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ENTANGLEMENT AND DECOHERENCE IN MANY-BODY PHYSICS

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DOTTORANDO: Ugo Marzolino

Responsabile dottorato di ricerca: Chiar.mo prof. Paolo Camerini (Univ. Trieste)

FIRMA: ______________________________

Tutore e Relatore: Dott. Fabio Benatti (Univ. Trieste)

FIRMA: ______________________________

Correlatore: Dott. Roberto Floreanini (INFN Trieste)

FIRMA: ______________________________

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## Contents

### I  Introduction

1  Environments and quantum noise  
   1.1  Density matrix  
   1.2  Closed systems  
   1.3  Master equation approach  
      1.3.1  Markovian vs non-Markovian dynamics  
      1.3.2  Brownian motion: damped harmonic oscillator  
      1.3.3  Long time scales  

2  Entanglement  
   2.1  Definition and properties  
      2.1.1  Local operators  
      2.1.2  Partial trasposition  
   2.2  Environment induced entanglement generation  
   2.3  Algebraic entanglement  
      2.3.1  Relative entanglement of distinguishable particles  
      2.3.2  What happens with identical particles  
      2.3.3  Algebraic definition  
      2.3.4  Applications  

### II  Results

3  Environment induced entanglement between two atoms  
   3.1  Coarse graining approach  
   3.2  Phononic bath  

---

<table>
<thead>
<tr>
<th>Level</th>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Introduction</td>
<td>5</td>
</tr>
<tr>
<td>1</td>
<td>Environments and quantum noise</td>
<td>11</td>
</tr>
<tr>
<td>1.1</td>
<td>Density matrix</td>
<td>11</td>
</tr>
<tr>
<td>1.2</td>
<td>Closed systems</td>
<td>12</td>
</tr>
<tr>
<td>1.3</td>
<td>Master equation approach</td>
<td>13</td>
</tr>
<tr>
<td>1.3.1</td>
<td>Markovian vs non-Markovian dynamics</td>
<td>16</td>
</tr>
<tr>
<td>1.3.2</td>
<td>Brownian motion: damped harmonic oscillator</td>
<td>17</td>
</tr>
<tr>
<td>1.3.3</td>
<td>Long time scales</td>
<td>22</td>
</tr>
<tr>
<td>2</td>
<td>Entanglement</td>
<td>24</td>
</tr>
<tr>
<td>2.1</td>
<td>Definition and properties</td>
<td>24</td>
</tr>
<tr>
<td>2.1.1</td>
<td>Local operators</td>
<td>26</td>
</tr>
<tr>
<td>2.1.2</td>
<td>Partial trasposition</td>
<td>26</td>
</tr>
<tr>
<td>2.2</td>
<td>Environment induced entanglement generation</td>
<td>27</td>
</tr>
<tr>
<td>2.3</td>
<td>Algebraic entanglement</td>
<td>29</td>
</tr>
<tr>
<td>2.3.1</td>
<td>Relative entanglement of distinguishable particles</td>
<td>30</td>
</tr>
<tr>
<td>2.3.2</td>
<td>What happens with identical particles</td>
<td>32</td>
</tr>
<tr>
<td>2.3.3</td>
<td>Algebraic definition</td>
<td>34</td>
</tr>
<tr>
<td>2.3.4</td>
<td>Applications</td>
<td>36</td>
</tr>
<tr>
<td>3</td>
<td>Environment induced entanglement between two atoms</td>
<td>42</td>
</tr>
<tr>
<td>3.1</td>
<td>Coarse graining approach</td>
<td>44</td>
</tr>
<tr>
<td>3.2</td>
<td>Phononic bath</td>
<td>47</td>
</tr>
</tbody>
</table>
3.2.1 Environment induced entanglement generation . . . . . . . . . . 49
3.3 Electromagnetic bath . . . . . . . . . . . . . . . . . . . . . . . . . . . 52
3.3.1 Environment induced entanglement generation . . . . . . . . . . 57

4 Reconstruction of master equation parameters 60
4.1 Cumulants reconstruction through tomography . . . . . . . . . . . . . 62
4.1.1 An alternative procedure . . . . . . . . . . . . . . . . . . . . . . . 66
4.2 Markovian master equations . . . . . . . . . . . . . . . . . . . . . . . . 67
4.3 Convolutionless non-Markovian master equations . . . . . . . . . . . . . 69
4.3.1 A benchmark model . . . . . . . . . . . . . . . . . . . . . . . . . 71
4.3.2 Time independent coefficients . . . . . . . . . . . . . . . . . . . . . 72
4.3.3 Master equation parameters . . . . . . . . . . . . . . . . . . . . . . 77

5 Quantum metrology 85
5.1 Interferometry . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 86
5.2 Spin inequalities . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 88
5.2.1 Collective spin inequalities and entanglement . . . . . . . . . . . . . 88
5.2.2 Spin-squeezing . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 91
5.3 Quantum Fisher information . . . . . . . . . . . . . . . . . . . . . . . . 97
5.3.1 Sub-shot-noise . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 99
5.4 Heisenberg limit . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 103
5.5 Fluctuating particle number . . . . . . . . . . . . . . . . . . . . . . . . 103
5.6 Localization and identification of particles . . . . . . . . . . . . . . . . . 108

III Conclusions 112

A Some integrals 117

B Weyl-Wigner-Moyal representation 120
B.1 Symplectic tomography . . . . . . . . . . . . . . . . . . . . . . . . . . . 121

C Sampling theorems 123

D Coherent states 126
D.1 Contraction of the Lie algebra U(2) to the Heisenberg Lie algebra h(4) . . 128
## E Estimation theory

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>E.1 Classical estimation theory</td>
<td>130</td>
</tr>
<tr>
<td>E.2 Quantum estimation theory</td>
<td></td>
</tr>
<tr>
<td>E.2.1 Unitary paths of states</td>
<td>133</td>
</tr>
<tr>
<td>E.2.2 Generalizations</td>
<td>135</td>
</tr>
</tbody>
</table>

**Bibliography** ...

136
Part I

Introduction
Quantum mechanics was originally formulated for microscopic systems. In many textbook the theory is still referred to closed systems, underlying reversible Hamiltonian evolutions. The time evolution of closed systems is described by a one parameter (i.e. time) unitary group, satisfying the usual Schrödinger equation. Real systems are actually never isolated from their environment. At least a weak interaction with the environment should always be taken into account, in order to model realistic physical system, such as those realized in the laboratories. Environment effects derive from non negligible couplings to surrounding degrees of freedom. The presence of a measurement apparatus can as well couple the system with external degrees of freedom. A quantum system interacting with its environment is called an open quantum system. An environment with an infinite number of degrees of freedom is usually called reservoir. In this case the frequencies of the reservoir modes form a continous set and the theromodynamic limit is performed. This limit gives us an irreversible time evolution. Indeed, information (e.g. von Neumann entropy) flows from the system to the infinite environment which behaves as a sink without giving back the complete information. Furthermore, bath or heat bath will refer to a reservoir in thermal equilibrium at temperature $T = \frac{1}{k_B \beta}$.

A brute force approach to find the time evolution of a system interacting with an environment is to solve the microscopic Hamiltonian dynamics. Typical environments in laboratories, e.g. the surrounding molecules at the room temperature, are huge systems. The approximation of infinite degrees of freedom is highly plausible. Therefore, the solution of the microscopic dynamics is a very hard or impossible task within nowadays techniques. Even in the unlikely scenario of solvable microscopic dynamics, it may be useless to compute it. Indeed, we are interested only in the system dynamics and how it is influenced by the environment. We do not care of all the microscopic details, which include much more information than we need. Thus, solving the microscopic dynamics is an unnecessary and a computationally too expensive task. In order to overcome this difficulties, we can look for an effective description of the reduced state dynamics, pertaining only to the system. The time-evolution of the reduced state is computed averaging out the irrelevant environmental degrees of freedom. One of the standard and most developped approach is to find a dynamical equation, whose solution represents the reduced quantum state of the system. This equation is called master equation. In the case of Hamiltonian dynamics, it reduces to the usual Schrödinger equation. This is a useful tool to avoid to compute the microscopic dynamics. However, only when the coupling between system and environment is weak, a master equation can be derived, in the most general case one needs other approaches.

Over the years the theory of open quantum systems has gained interest and enthusiasm in many fields of physics. Since the very beginning high energy physics has been representing a source of applications and inspiration, e.g. inelastic collisions [116, 117].
quantum cosmology [122, 123, 124], subnuclear physics (see references in [98]). More recently, quantum optics [85] has offered a test ground, because of the growing accuracy of experiments. Two of the most recent optical applications are ions trapped in an external, and possibly periodic, potential and atoms in a cavity (cavity QED). In these cases environmental degrees of freedom may be given by impurities, fluctuations of the external potential or a non perfectly isolated cavity. Chemistry and biology have as well encountered the need to describe real systems as open quantum systems [146, 167, 171]. In the last years, one of the most intriguing and promising development in atomic physics and statistical physics is the description of the Bose-Einstein condensates (BEC) [43, 45, 46, 47, 48], i.e. many identical Bosons filling the same ground state of an external potential. BEC represent an appealing benchmark for several physical phenomena, such as quantum coherence in macroscopic or mesoscopic systems. Indeed, BECs are very interesting also from the point of view of open quantum systems. A BEC may be considered an environment of a smaller system. Furthermore, a BEC may feel environmental effects, due to imperfections of the potential or to the presence of non condensed particles due to its evaporation.

One of the most discussed phenomena induced by the interaction with an environment is decoherence. Decoherence is the damping of the off-diagonal elements of the density matrix, that describes the state of the system. The name is justified by the fact that quantum coherence is encoded in the off-diagonal elements. Once they are damped to zero, any quantum coherence is lost and the state becomes a purely statistical mixture of eigenvectors whose probabilities are the eigenvalues. Indeed, the decoherence and the loss of quantum coherence are base dependent. The basis developing decoherence depends on the interaction with the environment [88, 97]. Some environments cause decoherence of a quantum particle in the overcomplete basis of coherent states. This phenomenon is related to the problem of quantum to classical transition, since the coherent state are those closest to the points in classical phase-space. The role of decoherence in the emergence of classicality in quantum systems is discussed in [88, 97, 121]. However, this discussion is still open. A generalization of coherent states can be defined also for finite dimensional systems [10]. However, the environment does not only destroy quantum features. It can also enhance them, especially at small times. An example is the generation of entanglement due to the pure dissipation. Quantum features, such as entanglement, may be also protected at large times, e.g. if there are decoherence-free subspaces. Entanglement and other quantum features, such as non locality due to the indistinguishability of identical particles, are behind quantum information protocols improving classical performances. As an example of these quantum protocols we shall discuss quantum metrological schemes. Thus, it is important to protect those features, enhance them or correct their dissipation in a noisy dynamics. To this purpose, much attention has been paid to engineering and controlling environments in the recent years. These researches are known as quantum
control and quantum error correction [55, 101].

In order to implement these proposals, physical systems, e.g. those mentioned above, are usually modelled using several settings. Qubits, namely two level systems, are the simplest finite dimensional systems. Due to the simplicity of their structures, e.g. the small Hilbert space and the algebra of observables, much is known about the entanglement. Moreover, the simplest states describing infinite dimensional systems are the coherent, or Gaussian, states. Because they are defined by a finite number of free parameters, they are simple to deal with and many properties, e.g. pertaining entanglement, are known. In this framework a special role is played by dynamics that preserve Gaussianity. They are pratically quadratic Hamiltonian, i.e. harmonic oscillators, and quadratic noises. Models of identical particles has been recently studied. For instance, ultracold atomic gases [49, 50, 51] are used to engineer and simulate many physical phenomena, such as BEC [41, 43, 45, 46, 47, 48], superfluidity [41, 43, 45, 46, 47, 51], superconductivity (BCS theory) [41, 44, 45], BEC/BCS crossover [45, 50, 51], quantum phase transitions [42]. Quantum gases consist of identical particles. A lot of efforts have been done in this field, although some theoretical features, such as entanglement, are less under control than in the above mentioned systems. Several real systems can be modelled in terms of qubits, harmonic oscillators, and identical particles. We find instances in atomic, molecular, nano physics and optics. Therefore, we shall focus on the effects of quantum noises in these three models. For instance, we shall describe the environment induced entanglement generation of two qubits and two harmonic oscillators and the decoherence in generalized coherent states for identical Bosons.

Let us turn back to the description of open quantum systems. As mentioned above, master equations can be found only under some assumptions. The first assumption is to consider an initial state which is completely uncorrelated (technically called simply separable) between the system and the environment. This condition is sufficient to get a time evolution which acts linearly on the reduced state. With this unique assumption, only few dynamics have been derived exactly. In the special case of a quantum register (\(N\) qubits) in a purely dephasing dynamics [125], the exact reduced dynamics is computed. Exact master equations have been derived for the evolution of a Brownian particle linearly coupled to a harmonic oscillator bath, for instance via path integral methods [122, 124] or phase-space and Wigner function computations [113, 126]. Analogous results are derived by means of quantum trajectories, either exactly or in weak coupling approximation [130, 141, 142, 36, 37]. In the framework of path integral methods, master equations have been derived both for states initially correlated to the environment [128, 129], and for uncorrelated initial states in the case of weak non linear interactions [123]. In general, all these master equations cover only few cases and are not simple to solve. Other techniques provide the time evolution of the reduced state without passing through a master equation.
and in some cases even for states initially correlated to the environment: e.g. path integral computations [102] and phase-space quasi-distributions [9, 136]. Recent works provide non linear master equations for a quantum system interacting with a classical nonequilibrium environment, by means of a thermodynamical approach [172, 173, 174, 175].

We need further working assumptions in order to compute master equations. The most common are rather technical and we shall discuss them later. Weak couplings with the environment allow perturbation expansions. Environmental correlations decaying faster than the typical time scale of the system allow us to neglect correlations between the environment and the system at any time. Markovian approximations hold at large times and neglect memory and short time effects. Markovian dynamics are the one that are prevalenty discussed in the literature. Their mathematical structure is much more known and one can define them adopting an axiomatic approach. Different approximations, Markovian or non Markovian, may give different master equations with different descriptions of the same phenomena [87]. In the case of composite systems, a crucial distinction is between local and global environment. Local environments can not correlate non-interacting systems, global ones can. For this reason we will be more interested in global environments. Moreover, there are several Markovian approximations. The most used one, known as weak coupling (à la Davies), describes the dynamics at a very large time scale, i.e. by means of a very rough coarse graining time. They behave as local environments. It is challenging to develop Markovian approximations at earlier time scales and finer coarse graining, as we shall show. These new approximations describe new phenomena as correlation, e.g. entanglement, generation between different qubits or harmonic oscillators. The landscape of non Markovian approximations is even more complicated. Moreover, in many practical cases a master equation is assumed phenomenologically. Thus, it is crucial to guess the right structure and approximation which capture the interesting phenomena. To this purpose, it is very useful to find some experimentally feasible procedures in order to estimate the parameters of a Markovian or non Markovian master equation and to discriminate and to test different approximations.

Many features of open quantum systems are discussed and reviewed in [83, 84, 85, 88, 87, 89, 92, 93, 95, 98, 99, 100]. Markovian approximations are treated in [83, 89, 92, 98, 99], in particular [98] focuses on the role of complete positivity. Dissipative dynamics of harmonic oscillators are reviewed in [93, 94, 95]. Dissipative dynamics induced by collisions with environmental particles are discussed in [100]. Quantum optics applications are described in [85], while the environment induced emergence of classicality is described in [88]. A wide variety of connected issues are discussed in [84, 87].

