statistical Mechanics: Theory and Experiment* **2004.06**, P06002 (2004).

[9] T. Nishioka, S. Ryu and T. Takayanagi. Holographic entanglement entropy: an overview. *Journal of Physics A: Mathematical and Theoretical* **42**, 504007 (2009).

[10] R. Horodecki, P. Horodecki, M. Horodecki and K. Horodecki. Quantum entanglement. *Reviews of modern physics*, **81**, 865 (2009).

[11] S.J. Blundell and K.M. Blundell. *Concepts in thermal physics* (Oxford University Press, 2010).

[12] M.A. Nielsen and I. L. Chuang. *Quantum computation and information* (Cambridge University Press, 2000).

[13] A.L. Fetter and J.D. Walecka. *Quantum theory of many-particle systems* (Dover, 2003).