The main body of the thesis is divided in three parts. The first part consists of two introductory chapters: chapter 1 about dissipative quantum dynamics and chapter 2 about entanglement. The topics of these chapters are standard ones in the theory of open quan-
tum systems, respectively quantum information theory. However, we will discuss some open problems, like the difference between the Markovian and the non-Markovian noisy dynamics and the validity of some Markovian approximations at large times; more in general, we shall introduce an algebraic definition of entanglement with applications to identical particles. In the second part of the thesis, some original results are discussed. In chapter 3, we shall consider the generation of entanglement between two two-level atoms induced by the interaction with a common environment. We shall derive a new Markovian approximation which, unlike the usual Markovian dynamics, captures the entanglement generation between unequal atoms. In chapter 4, we shall study some experimental procedures based on symplectic tomography, that serve to reconstruct the parameters characterizing the Gaussian dissipative dynamics of a harmonic oscillator. In chapter 5, we shall deal with quantum metrology, namely quantum enhancement of experimental estimations, in relation to spin inequalities and spin squeezing. We shall show that a quantum enhancement of metrological protocols with identical Bosons comes from several sources of non-locality, avoiding the need of an entangled initial state. The third part summarizes the results and in appendices some useful tools are briefly reviewed.
Environments and quantum noise

In this chapter, we shall review the mathematical description of quantum states and their dynamics.

1.1 Density matrix

The mathematical framework for a quantum system is a Hilbert space $\mathcal{H}$. The best description of the quantum system, called pure state, is a normalized element belonging to the Hilbert space: $|\psi\rangle \in \mathcal{H}$ and $\langle \psi | \psi \rangle = 1$. We call $\mathcal{B}(\mathcal{H})$ the space of bounded linear operators acting on $\mathcal{H}$. Any pure state $|\psi\rangle$ can be equivalently described by a rank-one projector $|\psi\rangle\langle\psi| \in \mathcal{B}(\mathcal{H})$. Mixed states are defined as statistical distributions of rank-one projectors: $\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$, $p_j \geq 0$ and $\sum_j p_j = 1$. The normalization of $|\psi_j\rangle$, i.e. $\langle \psi_j | \psi_j \rangle = 1$, implies the normalization of the mixed state, i.e. $\text{Tr}\rho = 1$. A pure state is a particular mixed state, whose $p_j$’s are all vanishing but one. An operator $\rho$ is called density matrix, or density operator.

**Definition 1.1.1.** An operator $X^\dagger = X \in \mathcal{B}(\mathcal{H})$ is positive semi-definite if

$$\langle \phi | X | \phi \rangle \geq 0 \quad \forall \phi \in \mathcal{H}, \quad (1.1)$$

and we write $X \geq 0$.

Any density operator is positive semi-definite. Moreover, any positive operator $\rho \geq 0$ can be written by means of its spectral decomposition as $\rho = \sum_j \lambda_j |j\rangle\langle j|$, where $\lambda_j$ are the eigenvalues and $|j\rangle$ the normalized eigenvectors. Since $\rho$ is positive, $\lambda_j \geq 0$. If $\rho$ is normalized $\text{Tr}\rho = 1$ then $\sum_j \lambda_j = 1$. Thus any positive semi-definite and normalized operator is a density matrix.
Quantum observables are given by Hermitian operators $X = X^\dagger \in \mathcal{B}(\mathcal{H})$. The average of an observable $X$ with respect to a state $\rho = \sum_j p_j |\psi_j\rangle\langle \psi_j|$ is given by

$$\langle X \rangle_\rho = \text{Tr}(\rho X) = \sum_j p_j \langle \psi_j | X | \psi_j \rangle.$$  \hfill (1.2)

The previous definitions constitute the bulk of the statistical interpretation of quantum mechanics.

Density operators form a convex subset $S \subset \mathcal{B}(\mathcal{H})$ which we shall refer to as the state-space. Namely, combining different mixtures $\sigma_j \in S$ with weights $\lambda_j > 0$, $\sum_j \lambda_j = 1$, into the convex combination $\sum_j \lambda_j \sigma_j$, the latter also belongs to $S$. Pure states are extremal elements of $S$, that is they can not be convexly decomposed, while with them, by linear convex combinations, one generates the whole of the state-space.

### 1.2 Closed systems

The dynamics of isolated systems described by pure states is given by the Schrödinger equation [15]

$$\frac{d}{dt} |\psi(t)\rangle = -\frac{i}{\hbar} H(t) |\psi(t)\rangle,$$  \hfill (1.3)

which straightforwardly turns into the Liouville-von Neumann for mixed states

$$\frac{d}{dt} \rho(t) = -\frac{i}{\hbar} [H(t), \rho(t)].$$ \hfill (1.4)

For sake of generality, we have chosen a time dependent Hamiltonian. The found solution of these equations is

$$|\psi(t)\rangle = U_{t,0} |\psi(t_0)\rangle, \quad \rho(t) = U_{t,0} \rho(t_0) U_{t,0}^\dagger, \quad U_{t,0} = T e^{-\frac{i}{\hbar} \int_{t_0}^t ds H(s)}$$ \hfill (1.5)

where $|\psi(t_0)\rangle$ and $\rho(t_0)$ are the initial states and $T$ is the time ordered product. We define the Hamiltonian generator on the state-space as follows

$$\mathcal{L}(t)[\rho(t)] = -\frac{i}{\hbar} [H(t), \rho(t)],$$  \hfill (1.6)

so that the dynamics is the exponential of the generator

$$\rho(t) = \gamma_{t,0} [\rho(t_0)] = T e^{\int_{t_0}^t ds \mathcal{L}(s)} [\rho(t_0)].$$ \hfill (1.7)

Since the Hamiltonian is Hermitian $H^\dagger(t) = H(t)$, the dynamics is unitary: $U_{t,0}^{-1} = U_{t,0}^\dagger$. 


If the Hamiltonian is time independent, the dynamics reads

\[ U_{t,0} = U_{t-t_0} = e^{-\frac{i}{\hbar}(t-t_0)\mathcal{H}}, \quad \gamma_{t,0} = \gamma_{t-t_0} = e^{i(t-t_0)\mathcal{L}}. \]  

(1.8)

In this case, the evolution operators form a one parameter group: \( U_t, U_s = U_{t+s} \) and \( \gamma_t, \gamma_s = \gamma_{t+s} \forall t, s \in \mathbb{R} \). This feature implies the reversibility of the dynamics, since \( U_{-t} = U_{t}^{-1} \) and \( \gamma_{-t} = \gamma_{t}^{-1} \), setting \( s = -t \) in the group property.

We can pass from the Schrödinger picture, discussed until now, to the Heisenberg picture, by means of the duality relation

\[ \text{Tr}(\gamma_{t,0}[\rho]X) = \text{Tr}(\rho \gamma_{t,0}^* [X]), \]  

where

\[ \gamma_{t,0}^*[X] = U_{t,0}^\dagger \rho_0 U_{t,0} = T e^{\int_{t_0}^{t} ds \mathcal{L}(s)} [X] \]  

(1.10)

is the solution of

\[ \frac{d}{dt} X(t) = \frac{i}{\hbar} [H(t), X(t)]. \]  

(1.11)

For time independent Hamiltonian, the Heisenberg time evolution reads \( \gamma_{t,0}^* = \gamma_{-t} = e^{i(t-t_0)\mathcal{L}} \). In the Schrödinger picture density operators evolve in time while observables are fixed, vice versa in the Heisenberg picture.

### 1.3 Master equation approach

We now consider a quantum system interacting with an environment. The Hilbert space of the whole system is the tensor product \( \mathcal{H}_S \otimes \mathcal{H}_E \) and its state is described by a density operator \( \rho_{S+E} \in \mathcal{B}(\mathcal{H}_S \otimes \mathcal{H}_E) \). The system alone is described by the reduced state \( \rho_S = \text{Tr}_E(\rho_{S+E}) \), obtained by tracing out the environmental degrees of freedom. \( \text{Tr}_E(\cdot) = \sum_j \langle e_j| \cdot |e_j \rangle \) is the partial trace over the Hilbert space \( \mathcal{H}_E \) and \( |e_j \rangle \) are an orthonormal basis of \( \mathcal{H}_E \). In order to get a dynamical equation for the reduced state, we trace the environmental degrees of freedom in the Liouville-von Neumann equation of the whole system:

\[ \frac{d}{dt} \rho_S(t) = -\frac{i}{\hbar} \text{Tr}_E[H(t), \rho_{S+E}(t)]. \]  

(1.12)

In general, the right hand side can not be easily written as an operator acting on the reduced evolved state \( \rho_S(t) \):
\[
\frac{d}{dt} \rho_S(t) = \mathbb{L}[\rho_S]. \tag{1.13}
\]
To this purpose, some assumptions are required. We can write the dynamical equation in the Heisenberg picture, by means of the duality relation (1.9):
\[
\frac{d}{dt} X(t) = \mathbb{L}^\ast[X]. \tag{1.14}
\]

Maps describing dynamics should satisfy some mathematical properties, according to the assumptions. One special instance is given by time independent generators \(\mathbb{L}\). The corresponding dynamical maps \(\gamma_t = e^{t\mathbb{L}}\) satisfy the semigroup property
\[
\gamma_t \gamma_s = \gamma_{t+s} \quad \forall t, s \geq 0,
\]
and are termed quantum dynamical semigroups. They are linear maps and the time evolution does not depend on the initial state at any time. The strong continuity in time of a quantum dynamical semigroup is necessary for the existence of a generator [13]. Moreover all quantum dynamical maps must preserve the Hermiticity and the trace of the reduced density matrix. It is necessary in order to send density matrices into density matrices. These conditions suffice to fix the generator of a quantum dynamical semigroup.

**Theorem 1.3.1.** Let \(\gamma_t^\ast : \mathcal{B}(\mathcal{H}_S) \mapsto \mathcal{B}(\mathcal{H}_S), \ t \geq 0,\) form a time-continuous semigroup of Hermiticity preserving and trace preserving linear maps. Then, the semigroup has the form \(\gamma_t = e^{t\mathbb{L}}\) in the Schrödinger picture and \(\gamma_t^\ast = e^{t\mathbb{L}^\ast}\) in the Heisenberg picture whose generators are
\[
\mathbb{L}[\rho_S] = -i[H, \rho_S] + \sum_{i,j=1}^{n^2-1} C_{ij} \left( F_i^\dagger \rho_S F_i - \frac{1}{2} \{ F_i F_i^\dagger, \rho_S \} \right), \tag{1.15}
\]
\[
\mathbb{L}^\ast[X] = i[H, X] + \sum_{i,j=1}^{n^2-1} C_{ij} \left( F_j X F_i^\dagger - \frac{1}{2} \{ F_j F_i^\dagger, X \} \right). \tag{1.16}
\]
where \(n\) is the dimension of \(\mathcal{H}_S\), the matrix of coefficient \(C_{ij}\), called Kossakowski matrix, is Hermitian, \(H = H^\dagger\), and the so-called Lindblad operators \(F_j\) are such that \(F_n^\dagger = 1_n/\sqrt{n}\) and \(\text{Tr}(F_j^\dagger F_k) = \delta_{jk}, 0 \leq j, k \leq n^2,\) while \(\{ , \}\) represents anticommutation.

This theorem is proved in [106].

Another important condition that all the dynamical maps should satisfy is the positivity, defined in the following definition.

**Definition 1.3.1.** A map \(\gamma : \mathcal{B}(\mathcal{H}) \mapsto \mathcal{B}(\mathcal{H})\) is positive if it sends positive operators into positive operators.
Positivity is required in order to maintain the probability interpretation of quantum mechanics. Indeed, the spectrum of any time-evolving density matrix must remain positive at all times, and this is guaranteed if the dynamics is positive. A complete characterization of positive maps is a challenging task. Sufficient conditions for positive quantum dynamical semigroups are known [103, 135, 139, 140], while necessary conditions are still unknown.

A much more stringent condition is the complete positivity, which is essential for quantum dynamical semigroups. This condition prevents physical inconsistencies when the system is coupled to an arbitrary auxiliary one. A map is completely positive if its action combined to the identity operation \( I \) on an auxiliary system is positive [13] (pag. 155 Definition 8.5).

**Definition 1.3.2.** A linear map \( \gamma : \mathcal{B}(\mathcal{H}) \mapsto \mathcal{B}(\mathcal{H}) \) is completely positive, if and only if \( \gamma \otimes I \) is positive on \( \mathcal{B}(\mathcal{H}) \otimes M_m(\mathbb{C}) \) for all \( m \geq 1 \).

Actually, in the case of finite-dimensional \( \mathcal{H} \) it is enough to check the positivity for \( m = \text{dim}(\mathcal{H}) \) [13] (pag. 156 Theorem 8.8).

**Theorem 1.3.2.** If \( \mathcal{H} = \mathbb{C}^n \), then a linear map \( \gamma : \mathcal{B}(\mathcal{H}) \mapsto \mathcal{B}(\mathcal{H}) \) is completely positive, if and only if \( \gamma \otimes I \) is positive on \( \mathcal{B}(\mathcal{H}) \otimes M_m(\mathbb{C}) \).

Furthermore, the most general form of completely positive maps is known [13, 58].

**Theorem 1.3.3.** A linear map \( \mathcal{B}(\mathcal{H}) \mapsto \mathcal{B}(\mathcal{H}) \) is completely positive, if and only if it is expressible in Kraus-Stinespring form

\[
\gamma[X] = \sum_{\alpha} V_{\alpha}^\dagger X V_{\alpha},
\]

where \( V_{\alpha} \in \mathcal{B}(\mathcal{H}) \) are such that \( \sum_{\alpha} V_{\alpha}^\dagger V_{\alpha} \) converges. If it converges to \( 1_n \), \( \gamma \) is termed unital.

Suppose one has a linear map on \( \mathcal{B}(\mathcal{H}) \) given in the form

\[
\gamma[X] = \sum_{\alpha\beta} C_{\alpha\beta} W_{\alpha}^\dagger X W_{\beta},
\]

with \( W_{\alpha} \in \mathcal{B}(\mathcal{H}) \) and \( C_{\alpha\beta} \) making a hermitian matrix of coefficients such that \( \sum_{\alpha\beta} C_{\alpha\beta} W_{\alpha}^\dagger W_{\beta} \) converges. By diagonalizing \( [C_{\alpha\beta}] = U^\dagger \text{diag}(d_1, d_2, \ldots) U \), one recovers (1.18) if and only
if \([C_{\alpha\beta}]\) is positive definite and thus \(d_i > 0\); indeed, \(C_{\alpha\beta} = \sum_j d_j U^*_{ja} U_{j\beta}\) and this serves to redefine \(V_j = \sum_\alpha \sqrt{d_j} U^*_{ja} W_\alpha\).

Complete positivity is fully characterized in quantum dynamical semigroup by the positivity of the Kossakowski matrix.

**Theorem 1.3.4.** The semigroup \(\{\gamma_t\}_{t\geq 0}\) consist of completely positive maps if and only if the Kossakowski matrix is positive definite.

This theorem is proved in [106] for finite dimensional Hilbert spaces \(\mathcal{H}\) and in [107] for infinite dimensional Hilbert spaces \(\mathcal{H}\) and bounded generators.

### 1.3.1 Markovian vs non-Markovian dynamics

Quantum dynamical semigroups are referred to Markovian dynamics. In fact, they transform density operators into density operators without any memory of the earlier evolution. They act linearly on any initial density operator. Generalization of such master equations are time dependent generators acting locally in time \(\rho_S \mapsto L_t[\rho_S(t)]\) and generators with a convolution integral \(L[\rho_S] = \int ds L_{t-s}[\rho_S(s)]\). We note that the literature about non-Markovian master equations may lead to some ambiguity. Indeed, some authors classify as Markovian those master equations with convolutionless local in time generators and as non-Markovian only those master equations whose generator contains a convolution integral. It has recently been proved in [170] that these latter generators can be mapped into convolutionless ones, following a so-called local approach. Non-Markovianity becomes then characterized by the dependence of the convolutionless generator on \(t - t_0\) where \(t_0\) is the initial time. According to this approach a time-dependent convolutionless generator could be considered as the generator of a Markovian reduced dynamics. A sensible definition of (non-)Markovian master equation may come as a generalization of (non-)Markovian processes in probability theory. A Markovian process is a (discrete or continuous) chain of random variables where the transition probabilities between two consecutive variables do not depend on the previous variables, otherwise the process is called non-Markovian. This definition has a natural generalization in quantum processes. Generators, namely the time derivative of the quantum process, which are local in time, either time independent and time dependent, give Markovian master equations. Generators containing convolution integrals give non-Markovian master equations. However, following a consistent part of literature, e.g. [122, 113, 126, 141, 142, 123, 143], we will term non-Markovian also time-evolutions generated by convolutionless time-dependent generators.

The simplest case of quantum dynamical semigroup is the only one which is discussed within a general theory [83, 98]. Several approximation techniques leading to quantum
dynamical semigroup from a microscopic Hamiltonian are well known [87, 89, 98, 100]. Notwithstanding, only few Markovian dynamics are analytically solved and general discussions are constrained by asymptotic or short time evolutions or by numerical tools. Since only few non-Markovian exact master equations are known, it would be highly desirable to find an approximation scheme fully capturing non-Markovian features. Standard techniques are described in [87]. In [137], a method based on superoperator algebra allows to solve the non-Markovian Brownian motion. In [90, 147, 150] projection operator techniques have been employed to generalize the Lindblad approach to the non-Markovian case. In [151, 165], it is discussed an approximation on the system-bath interaction allowing a completely positive time evolution. In general, different approximations may lead to physically different dynamics [87].

Linear master equations come from the almost ubiquitous assumption of no initial correlations between the system and the environment. The linearity corresponds to a unique dynamical map for any possible initial reduced state. Among the initial states, one must always consider the possibility of compound states involving auxiliary systems, these latter are left unchanged by the time evolution. This is the physical motivation for requiring complete positivity. Careless Markovian approximation may not satisfy necessary properties such as complete positivity or even positivity [98]. Rather than checking a posteriori the complete positivity, it is desirable to find approximations a priori providing completely positive dynamics. Such an approximation is the so called weak coupling limit [83, 87, 98, 104, 105, 109]. We shall develop and discuss another one which is, in a sense, finer. On the other hand, a general derivation of non-Markovian master equations is missing. A recent work [164] discusses the structure of generators involving convolution integrals which give rise to completely positive dynamics.

If initial correlations between the system and the environment are allowed, complete positivity is not required any more [160]. The lack of complete positivity implies the lack of positivity during the evolution of initial states which are entangled with some auxiliary system. If the system is initially correlated with the environment, it can not be too much correlated with another system [63, 67]. This is the physical reason for relaxing the assumption of complete positivity.

1.3.2 Brownian motion: damped harmonic oscillator

In this section, we shall discuss a class of Gaussian Shape Preserving (GSP) master equations with unknown coefficients modeling a one-dimensional damped harmonic oscillator. It is a solvable model which serves as an example of the previous discussions. We focus on the following general master equations:
\[
\frac{d\rho(t)}{dt} = L[\rho(t)] = -\frac{i}{\hbar}[H,\rho(t)] + \frac{1}{2\hbar} \sum_j \left( [V_j(t)\rho(t), V_j^\dagger(t)] + [V_j(t),\rho(t)V_j^\dagger(t)] \right),
\] (1.20)

where \( \rho(t) \) is the reduced density operator of the system. The master equation (1.20) is a straight generalization of the Markovian dynamics (1.15), where the non-unitary time evolution of a quantum system is described by (1.20) dropping the time-dependence in the operators \( V_j \). Microscopic derivations of master equations give Markovian time-independent behaviour only within some approximations \([91, 106, 107]\). Thus, more realistic systems may be described by a time-dependent dissipative generator, even though the microscopic Hamiltonian does not depend on the time. The interaction with the environment may also contribute with a Hamiltonian correction, called Lamb shift. The time-dependence which may be introduced by the Lamb shift term has been neglected. This is typically justified as most of the times either the Lamb shift is negligible or the Hamiltonian part of the dissipative generator reaches its asymptotic value on a much shorter timescale compared to the non unitary part \([87]\). We shall show that equation (1.20) is formally solvable if the Lindblad operators \( V_j \) and the system Hamiltonian \( H \) are, respectively, at most first and second degree polynomials in position \( q \) and momentum \( p \) coordinates.

For systems like a harmonic oscillator or a field mode in an environment of harmonic oscillators (i.e. collective modes or a squeezed bath), \( H \) can be chosen of the general quadratic form

\[
H = H_0 + \frac{\delta}{2}(qp + pq), \quad H_0 = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}q^2,
\] (1.21)

where \( \delta \) is the strength of the bilinear term in \( q \) and \( p \), \( m \) is oscillator mass, and \( \omega \) its frequency. The operators \( V_j \), which model the environment, are linear polynomials in \( q \) and \( p \):

\[
V_j(t) = a_j(t)p + b_j(t)q, \quad j = 1, 2,
\] (1.22)

with \( a_j(t) \) and \( b_j(t) \) complex numbers. The sum goes from 1 to 2 as there exist only two linear independent operators \( V_1(t), V_2(t) \), in the linear space of first degree polynomials in \( p \) and \( q \). We can safely omit generic constant contributions in \( V_j(t) \) as they do not influence the dynamics of the system.

Given this choice of operators, the Markovian master equation (1.20) can be rewritten as:

\[
\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[H_0,\rho(t)] - \frac{i(\lambda(t) + \delta)}{2\hbar} [q,\rho(t)p + pp\rho(t)] +
\]
1.3 - Master equation approach

\[ + \frac{i(\lambda(t) - \delta)}{2\hbar} [p, \rho(t)q + q\rho(t)] - \frac{D_{pp}(t)\hbar^2}{\hbar^2} [q, [q, \rho]] + \]

\[ - \frac{D_{qq}(t)}{\hbar^2} [p, [p, \rho(t)]] + \frac{D_{qp}(t)}{\hbar^2} ([q, [p, \rho(t)]] + [p, [q, \rho(t)]]), \]

(1.23)

where \( \lambda(t) = -\text{Im} \sum_{j=1,2} a^*_j(t)b_j(t) \) is the unknown friction constant and

\[ D_{qq}(t) = \frac{\hbar}{2} \sum_{j=1,2} |a_j(t)|^2, \quad D_{pp}(t) = \frac{\hbar}{2} \sum_{j=1,2} |b_j(t)|^2, \quad D_{qp}(t) = -\frac{\hbar}{2} \text{Re} \sum_{j=1,2} a^*_j(t)b_j(t) \] (1.24)

are the unknown diffusion coefficients. The master equation in (1.23) represents a natural generalization of the time-independent master equation discussed in [95, 116, 117] which describes a GSP evolution of a quantum state. In the time-dependent case a wide range of models obeys a GSP master equation of the form (1.23) [113, 124, 126, 128, 129, 141, 142, 36, 37]. The friction and diffusion coefficients of the Markovian, time-independent, generators satisfy the following constraints which ensure the complete positivity of the time evolution [95, 116, 117]:

\[ D_{qq} > 0, \quad D_{pp} > 0, \quad D_{qq}D_{pp} - D_{qp}^2 \geq \frac{\lambda^2\hbar^2}{4}. \] (1.25)

If the same conditions hold for the coefficients of a convolutionless non-Markovian generator, at any time, the generator gives a so-called Lindblad type dynamics [143].

Markovian GSP master equations of the form equation (4.9) are used in quantum optics and nuclear physics [114, 115, 118], and in the limit of vanishing \( \omega \) can be employed for a phenomenological description of quantum Brownian motion [111, 145, 154]. Also, in the case of a high-temperature Ohmic environment the time-dependent master equation derived in [122, 126] can be recast in this time-independent shape. It must be noted however that in the high-temperature limit the third constrain in (1.25) seems to be violated. Nevertheless, even if \( D_{qq} = 0, \ D_{qp} = 0 \) and \( \lambda \neq 0 \), \( D_{pp} \) diverges only linearly with temperature. Therefore, we can recover the complete positivity by means of a suitable renormalization. This renormalization consists in adding a suitable subleading term \( D_{qq} \) (e.g. \( D_{qq} \propto T^{-1} \)). Otherwise, we can consider an high frequency cut-off for the environment [122, 126]. In this way the master equation is not Markovian anymore. Anyway, since it involves only regular functions, it should give a completely positive dynamics (as the microscopic unitary group does).

Even though Markovian evolutions have been extensively investigated (see e.g. [83, 85, 87, 92, 93, 95, 98]), in general real noisy dynamics are far from being Markovian. Exact non-Markovian master equations have been derived for a Brownian particle linearly coupled to a harmonic oscillator bath via e.g. path integral methods [122, 124] or
phase-space and Wigner function computations [113, 126]. Analogous results have been obtained employing quantum trajectories, either exactly or in weak coupling approximation [130, 141, 142, 36, 37]. In the framework of path integral methods, master equations have been derived both for initially correlated states [128, 129], and for factorized initial states in the case of weak non linear interactions [123].

**Gaussian states evolution**

We now investigate the evolution of an initial Gaussian state according to the equation (1.23). In particular we derive invertible expressions for the cumulants of the state at a time \( t \) in terms of the parameters of the master equation. Due to the Gaussian shape preservation, the evolved state at time \( t \) is completely determined by its first and second order momenta. Due to the linearity of the \( V_j(t) \)'s in phase-space, the time-evolution of the first and second order cumulants can be decoupled. We then obtain the following two sets of solvable equations:

\[
\begin{align*}
\frac{d}{dt} \langle q \rangle_t &= -(\lambda(t) - \delta) \langle q \rangle_t + \frac{1}{m} \langle p \rangle_t, \\
\frac{d}{dt} \langle p \rangle_t &= -m\omega^2 \langle q \rangle_t - (\lambda(t) + \delta) \langle p \rangle_t, \\
\frac{d}{dt} \Delta q^2_t &= -2(\lambda(t) - \delta) \Delta q^2_t + \frac{2}{m} \sigma(q, q)_t + 2D_{qq}(t) \\
\frac{d}{dt} \Delta p^2_t &= -2(\lambda(t) + \delta) \Delta p^2_t - 2m\omega^2 \sigma(q, p)_t + 2D_{pp}(t) \\
\frac{d}{dt} \sigma(q, p)_t &= -m\omega^2 \Delta q^2_t + \frac{1}{m} \Delta p^2_t - 2\lambda(t) \sigma(q, p)_t + 2D_{qp}(t)
\end{align*}
\]

Equations (1.26)-(1.27) can be expressed in compact matrix form as

\[
\frac{d}{dt} S(t) = (M - \lambda(t)1_2) S(t), \\
\frac{d}{dt} X(t) = (R - 2\lambda(t)1_3) X(t) + D(t),
\]

where \( 1_2(3) \) is the 2(3)-dimensional identity matrix. The vectors \( S(t) \) and \( X(t) \) correspond, respectively, to the first and second order cumulants

\[
S(t) = \frac{1}{\sqrt{\hbar}} \left( \frac{\sqrt{m\omega \langle q \rangle_t}}{\sqrt{m\omega}}, \frac{\sqrt{m\omega \langle p \rangle_t}}{\sqrt{m\omega}} \right), \\
X(t) = \frac{1}{\hbar} \left( \frac{m\omega \Delta q^2_t}{(m\omega)}, \frac{\Delta p^2_t/(m\omega)}{(\sigma_{q,p})_t} \right),
\]
The matrices $M$ and $R$ contain the Hamiltonian parameters

$$
M = \begin{pmatrix}
\delta & \omega \\
-\omega & -\delta
\end{pmatrix}, \quad R = \begin{pmatrix}
2\delta & 0 & 2\omega \\
0 & -2\delta & -2\omega \\
-\omega & \omega & 0
\end{pmatrix}
$$

(1.31)

and, finally, $D(t)$ is the diffusion vector

$$
D(t) = \frac{2}{\hbar} \begin{pmatrix}
m\omega D_{qq}(t) \\
D_{pp}(t) \\
m\omega D_{qp}(t)
\end{pmatrix},
$$

(1.32)

The dynamical evolution of the first cumulants (1.28) depends only on $\lambda(t)$ whereas that of the second cumulants, equation (1.29), depends on the whole set of coefficients.
1.3.3 Long time scales

Despite the growing interest in non-Markovian dynamics in optics [85, 131], chemical physics [146, 171], biology [167, 171] and mathematical physics [164], they are much more complicated and much less known than Markovian dynamics. Furthermore, there are still some open problems with Markovian approximations. Indeed, they hold on large time-scales, where memory effects are negligible. Some subtle problems concern these time scales and whether they correctly approximate the asymptotic state.

We consider a system, interacting with its environment whose coupling constant is $\lambda$. The standard weak coupling approximation provides a dynamical semigroup $e^{\lambda t L(2)}$ and holds for small $\lambda$ and times scaling as $\frac{1}{\lambda^2}$ [104, 105, 87, 98, 99]. The time scaling should be large enough to neglect the non-Markovian memory effects. The error between the weak coupling limit and the exact dynamics is of the order of $O(\lambda^2)$, for any finite time $t \in [0, \infty)$ and $\lambda \in [0, \Lambda]$ [104, 105, 110, 112, 119]: under suitable hypotesis, it is proved [110, 112] that

$$\left\| \rho(t) - e^{\lambda^2 t L(2)} \rho(0) \right\| \leq \lambda^2 \beta_2(\lambda^2 t) \sup_{s \in [0, t]} \left\| e^{\lambda^2 s L(2)} \rho(0) \right\|,$$

where $\rho(t)$ is the exact evolution and $\beta_2(\cdot)$ is a positive and bounded function on a compact set. Therefore, the approximation gets closer to the exact dynamics when $\lambda$ approaches zero. In this limit, the time scale is pushed forward. However, if the environment is at temperature $T$, for any even small $\lambda$ there is a temperature $T$ below which the weak coupling limit is not applicable. For small $\lambda$, a perturbation expansion in $\lambda$ has been obtained whose first order is the standard weak coupling limit [110, 112, 119]. This expansion consists in two kinds of corrections to the weak coupling limit. The first one is a correction to the generator of the semigroup $e^{\sum_{j=1}^{\infty} \lambda^j L(j)}$. This correction does not change the magnitude of the approximation but pushes the time scale of the approximation forward: for instance, under some hypotesis [110, 112]

$$\left\| \rho(t) - e^{\lambda^2 t L(2) + \lambda^4 t M(t)} \rho(0) \right\| \leq \lambda^2 (a + b \lambda^4 t) \sup_{s \in [0, t]} \left\| e^{\lambda^2 s L(2) + \lambda^4 s M(t)} \rho(0) \right\|,$$

where $a$ and $b$ are constants, for any finite time $t \in [0, \infty)$ and $\lambda \in [0, \Lambda]$. The latter estimation shows that this refined approximation holds at times scaling as $\frac{1}{\lambda^4 t}$. The second kind of correction to the weak coupling limits deviates from the property of exponential semigroup: $\left(1 + \sum_{j=1}^{\infty} \lambda^j M(j)(t)\right) e^{\sum_{j=1}^{\infty} \lambda^j L(j)} \left(1 + \sum_{j=1}^{\infty} \lambda^j N(j)(t)\right)$. The terms $M(j)(t)$ and $N(j)(t)$ rapidly reach their asymptotic values $M(j)(\infty)$ and $N(j)(\infty)$. Thus, they carry non-Markovian effects. In particular, the terms $M(j)(t)$ are responsible for a slippage of the initial state $\rho(0)$, and the terms $N(j)(t)$ give non-Markovian oscillations on a fast
time scale. Adding the first non-Markovian corrections, the error of the approximation is estimated, under suitable hypotheses, by [110, 112]

\[ \left\| \rho(t) - \left( 1 + \lambda^2 \mathcal{M}^{(2)}(t) \right) e^{i z(L^{(2)} + i z L^{(4)})} (1 + \lambda^2 \mathcal{M}^{(2)}(t)) \rho(0) \right\| \leq \lambda^4 \beta_4(\lambda^2 t) \sup_{s \in [0, t]} \left\| e^{i z(L^{(2)} + i z L^{(4)})} \rho(s) \right\|, \]

where \( \beta_4(\cdot) \) is a positive and bounded function on compacts, for any finite time \( t \in [0, \infty) \) and \( \lambda \in [0, \Lambda] \). This estimation shows that the non-Markovian corrections restore the earlier time scale \( 1/\lambda^2 \), but improve the performance of the approximation: \( O(\lambda^4) \) instead of \( O(\lambda^2) \).

In order to get a better approximation and to describe a longer time scale, we can consider either smaller values of \( \lambda \) or additional terms in the expansion. However, all the estimations hold for times in compact sets. The problem of whether the weak coupling limit or its refinements capture the right asymptotic time behaviour is still open. In the following we will tackle the opposite problem. The weak coupling limit mainly captures the behaviour on the times scaling as \( 1/\lambda^2 \). Therefore, some phenomena might not emerge, as if they already approached the asymptotic behaviour. The phenomenon we will look for is the entanglement generation between unequal qubits or harmonic oscillators induced by a common environment. We will develop a refinement of the weak coupling limit suitable to time scales shorter than \( 1/\lambda^2 \). The time scaling is fixed by a phenomenological parameter, which describes the amplitude of the time interval we want to resolve in a coarse graining approach. The standard weak coupling limit is restored for infinitely large intervals.
Chapter 2

Entanglement

Entanglement is one of the most intriguing features of quantum mechanics. It was first discussed by Einstein, Podolsky and Rosen in [23] and then by Schrödinger in [24]. In the last decades, entanglement has found applications in the foundation of quantum mechanics, in quantum information theory and quantum computing and communication. It is not clear whether entanglement is really necessary for the speed up of quantum processing compared to the classical processing. However, almost all efficient quantum computation protocols are helped by entanglement. The vast majority of works on quantum protocols deal with distinguishable qubits or distinguishable continuous variable systems [55, 62]. In the present thesis, we shall consider quantum metrology with identical particles as an application of entanglement.

In this chapter we shall review some concepts regarding entanglement. We shall start with the usual notion of entanglement, based on the tensor product structure of the Hilbert space and of the states. This definition is natural for distinguishable particles. In the last section, we shall present a generalized definition of entanglement, based on subalgebras of observables. This generalization is more suitable for identical particles, where each single particle is not addressable and the tensor product structure is either unphysical or virtual.

2.1 Definition and properties

We consider a quantum system made up of $n$ parties. A general state $|\psi\rangle$, belongs to the Hilbert space $\mathcal{H} = \bigotimes_{j=1}^{N} \mathcal{H}_j$. $\mathcal{H}_j$ are Hilbert spaces pertaining to each party. The tensor product structure of the Hilbert space reflects the structure of the states and plays a crucial role for the entanglement definition.
Definition 2.1.1 (separable and entangled pure states). A pure state $|\psi\rangle \in \bigotimes_{j=1}^{N} \mathcal{H}_j$ is separable if there are states $|\psi_j\rangle \in \mathcal{H}_j$, $j = 1, 2, \ldots, n$, such that $|\psi\rangle = \bigotimes_{j=1}^{N} |\psi_j\rangle$. Otherwise, the state is called entangled.

Entanglement is fully encoded in the eigenvalues of the reduced density matrices of the subsystems. Conversely, the reduced density matrices characterize uniquely the entanglement of pure states. The reduced density matrix of each subsystem describes a pure state if and only if the global pure state is separable. Otherwise, if at least one of the reduced density matrices is a statistical mixture, the total pure state is entangled. This is the Schrödinger’s characterization of entanglement: the subsystems of entangled pure states can not be described independently of each other. One of the mathematical properties of this physical feature is the following theorem, known as Schmidt decomposition [55].

Theorem 2.1.1 (Schmidt decomposition or biorthonormal decomposition). For any pure state $|\psi\rangle \in \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, there are two orthonormal basis, $\{|l_A\rangle\}$ and $\{|l_B\rangle\}$, respectively spanning the Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, such that

$$|\psi\rangle = \sum_{l} \sqrt{\lambda_l} |l_A\rangle \otimes |l_B\rangle,$$

(2.1)

where $\lambda_l$ are non-negative real numbers satisfying $\sum_{l} \lambda_l = 1$, known as Schmidt coefficients.

The states $\{|l_A\rangle\}$ and $\{|l_B\rangle\}$ are the eigenvectors of the reduced density matrices $\rho_A = \text{Tr}_B |\psi\rangle\langle \psi|$ and $\rho_B = \text{Tr}_A |\psi\rangle\langle \psi|$, whose eigenvalues are $\lambda_l$.

Such a decomposition can be generalized to systems with more than two parts, but in general the states involved are no longer an orthonormal basis of the local Hilbert spaces [55, 56].

Up to now, we have dealt with pure states. We now switch to mixed states. The following definition generalized the notion of entanglement to mixed states.

Definition 2.1.2 (separable and entangled mixed states). A mixed state $\rho \in \mathcal{B}(\mathcal{H})$, $\mathcal{H} = \bigotimes_{j=1}^{N} \mathcal{H}_j$, is separable if there are states $\rho_j \in \mathcal{B}(\mathcal{H}_j)$, $j = 1, 2, \ldots, N$ and a probability distribution $\{p_k\}$, such that

$$\rho = \sum_{k} p_k \bigotimes_{j=1}^{N} \rho_j^{(j)},$$

(2.2)

Otherwise the state is entangled.

In other words a mixed state is separable if it is a convex combination of separable pure states, otherwise it is entangled. This definition cover the definition 2.1.1, when dealing
with pure states. As a special case of separable mixed state we introduce the following definition.

**Definition 2.1.3** (simply separable mixed states). A mixed state \( \rho \in \mathcal{B}(\mathcal{H}), \mathcal{H} = \bigotimes_{j=1}^{N} \mathcal{H}_j \), is simply separable if there are states \( \rho_j \in \mathcal{B}(\mathcal{H}_j), j = 1, 2, \ldots, N \), such that

\[
\rho = \bigotimes_{j=1}^{N} \rho_j.
\]

For global mixed states, entanglement is not clearly encoded in the eigenvalues of the reduced density matrices. Indeed, the degree of mixedness of the global state as well contributes to the mixedness of the reduced density matrices. For instance the completely mixed state is separable, even if each of its reduced density matrices completely mixed.

### 2.1.1 Local operators

The so-called local operations recur quite frequently in the theory of entanglement. Since entanglement is a global feature of the state, it is expected that operations acting locally on each part of the systems can not increase the entanglement.

**Definition 2.1.4** (local operators). An operator \( O \in \mathcal{B}(\mathcal{H}), \mathcal{H} = \bigotimes_{j=1}^{N} \mathcal{H}_j \), is called local if it can be written as \( O = \bigotimes_{j=1}^{N} O_j, O_j \in \mathcal{B}(\mathcal{H}_j) \). If \( O_j \) are unitary operators, \( O \) is termed unitary local operator.

The following corollary is a direct consequence of the Schmidt decomposition.

**Corollary 2.1.1.** Any unitary local operator \( U \in \mathcal{B}(\mathcal{H}) \) preserves the eigenvalues of all the reduced density matrices.

Thus, any unitary local operator preserves the entanglement and the mixedness of every global states. A non-unitary local operator tipically increases the mixedness and decreases the entanglement of the global state.

### 2.1.2 Partial trasposition

A useful tool to detect bipartite entanglement is the so-called partial trasposition. This technique does not require to compute the reduced density matrix. We consider a bipartite Hilbert space \( \mathcal{H}_A \otimes \mathcal{H}_B \) and its basis \( |j_A\rangle \otimes |j_B\rangle \), being \( |j_{A,B}\rangle \) a basis of the Hilbert space \( \mathcal{H}_{A,B} \). We now define the partial trasposition, i.e. the trasposition only on the Hilbert space of one party.
**Definition 2.1.5** (Partial trasposition). The partial trasposition on the first subsystem of a bipartite state \( \rho \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \) is defined as

\[
\langle l_A | \otimes \langle l_B | \mathbb{T} \otimes \mathbb{I} [\rho] | j_A \rangle \otimes | j_B \rangle = \langle j_A | \otimes \langle l_B | \rho | l_A \rangle \otimes | j_B \rangle.
\] (2.4)

Analogously for the second subsystem

\[
\langle l_A | \otimes \langle l_B | \mathbb{I} \otimes \mathbb{T} [\rho] | j_A \rangle \otimes | j_B \rangle = \langle l_A | \otimes \langle j_B | \rho | j_A \rangle \otimes | l_B \rangle.
\] (2.5)

The following theorem gives a sufficient criterion for the entanglement.

**Theorem 2.1.2.** If a state is separable \( \rho = \sum_m p_m \rho_m^{(A)} \otimes \rho_m^{(B)} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \), than it remains positive under partial trasposition:

\[
\mathbb{T} \otimes \mathbb{I} [\rho] \geq 0, \quad \mathbb{I} \otimes \mathbb{T} [\rho] \geq 0.
\] (2.6)

The latter theorem holds for any dimension of the Hilbert spaces \( \mathcal{H}_{A,B} \) [65]. The same condition is also necessary for low dimensions \( \text{dim}(\mathcal{H}_A \otimes \mathcal{H}_B) \leq 6 \), that is \( \text{dim}(\mathcal{H}_A) = \text{dim}(\mathcal{H}_B) = 2 \), or \( \text{dim}(\mathcal{H}_{A,B}) = 6 \) [66].

**Theorem 2.1.3.** If a state \( \rho \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \), \( \text{dim}(\mathcal{H}_A \otimes \mathcal{H}_B) \leq 6 \), remains positive under partial trasposition:

\[
\mathbb{T} \otimes \mathbb{I} [\rho] \geq 0, \quad \mathbb{I} \otimes \mathbb{T} [\rho] \geq 0,
\] (2.7)

that the state is separable \( \rho = \sum_k p_k \rho_k^{(A)} \otimes \rho_k^{(B)} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \).

The transposition is a positive but not completely positive map. Indeed, the transposition of the whole Hilbert space preserves positivity. However, the transposition on a subsystem, i.e. partial transposition, does not preserve the positivity of some entangled states. Thus, transposition is not a completely positive map. The transposition is a prototypical example of positive but not completely positive map, that is useful to detect entanglement.

### 2.2 Environment induced entanglement generation

An interesting application of partial transposition is the criterion for the entanglement generation induced by Markovian environment at short times [138, 155]. We shall focus on the entanglement generation capability at small times of the dynamics generated by the equation (1.15). We shall consider the dissipative dynamics of two qubits, i.e. two two-level systems. Considering a local Hamiltonian \( H_0 = H_0^{(1)} \otimes 1_2^{(2)} + 1_2^{(1)} \otimes H_0^{(2)} \), an
interaction Hamiltonian $H_{\text{int}} = \sum_j H_j^{(1)} \otimes H_j^{(2)}$ and the Pauli matrices acting on each qubit $\{\sigma_j^{(\alpha)}\}_{\alpha=1,2,3}$, the generator of a Markovian master equation (1.15) can be written as

$$L[\rho] = -i[H_0 + H_{\text{int}}, \rho(t)] + \frac{1}{2} \sum_{\alpha, \beta=1}^3 \sum_{i, j=1}^C C_{ij}^{(\alpha \beta)} \left[ \sigma_j^{(\beta)} \rho(t) \sigma_i^{(\alpha)} - \frac{1}{2} \{\sigma_j^{(\beta)} \sigma_i^{(\alpha)}, \rho(t)\} \right]. \quad (2.8)$$

We are interested in the generation of entanglement induced by the interaction of two independent qubits with a common environment. We neglect direct interactions between the qubits, such that all the emerging correlations come from the interaction mediated by the environment. In other words, the microscopic interactions which underlie the master equation (2.8) do not include the two body interaction between the qubits and the three body interaction among the qubits and the environment. Therefore, the interaction $H_{\text{int}}$ is mediated by the environment and the Lindblad operators in (2.8) are just Pauli matrices pertaining single qubits.

Then, without loss of generality, one can limit the considerations to pure, separable initial states, and therefore take:

$$\rho(0) = |\varphi\rangle\langle \varphi| \otimes |\psi\rangle\langle \psi|, \quad (2.9)$$

with $|\varphi\rangle, |\psi\rangle$ given single qubit states; indeed, if the dynamics is unable to create entanglement out of pure states, it will certainly not correlate their mixtures. Since we are dealing with a couple of two-level systems, one can use partial transposition as a criterion for entanglement creation. More precisely, the dynamics is able to create entanglement between the two atoms if and only if the operation of partial transposition spoils the positivity of the state $\rho(t)$.

The presence of negative eigenvalues in the partially transposed reduced density matrix $\rho(t)$ can be ascertained by looking at the sign of the average

$$Q(t) = \langle \chi | \rho(t) | \chi \rangle, \quad (2.10)$$

with $|\chi\rangle$ a four-dimensional vector. Indeed, choose $|\chi\rangle$ to be orthogonal to $|\varphi\rangle \otimes |\psi\rangle$, so that the above average initially vanishes, $Q(0) = 0$. Then, the two atoms, initially prepared in a state $\rho(0)$ as in (2.9), will surely become entangled if $|\chi\rangle$ can be further chosen so that $\partial_t Q(0) < 0$. From this condition, a simple test for entanglement creation involving the elements of the Kossakowski matrix $C_{i,j}^{\alpha \beta}$ and of the interaction Hamiltonian $H_{\text{int}}$ can then be extracted [138, 155]. We define the matrices $[C_{i,j}^{\alpha \beta}]_{i,j}$ and three-dimensional vectors $u, v \in \mathbb{R}^3$ containing the information about the starting factorized state (2.9) with components
\[ u_i = \langle \varphi | \sigma_i | \varphi_\perp \rangle, \quad v_i = \langle \psi_\perp | \sigma_i | \psi \rangle, \quad (2.11) \]

where \( | \varphi_\perp \rangle \) and \( | \psi_\perp \rangle \) are the orthonormal complements to the initial qubit states \( | \varphi \rangle \) and \( | \psi \rangle \), respectively. A sufficient condition for environment induced entanglement generation explicitly reads

\[ \left( u, C^{(11)} u \right) \left( v, (C^{(22)})^T v \right) < \left| \left( u, \text{Re} \left( C^{(12)} + iH_{\text{int}} \right) v \right) \right|^2, \quad (2.12) \]

where \( T \) means matrix transposition. Therefore, the Markovian dynamics generated by (2.8) will be able to initially entangle the two qubits if there exists an initial state of the form (2.9) for which the inequality (2.12) is satisfied. On the other hand, if the opposite inequality holds for every vectors \( u, v \)

\[ \left( u, C^{(11)} u \right) \left( v, (C^{(22)})^T v \right) > \left| \left( u, \text{Re} \left( C^{(12)} + iH_{\text{int}} \right) v \right) \right|^2, \quad (2.13) \]

i.e. if \( \partial_t Q(0) > 0 \) for every initial states, then the dynamics can not entangle the two qubits. Finally, if the relation (2.12) holds with the equality sign, we should look at higher derivatives of \( Q(t) \), in order to possibly detect entanglement generation.

### 2.3 Algebraic entanglement

The notion of entanglement can be defined and extended in an algebraic way. This algebraic definition is useful in several cases. In the following we first discuss examples where such a generalization is needed to capture some peculiar features in a more compact formalism. The first example shows that even for distinguishable particles entanglement is relative to the experimentally addressable degrees of freedom. This is due to the non-uniqueness of the tensor product structure and to the possibility to define virtual subsystems, that are non-local with respect to the original ones. The second example shows that one cannot directly extend the notion of separability from distinguishable to indistinguishable particles. This is essentially due to the fact that the tensor product (local) structure, that is naturally associated with distinguishable particles, loses its meaning for indistinguishable particles. Then, we shall argue that one can consistently define separability not in terms of tensor products, but in terms of commuting subalgebras of operators. In chapter 5, in the light of this definition, we shall examine some results concerning the metrological use of the Fisher information and of spin squeezing that, though obtained in the case of \( N \) distinguishable spin, have been used, by naive and direct extrapolation, to the case of \( N \) indistinguishable spins.
Notice that the definition of separability 2.1.2 is strictly dictated by the natural tensor product structure for the $N$-body system $\mathcal{H} = \bigotimes_{j=1}^{N} \mathcal{H}_j$. This tensor product structure reflects the multi-partition of the system into its $N$ parts and the identification of local operations.

### 2.3.1 Relative entanglement of distinguishable particles

We shall point out some subtleties about entanglement that are already known in literature [30], and are naturally captured by the algebraic definition we will state later. We can describe the states in terms of some quantum numbers, that are eigenvalues of a complete set of commuting observables [30, 31, 60, 61]. For composite systems, different choices of quantum numbers induce different tensor product structures. For instance, the ground state of the hydrogen atom can be factorized in the product of a function of the center of mass and a function of the relative degree of freedom [28]. The same wave function can not be written as a product of two functions, pertaining respectively to the electron and the proton variables. Another concrete example concerns the representation of Bell states as separable states [31, 60].

The Hilbert space of two qubits is $\mathbb{C}^4$. It can be represented as a tensor product of local Hilbert spaces: $\mathbb{C}^4 = \mathcal{H}_1 \otimes \mathcal{H}_2$, where $\mathcal{H}_j = \text{span}\{|0\rangle_j, |1\rangle_j\} = \mathbb{C}^2$ and $\{|0\rangle_j, |1\rangle_j\}$ are the eigenstates of the Pauli matrix $\sigma_j^{(3)}$ with eigenvalues $+1$ and $-1$ respectively. The Bell states

$$|\psi^\pm\rangle = \frac{|1\rangle_1 \otimes |0\rangle_2 \pm |0\rangle_1 \otimes |1\rangle_2}{\sqrt{2}}, \quad |\phi^\pm\rangle = \frac{|0\rangle_1 \otimes |0\rangle_2 \pm |1\rangle_1 \otimes |1\rangle_2}{\sqrt{2}}, \quad (2.14)$$

are entangled with respect to the chosen tensor product structure. We can describe the Bell state with respect to the quantum numbers of the observables $\sigma_1^{(1)} \otimes \sigma_1^{(2)}$, $\sigma_1^{(1)} \otimes \sigma_2^{(2)}$, $\sigma_3^{(1)} \otimes \sigma_3^{(2)}$ and $\sigma_2^{(1)} \otimes \sigma_2^{(2)}$. The first two operators act on the relative sign of the Bell states, while the other operators act on the number of excitations (the number of 1 (modulo 2)).

This reminds to what is done when one deals with the addition of angular momenta and writes the states in terms of the eigenstates of two different complete sets of commuting operators and thus two different sets of quantum numbers. In our case, instead of choosing the complete set of commuting operators $\{\mathbf{1}^{(1)} \otimes \sigma_3^{(2)}, \sigma_3^{(1)} \otimes \mathbf{1}^{(2)}\}$ we look at the common eigenstates of the complete set of commuting operators $\{\sigma_1^{(1)} \otimes \sigma_1^{(2)}, \sigma_3^{(1)} \otimes \sigma_3^{(2)}\}$. Since the eigenvalues of these operators are $\pm 1$, we define the labels $\eta = +, -$ and $\lambda = +, -$:

$$\sigma_1^{(1)} \otimes \sigma_1^{(2)}|\eta, \lambda\rangle = \lambda|\eta, \lambda\rangle, \quad \sigma_3^{(1)} \otimes \sigma_3^{(2)}|\eta, \lambda\rangle = \eta|\eta, \lambda\rangle. \quad (2.15)$$
We relabel \( \eta = + \) and \( \eta = - \) respectively as \( \chi = \phi \) and \( \chi = \psi \) and the previous eigenvector equations become

\[
\begin{align*}
\sigma_1^{(1)} \otimes \sigma_1^{(2)} |\psi, \pm\rangle &= \pm |\psi, \pm\rangle, \\
\sigma_1^{(1)} \otimes \sigma_1^{(2)} |\phi, \pm\rangle &= \pm |\phi, \pm\rangle, \\
\sigma_3^{(1)} \otimes \sigma_3^{(2)} |\psi, \pm\rangle &= -|\psi, \pm\rangle, \\
\sigma_3^{(1)} \otimes \sigma_3^{(2)} |\phi, \pm\rangle &= +|\phi, \pm\rangle.
\end{align*}
\]

The eigenstates are exactly the Bell states (2.14): \( |\chi, \lambda\rangle = |\chi^{-}\rangle \). Similarly to the case of addition of angular momenta, the common eigenstates of a complete set of commuting operators are a linear combination of the eigenstates of a different set of commuting operators.

Therefore, relative to these quantum numbers we can formally write the Bell states as factorized states \( |\chi\rangle \tilde{\otimes} |\lambda\rangle \), where \( \chi = \psi, \phi \) and \( \lambda = +, - \). The symbol \( \tilde{\otimes} \) is the tensor product in a different representation \( \mathbb{C}^4 = \mathcal{H}_\chi \tilde{\otimes} \mathcal{H}_\lambda \), where \( \mathcal{H}_\chi = \text{span}(|\psi\rangle, |\phi\rangle) = \mathbb{C}^2 \) and \( \mathcal{H}_\lambda = \text{span}(|+\rangle, |\rangle) = \mathbb{C}^2 \) are the local Hilbert spaces with respect to the new representation. The relative entanglement is a consequence of looking at observables which are non-local with respect to the original tensor product structure.

It is interesting to notice that the operator \( \sigma_1^{(1)} \otimes \sigma_1^{(2)} \) acts as an identity operator on the quantum number \( \chi \) and as an operator \( \sigma_3 \) on the degree of freedom \( \lambda \), and \( \sigma_3^{(1)} \otimes \sigma_3^{(2)} \) acts as an operator \( \sigma_3 \) on \( \chi \) and as an identity operator on \( \lambda \). Furthermore, \( \sigma_1^{(1)} \otimes \sigma_2^{(2)} \) acts as an identity operator on \( \chi \) and as an operator \( \sigma_2 \) on \( \lambda \), \( \sigma_2^{(1)} \otimes \sigma_3^{(2)} \) acts as an operator \( \sigma_2 \) on \( \chi \) and as an identity operator on \( \lambda \), \( \mathbf{1}^{(1)} \otimes \sigma_3^{(2)} \) acts as an identity operator on \( \chi \) and as an operator \( \sigma_1 \) on \( \lambda \), \( \sigma_1^{(1)} \otimes \mathbf{1}^{(2)} \) acts as an operator \( \sigma_1 \) on \( \chi \) and as an identity operator on \( \lambda \):

\[
\begin{align*}
\sigma_1^{(1)} \otimes \sigma_2^{(2)} |\psi, \pm\rangle &= \pm i |\psi, \mp\rangle, \\
\sigma_1^{(1)} \otimes \sigma_2^{(2)} |\phi, \pm\rangle &= \pm i |\phi, \mp\rangle, \\
\sigma_2^{(1)} \otimes \sigma_3^{(2)} |\psi, \pm\rangle &= -i |\psi, \pm\rangle, \\
\sigma_2^{(1)} \otimes \sigma_3^{(2)} |\phi, \pm\rangle &= +i |\phi, \pm\rangle, \\
\mathbf{1}^{(1)} \otimes \sigma_3^{(2)} |\psi, \pm\rangle &= |\psi, \pm\rangle, \\
\mathbf{1}^{(1)} \otimes \sigma_3^{(2)} |\phi, \pm\rangle &= |\phi, \pm\rangle, \\
\sigma_1^{(1)} \otimes \mathbf{1}^{(2)} |\psi, \pm\rangle &= |\psi, \mp\rangle, \\
\sigma_1^{(1)} \otimes \mathbf{1}^{(2)} |\phi, \pm\rangle &= |\phi, \mp\rangle.
\end{align*}
\]

Therefore, we can identify

\[
\begin{align*}
\mathbf{1}^{(1)} \otimes \sigma_3^{(2)} &= \mathbf{1}^{(1)} \tilde{\otimes} \mathbf{1}^{(2)}, & \sigma_1^{(1)} \otimes \sigma_2^{(2)} &= \mathbf{1}^{(1)} \tilde{\otimes} \sigma_3^{(2)}, & \sigma_1^{(1)} \otimes \sigma_1^{(2)} &= \mathbf{1}^{(1)} \tilde{\otimes} \mathbf{1}^{(2)}, \\
\sigma_1^{(1)} \otimes \mathbf{1}^{(2)} &= \mathbf{1}^{(1)} \tilde{\otimes} \mathbf{1}^{(1)}, & \sigma_3^{(1)} \otimes \sigma_3^{(2)} &= \sigma_2^{(1)} \tilde{\otimes} \mathbf{1}^{(2)}, & \sigma_3^{(1)} \otimes \sigma_2^{(2)} &= \sigma_3^{(1)} \tilde{\otimes} \mathbf{1}^{(2)}. \tag{2.18}
\end{align*}
\]

All the Hilbert spaces \( \mathcal{H}_{\chi,\lambda} \) are isomorphic to \( \mathbb{C}^2 \). Thus, choosing this common representation we get the isomorphism between the two different representations of the Bell states:
\[ |\psi^\pm\rangle = \frac{1}{\sqrt{2}} \left( |0\rangle \pm |1\rangle \right) \]
\[ |\phi^\pm\rangle = \frac{1}{\sqrt{2}} \left( |0\rangle \pm |1\rangle \right) \]
\[ |\psi\rangle \otimes |\phi\rangle \equiv |\psi\rangle |\phi\rangle \]
\[ \mathcal{H}_1 \otimes \mathcal{H}_2 \ni |\chi\rangle = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix} |\chi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2. \]  

### 2.3.2 What happens with identical particles

In general, the density matrix (2.2) is not an allowed quantum state for indistinguishable particles. For sake of simplicity, we shall consider two indistinguishable particles: if one could assign a density matrix \( \rho^{(1)} \) to the first particle and \( \rho^{(2)} \) to the second one, then the two would be effectively distinguishable by means of their states. Even states of the form
\[ \sum_k p_k \rho_k \otimes \rho_k \cdots \otimes \rho_k \]  
are not acceptable as states of indistinguishable particles, despite all particles being described by the same density matrix. The reason is that, according to the standard rules of quantum mechanics, a pure state \(|\psi_N\rangle\) of \(N\) identical particles must be symmetric or anti-symmetric combinations of tensor products of \(N\) single-particle vector states, while mixed states, i.e. density matrices, must be linear convex combinations of projectors \(|\psi_N\rangle\langle\psi_N|\) onto such symmetrized or anti-symmetrized states. The latter constraint is due to the fact that mixed states are mixtures (linear convex combinations) of pure states (projections). This excludes that the distinguishability of particles that is intrinsic in a state as (2.2) could be cured by simply symmetrizing the superscript \((j)\). Indeed, this would in the end always be a mixture of states where particles can be distinguished. In the formalism of
second quantization, mixtures of \( N \) indistinguishable particles must consist of projections onto vector states of the \( N \)-particle sector of the appropriate Fock space.

Therefore, the usual notion of separability is no longer applicable in the case of a system of identical particles. This problem has already been addressed and discussed in the literature, in several physical contexts (e.g. see [59, 60, 64, 71, 72, 73, 74, 31, 79, 80, 82] and reference therein). The way out resides in a dual point of view, where emphasis is given to the algebra of observables, instead of the set of states; the connection between these two points of view is given by the expectation value map that allows to express the average of an observable \( O \) as its trace with the corresponding density matrix, 

\[
\langle O \rangle = \text{Tr}(O \rho).
\]

As a concrete instance, consider the case of two qubits. The Hilbert space of two distinguishable qubits is four dimensional, \( \mathbb{C}^2 \otimes \mathbb{C}^2 \). Instead, the Hilbert space for two indistinguishable qubits is a symmetric 3-dimensional subspace in the case of Bosons, or an anti-symmetric 1-dimensional subspace for Fermions. Given an orthonormal basis \( \{|\downarrow_1\downarrow_2\rangle, |\downarrow_1\uparrow_2\rangle, |\uparrow_1\downarrow_2\rangle, |\uparrow_1\uparrow_2\rangle\} \) in \( \mathbb{C}^4 \), the symmetric sector is spanned by

\[
|\downarrow_1\downarrow_2\rangle, |\uparrow_1\uparrow_2\rangle, \frac{|\downarrow_1\uparrow_2\rangle + |\uparrow_1\downarrow_2\rangle}{\sqrt{2}},
\]

while the anti-symmetric one by \( \frac{|\downarrow_1\uparrow_2\rangle - |\uparrow_1\downarrow_2\rangle}{\sqrt{2}} \). It is easy to show that in general the state (2.2) for two indistinguishable qubits is not an allowed state. In fact, the density matrix (2.2) is

\[
\sum_k p_k \rho_k^{(1)} \otimes \rho_k^{(2)},
\]

If (2.23) has rank greater than three (one), it cannot be interpreted as the state of two indistinguishable qubits. A simple example is given by

\[
\rho^{(1)} \otimes \rho^{(2)}, \quad \text{where} \quad \rho^{(1)} = \begin{pmatrix} r_1 & 0 \\ 0 & 1 - r_1 \end{pmatrix}, \quad \rho^{(2)} = \begin{pmatrix} r_2 & 0 \\ 0 & 1 - r_2 \end{pmatrix}.
\]

The rank of \( \rho^{(1)} \otimes \rho^{(2)} \) is 4, unless one of the two states is a projection (\( r_1 = 0, 1 \) or \( r_2 = 0, 1 \)). If this is not the case, (2.24) can be written as the convex combination of 4 independent one dimensional projectors

\[
\rho^{(1)} \otimes \rho^{(2)} = \begin{pmatrix} r_1 r_2 & 0 & 0 & 0 \\ 0 & r_1(1 - r_2) & 0 & 0 \\ 0 & 0 & (1 - r_1)r_2 & 0 \\ 0 & 0 & 0 & (1 - r_1)(1 - r_2) \end{pmatrix}.
\]
while the spectral decomposition of a state of two indistinguishable qubits must use only three (one) projectors onto symmetrized (anti-symmetrized) orthogonal vectors.

The symmetrization or anti-symmetrization of states is automatically guaranteed by the formalism of second quantization. Before describing the more general algebraic notion of separable states which can be applied to indistinguishable particles, we set the framework for \( N \) Bosons in second quantization and shortly comment on certain aspects of locality. Let \( |0\rangle \) be the vacuum state and \( a_1^\dagger, a_2^\dagger \) the creation operators of a particle in the states \(| \downarrow \rangle \) and \(| \uparrow \rangle \), that is \( a_1^\dagger |0\rangle = | \downarrow \rangle, a_2^\dagger |0\rangle = | \uparrow \rangle \). Together with the annihilation operators \( a_1|0\rangle = a_2|0\rangle = 0 \), they obey the canonical commutation relations

\[
[a_j, a_l^\dagger] = \delta_{j,l},
\]

(2.26)

In other words, we are considering the second quantization of a single-particle with Hilbert space \( \mathbb{C}^2 \) which effectively describes \( N \) ultra-cold atoms confined by a double-well potential in the Bose-Hubbard approximation \([43, 46, 47, 48, 49, 50]\). Then, \(| \downarrow \rangle \) corresponds to one atom being being located within the left well and \(| \uparrow \rangle \) within the right one. The Fock space of this two-mode system is in general infinite dimensional and generated by orthonormal vectors of the form

\[
|n,m\rangle = \frac{(a_1^\dagger)^n(a_2^\dagger)^m|0\rangle}{\sqrt{n!m!}}, \quad n, m \geq 0.
\]

(2.27)

However, in the case of \( N \) Bosons in a double-well potential, if the total number is conserved by the dynamics, then the corresponding super-selection rule, constrains the system to an \( N + 1 \) dimensional symmetric Hilbert space generated by orthogonal vectors of the form

\[
|k, N-k\rangle = \frac{(a_1^\dagger)^k(a_2^\dagger)^{N-k}|0\rangle}{\sqrt{k!(N-k)!}}, \quad 0 \leq k \leq N.
\]

(2.28)

Notice that, by considering all polynomials \( P_1 \) in \( a_1, a_1^\dagger \), respectively \( P_2 \) in \( a_2, a_2^\dagger \) and, technically speaking, their norm closures, one obtains two commuting subalgebras \( \mathcal{A}_1 \) and \( \mathcal{A}_2 \), \([\mathcal{A}_1, \mathcal{A}_2] = 0\), of the algebra of all bounded Bosonic operators on the Fock space spanned by (2.27). This commutativity provides a notion of locality for indistinguishable particles that generalizes the tensor product structure for distinguishable particles. We shall refer to the pair \( \{\mathcal{A}_1, \mathcal{A}_2\} \) as an algebraic bipartition: a natural step is to speak of locality only relative to a chosen algebraic bipartition.

### 2.3.3 Algebraic definition

We are ready to define entanglement in an algebraic framework. This algebraic definition is justified by the experimental addressability of only some observables, and is a
natural approach in quantum statistical mechanics. Thus, entanglement should be related to the degrees of freedom and the observables we can measure. Let us consider a system of particles whose pure states span the Hilbert space \( \mathcal{H} \) and denote by \( \mathcal{B}(\mathcal{H}) \) the algebra of all bounded operators on it; the observables of the system clearly belong to this algebra. We shall introduce the notion of (bipartite) separability by considering couple of commuting subalgebras of \( \mathcal{B}(\mathcal{H}) \) instead of focusing on partitions of the system states. We then introduce the following definitions:

**Definition 2.3.1.** (Algebraic entanglement).

- An algebraic bipartition of the algebra \( \mathcal{B}(\mathcal{H}) \) is any pair \((\mathcal{A}_1, \mathcal{A}_2)\) of commuting subalgebras of \( \mathcal{B}(\mathcal{H}) \).

- An element (operator) of \( \mathcal{B}(\mathcal{H}) \) is said to be local with respect to the bipartition \((\mathcal{A}_1, \mathcal{A}_2)\) if it is the product \( A_1A_2 \) of an element \( A_1 \) of \( \mathcal{A}_1 \) and another \( A_2 \) of \( \mathcal{A}_2 \).

- A state \( \omega \) on the algebra \( \mathcal{B}(\mathcal{H}) \) will be called separable with respect to the bipartition \((\mathcal{A}_1, \mathcal{A}_2)\) if the expectation \( \omega(A_1A_2) \) of any local operator \( A_1A_2 \) can be decomposed into a linear convex combination of products of expectations:

\[
\omega(A_1A_2) = \sum_k \lambda_k \omega^{(1)}_k(A_1) \omega^{(2)}_k(A_2), \quad \lambda_k \geq 0, \quad \sum_k \lambda_k = 1, \quad (2.29)
\]

where \( \omega^{(1)}_k \) and \( \omega^{(2)}_k \) are states on \( \mathcal{B}(\mathcal{H}) \); otherwise the state \( \omega \) is said to be entangled with respect to the bipartition \((\mathcal{A}_1, \mathcal{A}_2)\).

Notice that the two subalgebras \( \mathcal{A}_1 \) and \( \mathcal{A}_2 \) need not reproduce the whole algebra \( \mathcal{B}(\mathcal{H}) \), i.e. in general \( \mathcal{A}_1 \cup \mathcal{A}_2 \subseteq \mathcal{B}(\mathcal{H}) \). In this respect, the term bipartition is not strictly appropriate and has been adopted for sake of simplicity. However, in the case of the system discussed below, the considered mode partitions actually generate the whole algebra \( \mathcal{B}(\mathcal{H}) \). On the other hand, we can straightforwardly generalize this definition to an algebraic multipartition, identifying many commuting subalgebras \( \{\mathcal{A}_j\}, [\mathcal{A}_j, \mathcal{A}_l] \subseteq \delta_{ij}\mathcal{A}_j \).

As we shall see in the following sections, this generalized definition of separability results meaningful both for systems composed of distinguishable particles and for those made of identical ones.
### 2.3.4 Applications

#### Distinguishable particles

We now show that the algebraic notion of entanglement recovers the usual definition, for distinguishable particles. We consider the Hilbert space $\mathcal{H} = \bigotimes_{j=1}^N \mathcal{H}_j$ and the algebraic multipartition $\{\mathcal{A}_j\}_{j=1}^N$, where $\mathcal{A}_j = \{1^{(1)} \otimes \cdots \otimes 1^{(j-1)} \otimes O^{(j)} \otimes 1^{(j+1)} \otimes \cdots \otimes 1^{(N)}\}$. It is easy to apply the definition 2.3.1, getting the usual notion of separable states 2.1.2 and local operators 2.1.4.

We move back to the possibility of writing Bell states as separable states, in the light of the algebraic definition of entanglement. Consider the Hilbert space $\mathcal{H}_4 = \mathcal{H}_2 \otimes \mathcal{H}_2$ and the subalgebras $\mathcal{A}_1 = \{O^{(1)} \otimes 1^{(2)}\}$, $\mathcal{A}_2 = \{1^{(1)} \otimes O^{(2)}\}$, $\mathcal{B}_1 = \{1^{(1)} \otimes 1^{(2)}\}$, $\mathcal{B}_2 = \{1^{(1)} \otimes 1^{(2)}\}$, $\mathcal{G}_1 = \{1^{(1)} \otimes 1^{(2)}\}$, $\mathcal{G}_2 = \{1^{(1)} \otimes 1^{(2)}\}$.

According to the definition 2.3.1, the Bell states (2.14) are entangled with respect to the algebraic bipartition $(\mathcal{A}_1, \mathcal{A}_2)$ while they are separable with respect to the algebraic bipartition $(\mathcal{B}_1, \mathcal{B}_2)$, as explicitly shown in 2.3.1. The change in the entanglement properties comes from the non-local transformation connecting the two algebraic bipartitions.

#### $N$ two-mode Bosons confined in a double well potential

We apply the previous definition to the case of identical particles, focussing on $N$ two-mode Bosons. This system is quite simple and is able to model ultracold Bosonic atoms trapped in a double well potential. In the following we shall study applications in quantum metrology, and the role of entanglement there.

The dynamics of cold atoms confined in an optical trap can be very well approximated by a Bose-Hubbard type Hamiltonian; in the case of a double-well potential, it reads:

$$H_{BH} = \epsilon_1 a_1^\dagger a_1 + \epsilon_2 a_2^\dagger a_2 + U_1(a_1^\dagger)^2 a_1^2 + U_2(a_2^\dagger)^2 a_2^2 - T(a_1^\dagger a_2 + a_1 a_2^\dagger), \quad (2.30)$$

where $a_{1,2}, a_{1,2}^\dagger$ annihilate and create atom states in the first, second well, respectively, and satisfy the Bose commutation relations $[a_i, a_j^\dagger] = \delta_{ij}, i, j = 1, 2$. Of the contributions to $H_{BH}$, the last one corresponds to a hopping term depending on the tunneling amplitude $T$, the first two are due to the trapping potential and are proportional to the depth $\epsilon_{1,2}$ of the wells. Finally, the remaining terms, quadratic in the number operators $a_i^\dagger a_i$, take into account repulsive Coulomb interactions inside each well.

We are using here a formalism of second-quantization, where the creation operator $\hat{\psi}^\dagger(x)$ of an atom at position $x$ can be decomposed in general as

$$\hat{\psi}^\dagger(x) = \sum_{i=1}^\infty \phi_i(x) a_i^\dagger, \quad (2.31)$$
and \( a_i^\dagger \) creates an atom in the state \( |\phi_i\rangle = a_i^\dagger |0\rangle \) with wavefunction \( \phi_i(x) = \langle x|\phi_i\rangle \); the set \( \{ |\phi_i\rangle \}_{i=1}^\infty \) is therefore a complete set of orthonormal single-particle atom states. The Bose-Hubbard Hamiltonian (2.30) results from a tight binding approximation, where only the first two of the basis vectors are relevant; in this case \( \phi_{1,2}(x) \) are orthogonal functions, \( \phi_1 \) localized within the first well, \( \phi_2 \) within the second one.

The total number \( N \) of atoms is conserved by (2.30). Therefore, the Hilbert space of the system is \( N + 1 \)-dimensional and can be spanned by Fock states of the form (2.28) describing the situation in which the first well is filled with \( k \) atoms, while the other one contains \( N - k \) particles. They are obtained by the action of the creation operators on the vacuum. These states turn out to be eigenstates of the Bose-Hubbard Hamiltonian when the tunneling term can be neglected, i.e. in the Mott insulator phase \( (U_{1,2}/T \gg 1) \).

Notice that in this formalism, symmetrization of the elements of the Hilbert space, as required by the identity of the particles filling the two wells, is automatically guaranteed by the commutativity of the two creation operators. Furthermore, all polynomials in \( a_1, a_1^\dagger \) and similarly all polynomials in \( a_2, a_2^\dagger \) (together with their respective norm closures), form two algebras, \( \mathcal{A}_1, \mathcal{A}_2 \), respectively \( \mathcal{A}_2 \), that result commuting: \( [\mathcal{A}_1, \mathcal{A}_2] = 0 \); they are subalgebras of the algebra \( \mathcal{A} \) of all operators on the Fock space spanned by the states (2.28). Strictly speaking, polynomials in Bosonic creation and annihilation operators are not bounded, and the so-called Weyl algebras of the corresponding exponentials should be used; however, the following discussion is not affected by working with algebras of unbounded operators. According to the definition introduced in the previous section, they define a bipartition of \( \mathcal{A} \) and therefore can be used to provide the notion of separability for the states describing the identical atoms in the trap, generalizing the one usually adopted for distinguishable particles.

With respect to this natural mode bipartition, \( (\mathcal{A}_1, \mathcal{A}_2) \), the Fock states (2.28) turn out to be separable states. Indeed, for any polynomial operator \( A_1(a_1, a_1^\dagger) \in \mathcal{A}_1 \) and \( A_2(a_2, a_2^\dagger) \in \mathcal{A}_2 \), the expectation value of the product \( A_1 A_2 \) on such states can always be written as the product of the separate averages of \( A_1 \) and of \( A_2 \); explicitly, one has:

\[
\langle k, N-k | A_1 A_2 | k, N-k \rangle = \frac{1}{k!(N-k)!} \langle 0 | a_1^{\dagger k} A_1 (a_1^\dagger)^k |0 \rangle \langle 0 | a_2^{N-k} A_2 (a_2^\dagger)^{N-k} |0 \rangle = \langle k | A_1 | k \rangle \langle N-k | A_2 | N-k \rangle ,
\]

(2.32)

where \( |k\rangle \equiv (a_1^\dagger)^k / \sqrt{k!} |0\rangle \) and \( |N-k\rangle \equiv (a_2^\dagger)^{N-k} / \sqrt{(N-k)!} |0\rangle \) are single-mode Fock states.

As a consequence, separable with respect to the bipartition \( (\mathcal{A}_1, \mathcal{A}_2) \) are also those mixed states that are diagonal with respect to the Fock basis (2.28), i.e. density matrices of the form:

\[
\rho = \sum_{k=0}^N p_k |k, N-k\rangle \langle k, N-k| , \quad p_k \geq 0 , \quad \sum_{k=0}^N p_k = 1 .
\]

(2.33)
Actually, all states separable with respect to the bipartition \((\mathcal{A}_1, \mathcal{A}_2)\) must be in diagonal form with respect to the Fock basis. An abstract proof of this fact can be easily given. In fact, one first observes that the algebra generated by the polynomials in the operators \(a_1, a_1^\dagger\) and \(a_2, a_2^\dagger\) coincides with the whole algebra of operators \(\mathcal{A}\). Then, being pure projections, the states \(|k, N-k\rangle\langle k, N-k|\) are the only extremal ones in the convex set of states satisfying the separability condition (2.29); thus, all others are necessarily a convex combination of them.

Nevertheless, a more direct proof can also be explicitly worked out. A generic density matrix representing a state for a two-mode system of \(N\) identical Bosons is of the form:

\[
\rho = \sum_{k,l=0}^{N} \rho_{kl} |k, N-k\rangle\langle l, N-l|, \quad \rho_{kk} \geq 0, \quad \sum_{k=0}^{N} \rho_{kk} = 1. \tag{2.34}
\]

Assume now the state \(\rho\) to be separable with respect to the bipartition \((\mathcal{A}_1, \mathcal{A}_2)\); this means that for any local operator \(A_1A_2\), with \(A_1 \in \mathcal{A}_1\) and \(A_2 \in \mathcal{A}_2\), one must have:

\[
\text{Tr}[\rho A_1A_2] = \sum_m \lambda_m \text{Tr}[\rho^{(1)}_m A_1] \text{Tr}[\rho^{(2)}_m A_2], \tag{2.35}
\]

where \(\rho^{(i)}_m\), \(i = 1, 2\), are density matrices of the generic form (2.34). Choose now \(A_1 = (a_1^\dagger)^m a_1^n\), with \(m < n\) and \(A_2 = (a_2^\dagger)^s a_2^r\), with \(s < r\) and \(m + r = n + s\); then, each factor in the sum above identically vanish. Indeed, one finds:

\[
\text{Tr}[\rho^{(1)}_m A_1] = \sum_{k,l=0}^{N} \rho^{(1)}_{m,kl} \langle k, N-k|A_1|l, N-l \rangle = \sum_{k=0}^{N} \rho^{(1)}_{m,kk} \langle k|A_1|k \rangle \equiv 0, \tag{2.36}
\]

and similarly, \(\text{Tr}[\rho^{(2)}_m A_2] \equiv 0\). However, using (2.34), one also have:

\[
\text{Tr}[\rho A_1A_2] = \sum_{k,l=0}^{N} \rho_{kl} \langle k|A_1|l \rangle \langle N-k|A_2|N-l \rangle = \sum_k \rho_{k,k-n+m} \alpha_{m,n}(k) \beta_{r,s}(k), \tag{2.37}
\]

where the coefficients \(\alpha\) and \(\beta\) are explicitly given by:

\[
\alpha_{m,n}(k) = \left[ (k-1) \cdots (k-n+1) \cdot (k-n+1)(k-n+2) \cdots (k-n+m) \right]^{1/2},
\]

\[
\beta_{r,s}(k) = \left[ (N-k)(N-k-1) \cdots (N-k-s+1) \times (N-k-s+1)(N-k-s+2) \cdots (N-k-s+r) \right]^{1/2}.
\]
Since $\text{Tr}[\rho A A]$ vanishes by hypothesis, by choosing $n = N - s$, one finally gets the condition:

$$
\rho_{nm} \left[ m! n! (N-m)! (N-n)! \right]^{1/2} = 0, \quad m < n;
$$

(2.38)
a similar condition holds for the case $m > n$. As a consequence, $\rho_{mn} = 0$ for all $m \neq n$, and thus the original density matrix in (2.34) results diagonal in the Fock representation. Furthermore, one easily checks that the states (2.33) satisfy the separability criterion for continuous variable systems introduced in [68].

Up to now we discussed entanglement shared by an algebraic bipartition induced by the modes, that we call *mode-entanglement*. We shall now discuss how the usual entanglement shared by the partition induced by the identification of the paricles changes for identical particles, and its relation with the mode-entanglement. For identical Bosons (Fermions), the projection $S(A)$ of the states onto the completely symmetized $S(H)$ (anti-symmetrized $A(H)$) subspace, where $H = \bigotimes_{j=1}^{N} \mathcal{H}$, is required. The symmetrization and anti-symmetrization give rise to unavoidable correlations which violates the separability conditions (2.1.1) and (2.1.2). Thus, we need to rediscuss the definition of particle-entanglement as it is usually formulated for distinguishable particles within the formalism of first quantization. For a slightly different discussion of the following definition, see [72, 74]. We will focus on the case of two particles, since the general case is not well addressed yet. We don’t need to go beyond the case of two particles to show the peculiar feature of the entanglement shared by identical particles and its relation with the mode-entanglement.

**Definition 2.3.2 (Particle-entanglement).** A pure state of two identical Bosons (Fermions) $|\psi_S\rangle \in S(H) \ (|\psi_A\rangle \in A(H))$ is separable if there are two orthonormal states $|\psi_j\rangle \in \mathcal{H}$, $\langle \psi_j | \psi_j \rangle = \delta_{jj}, \ j = 1, 2$ and $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \in \mathcal{H}$, such that $|\psi^2\rangle = S|\psi\rangle \ (|\psi^A\rangle = A|\psi\rangle)$. Otherwise, the state is called entangled.

A mixed state of identical Bosons (Fermions) $\rho^S \in B(S(H)) \ (\rho^A \in B(A(H)))$ is separable if it is a convex combination of separable pure states $|\psi^S_k\rangle \langle \psi^S_k |$ ($|\psi^A_k\rangle \langle \psi^A_k |$):

$$
\rho^S = \sum_k p_k |\psi^S_k\rangle \langle \psi^S_k |, \quad \rho^A = \sum_k p_k |\psi^A_k\rangle \langle \psi^A_k |.
$$

(2.39)

Otherwise the state is entangled.

The orthogonality condition $\langle \psi_1 | \psi_2 \rangle = 0$ always holds for Fermions but not for Bosons: every antisymmetrization of the product of two states is equal to the antisymmetrization of the product of two orthogonal states; it is not true for symmetrized states. There is a physical reason to exclude correlations induced by the symmetrization and anti-symmetrization from the definition of particle-entanglement. Indeed, identical particles which have never
interacted are described by symmetrized or anti-symmetrized states. However, physical correlations such as entanglement should arise from interactions.

Let us get back to mode-entanglement and its relation with particle-entanglement. Mode-entanglement shared by the algebraic bipartition \((A_1, A_2)\) reveals a non-locality between two different preparations of a state, for instance the spatial modes discussed above. A Bogolubov transformation, as

\[
a_1 = \frac{b_1 + b_2}{\sqrt{2}}, \quad a_2 = \frac{b_1 - b_2}{\sqrt{2}},
\]

(2.40)
corresponds to a change of basis in the single particle Hilbert space, from the one of spatially localized states, to the one of

\[
b_1^\dagger |0\rangle = \frac{1}{\sqrt{2}} (|\downarrow\rangle + |\uparrow\rangle), \quad b_2^\dagger |0\rangle = \frac{1}{\sqrt{2}} (|\downarrow\rangle - |\uparrow\rangle).
\]

(2.41)

Physically speaking, such states are eigenstates of the single particle Hamiltonian in the Bose-Hubbard approximation with a highly penetrable barrier. The change to the energy bipartition \((B_1, B_2)\) is non-local with respect to the spatial bipartition \((A_1, A_2)\). It corresponds to a locally unitary and completely symmetric transformation \(\bigotimes_{j=1}^N U \in \mathcal{B}(\mathcal{H})\), in a first quantized formalism. This kind of transformation leaves unchanged the entanglement shared by the particles. However, mode-entanglement is not invariant under Bogolubov transformation: it can be created or destroyed. Hence, the mode-entanglement is not a straightforward consequence of the particle-entanglement: it may come either from the particle-entanglement and from the symmetrization (anti-symmetrization) of the first quantized states. In general, we state the following proposition

**Proposition 2.3.1.** A state of two identical particles exhibits mode-entanglement under any Bogolubov transformation if and only if it exhibits particle-entanglement.

**Proof.** Since entangled mixed states are mixtures of some entangled pure states, we just need to prove the proposition for pure states. Any symmetrization or anti-symmetrization of products of orthogonal states in first quantization is equivalent to a Fock state of some commuting modes in second quantization. The proposition straightforwadly follows.
Part II
Results
Environment induced entanglement between two atoms

The result discussed in this chapter are published in [162, 166]. Quantum systems can be considered isolated from their environment only if the coupling with it can be neglected; if this is weak but not negligible, a reduced dynamics can be obtained by eliminating the degrees of freedom of the environment and by subsequently performing a so-called Markovian approximation [83, 87, 92, 98, 104, 105]. These systems are known as open quantum systems and their reduced dynamics is irreversible and satisfies a forward-in-time composition law: it is described by a so-called quantum dynamical semigroup that incorporates the dissipative and noisy effects due to the environment. Usually, the latter acts as a source of decoherence: in general, the corresponding reduced dynamics generically and irreversibly transforms pure states (one-dimensional projections) into mixtures of pure states (density matrices).

One of the most intriguing aspects of quantum coherence is entanglement [62], that is the existence of purely quantum mechanical correlations, which has become a central topic in quantum information for its many applications as a physical resource enabling otherwise impossible information processing protocols. With reference to the entanglement content of a state of two qubits embedded in the same heat bath, it is generally expected that it would be depleted by decoherence effects. However, this is not the only possibility: if suitably engineered, the environment can entangle an initial separable state of two dynamically independent systems; the reason is that, although not directly interacting between themselves, there can be an environment mediated generation of quantum correlations between two systems immersed in it.

This possibility has been demonstrated analytically for two qubits with the same os-
cillation frequency [134, 144, 161] and two identical harmonic oscillators [148] evolving according to a reduced master equation of the typical Lindblad form [91, 106, 107], obtained via the so-called weak-coupling limit, while for harmonic oscillators in a heat bath of other oscillators it has been derived from the exact time-evolution [157, 159]. This technique is based on the fact that the time-scale over which the dissipative effects are visible is so large that the free dynamics of the embedded systems can be averaged out [83, 87, 98, 104, 105], thus eliminating too rapid oscillations.

Noticeably, such a prescription guarantees that, unlike for reduced dynamics of Redfield type (see [98, 109]), the resulting quantum dynamical semigroups consist of completely positive maps [83, 91, 92, 104, 105]. Complete positivity ensures that the open quantum evolution is consistent with entanglement in the sense that not only the positivity of any initial density matrix of the open system is preserved in time, but also that of any initial state of the open system coupled to any other possible ancillary system external to the environment. Indeed, only complete positivity can guarantee the full physical consistency of the Markovian approximations that one may use to describe an open quantum dynamics; in other words, without complete positivity, it always occurs that at least one initial state carrying entanglement between the given system and an ancilla will assume negative eigenvalues in the course of time [98].

It turns out that, when two qubits or two harmonic oscillators embedded in the same environment have different oscillation frequencies $\omega_1 \neq \omega_2$, no matter how small the difference $\omega_2 - \omega_1$ is, the elimination of too rapid oscillations destroys the generation capability that the environment possesses when $\omega_1 = \omega_2$.

In the following, we study this behavior in the case of two qubits weakly interacting, via a Ohmic coupling, with a Bose heat bath of free Bosons at temperature $T = 1/\beta$. In many physical instancies, atoms can be treated in a non-relativistic approximation, as independent finite-level systems, with negligibly small size. On the other hand, the environment can be modeled by a set of weakly coupled quantum fields, typically the electromagnetic field or the phononic field, in a given temperature state. Although ignoring the internal atom dynamics and the full vectorial structure of the quantum field, this simplified setting is nevertheless perfectly adequate for studying the behaviour of physical systems like ions in traps, atoms in optical cavities and fibers, impurities in phonon fields [11, 14, 96].

We shall first relate the sharp dependence of the entanglement capability of the environment on the oscillation frequencies of the two qubits to the time coarse-graining underlying the derivation of the reduced dynamics and then show how a more refined time coarse-graining can guarantee both complete positivity and the entanglement generation capability of the environment even when $\omega_1 \neq \omega_2$. In this refined framework the sharp dependence on the atom frequencies of the entanglement capability of the environment
mentioned above looks more like a mathematical artifact than a real physical effect.

### 3.1 Coarse graining approach

As explained above, we shall study the behaviour of a system composed by two, unequal two-level atoms, that start interacting at time $t = 0$ with an environment made of a collection of independent, massless, scalar quantum fields at temperature $1/\beta$. We are interested in the evolution of the atoms as open quantum systems and not in the details of their internal dynamics; therefore, we shall model them, in a nonrelativistic way, as simple qubits, described in terms of a two-dimensional Hilbert space.

In absence of any interaction with the external fields, the single atom internal dynamics can thus be taken to be driven by a generic $2 \times 2$ hamiltonian matrix. As a result, the total atom Hamiltonian $H_S$ can be expressed as:

$$H_S = H_S^{(1)} + H_S^{(2)}, \quad H_S^{(\alpha)} = \frac{\omega_\alpha}{2} \vec{n} \cdot \sigma^{(\alpha)} = -\sum_{i=1}^{3} n_i \sigma_i^{(\alpha)}, \quad \alpha = 1, 2,$$

(3.1)

where $\sigma_i^{(1)} = \sigma_i \otimes 1$ and $\sigma_i^{(2)} = 1 \otimes \sigma_i$ are the basis operators pertaining to the two different atoms, with $\sigma_i, i = 1, 2, 3$ the Pauli matrices, $n_i$ the components of a unit vector, while $\omega_\alpha$ represent the gaps between the two energy eigenvalues of the two atoms.

As mentioned in the introductory remarks, the coupling of the atoms with the external fields is assumed to be weak. In our simplifying settings that ignore spinorial indices, the interaction term can then be described by a Hamiltonian $H'$ that is linear in both atom and field variables:

$$H' = \sum_{i=1}^{3} \left( \sigma_i^{(1)} \otimes \Phi_i[f^{(1)}] + \sigma_i^{(2)} \otimes \Phi_i[f^{(2)}] \right).$$

(3.2)

The operators $\Phi_i(t, \vec{x})$ represent the set of external quantum fields, which evolve in time as free fields with a Hamiltonian $H_B$. The atoms are assumed to have a spatial extension described by the two functions $f^{(\alpha)}(\vec{x}), \alpha = 1, 2$. To be more specific, we shall choose for the atoms a common profile $f(\vec{x})$ of spherically symmetric shape, with size $\varepsilon$:

$$f(\vec{x}) = \frac{1}{\pi^{3/2}} \frac{(\varepsilon/2)}{[|\vec{x}|^2 + (\varepsilon/2)^2]^{3/2}},$$

(3.3)

and position the first atom at the origin of the reference frame, so that $f^{(1)}(\vec{x}) \equiv f(\vec{x})$, while the second is displaced by an amount $\vec{\ell}$ with respect to it, $f^{(2)}(\vec{x}) = f(\vec{x} + \vec{\ell})$. Since the atom-field interaction takes place on the whole region occupied by the atoms, the field...
operators entering the interaction Hamiltonian above are smeared over the atom spatial extension:

$$\Phi_i[f^{(\alpha)}] = \int d^3x f^{(\alpha)}(\vec{x}) \Phi_i(0, \vec{x}) , \quad \alpha = 1, 2 . \tag{3.4}$$

The total Hamiltonian $H$ describing the complete system, the two atoms together with the external fields $\Phi_i$, can thus be written as

$$H = H_S + H_B + \lambda H' \equiv H_0 + \lambda H' , \tag{3.5}$$

with $\lambda$ a small coupling constant. Through the standard Liouville-von Neumann equation, $\partial_t \rho_{\text{tot}}(t) = -i[H, \rho_{\text{tot}}(t)]$, it generates the evolution in time of the state of the total system, described in general by a density matrix $\rho_{\text{tot}}$, starting at $t = 0$ from the initial configuration: $\rho_{\text{tot}}(0)$.

We shall assume the atom and the fields to be initially prepared in an uncorrelated state, with the fields in the temperature state $\rho_\beta$ and the atoms in a generic initial state $\rho(0)$, so that $\rho_{\text{tot}}(0) = \rho(0) \otimes \rho_\beta$. The reduced time evolution of the two atoms is then obtained by integrating over the unobserved field degrees of freedom and is formally given by the transformation map: $\rho(0) \mapsto \rho(t) \equiv \text{Tr}_B[\rho_{\text{tot}}(t)]$. This map is in general very complicated, because of nonlinearities and memory effects; nevertheless, it can be approximated by a linear, memoryless map when the coupling with the environment is small and its own internal dynamics is sufficiently fast [83, 87, 91, 92, 98, 99]. Indeed, in such cases the details of the internal environment dynamics result irrelevant, being the time scale of the subsystem evolution typically very long compared with the decay time of the correlations in the bath.

In order to derive the equation obeyed by the reduced density matrix $\rho(t)$ in the case at hand, it is convenient to work in the interaction representation

$$\tilde{\rho}_{\text{tot}}(t) = e^{itH_0} \rho_{\text{tot}}(t) e^{-itH_0} , \tag{3.6}$$

so that

$$\frac{\partial \tilde{\rho}_{\text{tot}}(t)}{\partial t} = -i\lambda \left[ H'(t), \tilde{\rho}_{\text{tot}}(t) \right] , \quad H'(t) = e^{itH_0} H' e^{-itH_0} . \tag{3.7}$$

One then focuses on the changes of the reduced state $\tilde{\rho}(t) \equiv \text{Tr}_B[\tilde{\rho}_{\text{tot}}(t)]$ over a time interval $\Delta t$; by taking the trace over the field variables of the integrated version of the equation (3.7) one gets (to lowest order in $\lambda$):

$$\frac{\tilde{\rho}(t + \Delta t) - \tilde{\rho}(t)}{\Delta t} = \frac{1}{\Delta t} \int_t^{t+\Delta t} ds \frac{\partial \tilde{\rho}(s)}{\partial s}$$

$$= -\lambda^2 \Delta t \int_t^{t+\Delta t} dt_1 \int_t^{t+\Delta t} dt_2 \text{Tr}_B\left([H'(t_1), [H'(t_2), \tilde{\rho}_{\text{tot}}(t)]]\right) +$$
+O(\lambda^4). \quad (3.8)

One notices that the variation of $\tilde{\rho}(t)$ starts to become relevant at order $\lambda^2$, i.e. on time scales of order $\tau = \lambda^2 t$. Then, one can equivalently write:

$$\frac{\tilde{\rho}(t + \Delta t) - \tilde{\rho}(t)}{\Delta t} = \frac{1}{\Delta t} \int_{\tau}^{t+\lambda^2 \Delta t} ds \frac{\partial \tilde{\rho}(s/\lambda^2)}{\partial s}, \quad (3.9)$$

so that in the limit of small $\lambda$ and for (finite) $\Delta t$ such that $\lambda^2 \Delta t \ll 1$ one can readily approximate the r.h.s. of (3.9) with $\partial_t \tilde{\rho}(t)$. Indeed, the error is bounded by $\lambda^2 \Delta t$.

At this point, one further observes that the environment, containing an infinite number of degrees of freedom, is much larger than the subsystem immersed in it, so that its dynamics is hardly affected by its presence. Further, if $\Delta t$ is chosen much larger than the decay time $\tau_B$ of the environment two-point time-correlation functions, one may approximate in the double integral of (3.8) $\tilde{\rho}_{SB}(t)$ with the uncorrelated state $\rho(t) \otimes \rho_\beta$, taking the initial state $\rho_\beta$ as a reference state for the bath [83, 87, 91, 92, 99]. Therefore, if $\tau_B \ll \Delta t$, one gets the following approximated master equation (in interaction representation):

$$\partial_t \tilde{\rho}(t) = -\frac{\lambda^2}{\Delta t} \int_1^{t+\lambda^2 \Delta t} dt_1 \int_1^{t_1} dt_2 \text{Tr}_B \left( [H'(t_1), [H'(t_2), \tilde{\rho}(t) \otimes \rho_\beta]] \right). \quad (3.10)$$

Returning to the Schrödinger representation, one finally gets the following linear, Markovian master equation for the two-atom state $\rho(t)$:

$$\frac{\partial \rho(t)}{\partial t} = -i[H_S, \rho] + D[\rho(t)], \quad (3.11)$$

where the bath-dependent contribution $D[\rho(t)]$ contains both the Hamiltonian and the dissipative term

$$D[\rho(t)] = -i[H_{12}, \rho(t)] + L[\rho(t)], \quad (3.12)$$

with

$$H_{12} = \frac{i\lambda^2}{2\Delta t} \int_0^{\Delta t} ds_1 \int_0^{s_1} ds_2 \theta(s_1 - s_2) \text{Tr}_B \left( \rho_\beta [H'(s_1), H'(s_2)] \right), \quad (3.13)$$

$$L[\rho(t)] = \frac{\lambda^2}{\Delta t} \text{Tr}_B \left( L(\rho(t) \otimes \rho_\beta) L - \frac{1}{2} \left[ L^2, \rho(t) \otimes \rho_\beta \right] \right), \quad L = \int_0^{\Delta t} ds H'(s), \quad (3.14)$$

the curly brackets representing the anticommutator, while $\theta(s)$ is the step function. A discussion on the validity of this so-called Markovian approximation is reported in [120].
There, a non-Markovian weak coupling approximation of the reduced dynamics is also introduced; it leads to a two-parameter family of dynamical maps, with a time-dependent generator [83]. We stress that this approach is completely different from the one discussed below, which instead describes the reduced two-atom dynamics in terms of a Markovian, one parameter semigroup. In particular, while in [120] the standard weak coupling limit can be reached only in the asymptotic, long-time regime, in the treatment presented below it can always be obtained for any time by letting the coarse-graining parameter become large.

It is important to observe that, for any interval $\Delta t$, the master equation (3.11)-(3.14) generates a quantum dynamical semigroup of completely positive maps. Indeed, the generator in the r.h.s. of (3.12), besides the Hamiltonian piece, contains a dissipative term which turns out to be itself completely positive, being the composition of two completely positive maps, the trace over the environment degrees of freedom and a linear operator on the total system, written in canonical (1.18) Kraus-Stinespring form [13, 58]. Notice that, on the contrary, in the usual weak coupling limit approach to the derivation of a Markovian master equation, complete positivity is ensured by an ergodic average prescription that eliminates fast oscillating terms [104, 105, 109].

The physical meaning of $\Delta t$ is that of a time-coarse graining parameter naturally associated to the slow dissipative time-scale $\tau = t\lambda^2$. More precisely, significant variations of the system density matrix due to the presence of the environment can only be seen after a time $\Delta \tau = \lambda^2 \Delta t$ has elapsed. Given the coupling constant $\lambda \ll 1$, the dissipative time-scale is set and actual experiments cannot access faster time-scales; furthermore, if $\Delta \tau \ll 1$ on the scale of $\tau$, then the experimental evidences are consistently described by a master equation as in (3.10). The weak-coupling limit consists in letting $\lambda \rightarrow 0$ [83, 87, 99]; then, variations of the system density matrix as in (3.10) are actually visible only if $\Delta t \rightarrow +\infty$. This allows one to average out all fast oscillations through the time ergodic average as in the standard weak-coupling limit approach [104, 105, 109]. Instead, if the system-environment coupling $\lambda$ is small, but not vanishingly small, then $\Delta t$ cannot be taken as infinitely large thus allowing one to keep contributions that would otherwise be washed out. In such cases, the usual weak-coupling limit techniques provide an approximation which is too rough to properly describe the dissipative time-evolution and one needs a more refined approach.

### 3.2 Phononic bath

The problem we are going to address in the following regards whether two non-interacting qubits with Hamiltonian
can become entangled when weakly coupled to free spinless Bosons in thermal equilib-
rium via a (finite volume) interaction of the form

\[ H' = \lambda \Phi[f]\left(\sigma^{(1)}_1 + \sigma^{(2)}_1\right), \quad \Phi[f] = \sum_k \left( f(k) a_k^\dagger + f^*(k) a_k \right). \]  

(3.16)

where \( a_k^\dagger \) and \( a_k \) denote the creation and annihilation operators of Bose modes with mo-
mmentum \( k \) and energy \( \omega(k) \), \( f(k) \) is a one-particle Bose state in momentum representation,
while \( \sigma^{(1)}_{1,3} = \sigma_{1,3} \otimes 1 \) and \( \sigma^{(2)}_{1,3} = 1 \otimes \sigma_{1,3} \) represent the first and third Pauli matrices for
the two qubits. For sake of simplicity, we consider the two qubits located at a same point
in space. With respect to the notation introduced in the previous section, it corresponds to
the choice \( \vec{f} = 0 \), that is \( f^{(1)} = f^{(2)} \), for the operators (3.4). The total system Hamiltonian
will then be

\[ H = H_S + H_B + H', \quad H_B = \sum_k \omega(k) a_k^\dagger a_k. \]  

(3.17)

This model is commonly used to describe two-level atoms immersed in a phononic bath
[41]. In the interaction picture we write

\[ H'(t) = \lambda \Phi_t[f]\left(\sigma^{(1)}_1 + \sigma^{(2)}_1\right), \quad \Phi_t[f] = \sum_k \left( f(k) e^{i\omega(k)t} a_k^\dagger + f^*(k) e^{-i\omega(k)t} a_k \right). \]  

(3.18)

In the Schrödinger representation, (3.10) yields the following memoryless master
equation (see [120, 132, 156]) of Kossakowski-Lindblad type [83, 87, 98]:

\[ \partial_t \rho(t) = -i\left[ H_S + \lambda^2 H_{\Delta t}, \rho(t) \right] + D_{\Delta t}[\rho(t)]. \]  

(3.19)

The environment contributes to the generator of the reduced dynamics with a Hamiltonian
\( H_{\Delta t} \) and a purely dissipative term \( D_{\Delta t}[\rho(t)] \); both of them depend on the environment
through the two-point time-correlation functions

\[ G(t_2 - t_1) = \text{Tr} \left( \rho_{\Delta t} \Phi_{t_1}[f] \Phi_{t_2}[f] \right) = G(t_1 - t_2)^*. \]  

(3.20)

The bath-induced Hamiltonian \( H_{\Delta t} \) contains a bath-mediated spin-spin interaction

\[ H_{\Delta t}^{\text{int}} = \sum_{i,j=1,2} h_{ij}(\Delta t) \sigma^{(1)}_i \sigma^{(2)}_j, \]  

(3.21)
where the $2 \times 2$ matrix $h_{\Delta t} = [h_{ij}(\Delta t)]$ is real, but not necessarily Hermitian. It is convenient to introduce the following matrices $[\Psi_{\epsilon j}] = \frac{1}{2} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}$, $\epsilon = \pm 1$; then $h_{\Delta t} = \Psi^\dagger H_{\Delta t}^{(12)} \Psi + \left( \Psi^\dagger H_{\Delta t}^{(21)} \Psi \right)^T$, where $H_{\Delta t}^{(ab)} = [H_{\Delta t}^{(ab)}(\Delta t)]$, $a, b = 1, 2$, with

$$H_{\Delta t}^{(ab)}(\Delta t) = -\frac{i}{2\Delta t} \int_0^{\Delta t} dt_1 \int_0^{\Delta t} dt_2 e^{i(\epsilon \omega_a t_1 - \epsilon' \omega_b t_2)} \text{sign}(t_2 - t_1) G(t_2 - t_1) ,$$

(3.22)

where $X^T$ denotes matrix transposition. Instead, the purely dissipative part can be written as

$$D_{\Delta t}[\rho(t)] = \sum_{a,b=1,2,i,j=1,2} (\Psi^\dagger D_{\Delta t}^{(ab)}(\Delta t) \Psi)_{ij} \left( \sigma_i^{(a)}(t) \sigma_j^{(b)}(t) - \frac{1}{2} \{ \sigma_j^{(b)}(t) \sigma_i^{(a)}(t) , \rho(t) \} \right) ,$$

(3.23)

where $D_{\Delta t}^{(ab)} = [D_{\Delta t}^{(ab)}(\Delta t)]$ with

$$D_{\Delta t}^{(ab)}(\Delta t) = \frac{1}{\Delta t} \int_0^{\Delta t} dt_1 \int_0^{\Delta t} dt_2 e^{i(\epsilon \omega_a t_1 - \epsilon' \omega_b t_2)} G(t_2 - t_1) .$$

(3.24)

The $4 \times 4$ Kossakowski matrix $C_{\Delta t}$ formed by the $2 \times 2$ blocks $C_{\Delta t}^{(ab)} = \Psi^\dagger D_{\Delta t}^{(ab)}(\Delta t) \Psi$, $a, b = 1, 2$, involves the Fourier transforms of the correlation functions (3.20) and is automatically positive definite; this fact guarantees that the master equation (3.19) generates a semigroup of dynamical maps $\gamma_{\Delta t}$ on the two-qubit density matrices which are completely positive [83, 87, 98, 92, 104, 105], whence, as discussed in the introduction, fully physically consistent.

### 3.2.1 Environment induced entanglement generation

Given two qubits weakly interacting with their environment, a sufficient condition for them to get entangled at small times by the completely positive reduced dynamics has been derived in [138, 155] and briefly reviewed in the section 2.2. It is based on the properties of the generator in (3.19), that is on the interaction Hamiltonian (3.21) and the dissipative contribution (3.23). We shall focus on an initial two qubit state of the form $\rho(0) = | \downarrow \rangle \langle \downarrow | \otimes | \uparrow \rangle \langle \uparrow |$, where $\sigma_3 | \uparrow, \downarrow \rangle = \pm | \uparrow, \downarrow \rangle$; then, the condition is as follows:

$$\delta = D_{\Delta t}^{(11)}(\Delta t) D_{\Delta t}^{(22)}(\Delta t) - |D_{\Delta t}^{(12)}| < 0 ,$$

(3.25)
where, from (3.22) and (3.24),

\[
D^{(12)}_\Delta = \frac{D^{(12)}(\Delta t) + (D^{(12)}(\Delta t))^*} {2}
\]  
\[
H^{(12)}_\Delta = H^{(12)}_- (\Delta t) + H^{(21)}_+ (\Delta t).
\]  

If \( \delta > 0 \), such a separable state cannot get entangled by the environment at small times [155].

We are interested in the capacity of the environment to generate entanglement, at least at small times with respect to the dissipative time-scale. Because of the positivity of the Kossakowski matrix \( C_\Delta \), the diagonal block matrices \( C^{(aa)}_\Delta (\Delta t) \) and \( D^{(aa)}_\Delta (\Delta t) \), \( a = 1, 2 \), are positive definite; therefore, the dissipative entanglement generation depends on the quantity \( D^{(12)}_\Delta \), but also on how it interferes with \( H^{(12)}_\Delta \) in (3.25). In the case at hand, it turns out that

\[
\left| D^{(12)}_\Delta + i H^{(12)}_\Delta \right|^2 = \left| D^{(12)}_\Delta \right|^2 + \left| H^{(12)}_\Delta \right|^2.
\]  

Indeed, using (3.20), one can check by explicit computation that the quantities

\[
e^{-i(\omega_2-\omega_1)\Delta t/2} D^{(12)}_\Delta, \quad e^{-i(\omega_2-\omega_1)\Delta t/2} H^{(12)}_\Delta
\]  

are both real. We shall thus concentrate on the purely dissipative entanglement generation, that is on the difference

\[
\tilde{\delta} = D^{(11)}_- (\Delta t) D^{(22)}_+ (\Delta t) - \left| D^{(12)}_\Delta \right|^2.
\]  

If \( \tilde{\delta} \) is negative, then also \( \delta \) in (3.25) is negative.

We shall consider (infinite volume) Ohmic correlation functions [125]

\[
G(t) = \int_0^{+\infty} d\omega \ e^{-\omega/\omega_c} \omega \left( \coth \frac{\beta \omega} {2} \cos \omega t - i \sin \omega t \right),
\]  

where \( \omega_c \) is a Debye cut-off; then, setting \( \text{sinc}(x) = \frac{\sin x} {x} \) and \( (a, \varepsilon) = (1, -), (2, +) \), one explicitly gets

\[
D^{(aa)}_{\varepsilon \varepsilon}(\Delta t) = \frac{e\Delta t} {2} \int_{-\infty}^{+\infty} d\omega \ \omega \ e^{\frac{-|\omega|} {\omega_c}} \frac{1} {e^{\beta \omega} - 1} \sin^2 \left( \frac{(\omega - \omega_\varepsilon)\Delta t} {2} \right)
\]  
\[
\left| D^{(12)}_\Delta \right| = \frac{\Delta t} {2} \int_{-\infty}^{+\infty} d\omega \ \omega \ e^{\frac{-|\omega|} {\omega_c}} \ coth \left( \beta \omega / 2 \right).
\]
\[ \text{sinc}\left(\frac{(\omega - \omega_1)\Delta t}{2}\right) \cdot \text{sinc}\left(\frac{(\omega - \omega_2)\Delta t}{2}\right). \quad (3.33) \]

The weak-coupling limit amounts to \( \Delta t \to +\infty \); since \( \lim_{\alpha \to +\infty} \alpha \cdot \text{sinc}(\alpha(x - x_0)) = \delta(x - x_0) \), one finds

\[
\lim_{\Delta t \to +\infty} D_{(\omega_1)}(\Delta t) = 4\pi e^{\frac{\omega}{\omega_c}} \frac{e^{-\omega_1/\omega_c}}{e^{\omega_1/\omega_c} - 1} \quad (3.34)
\]

\[
\lim_{\Delta t \to +\infty} |D_{(\omega_1)}(\Delta t)| = 2\pi \delta_{\omega_1\omega_2} \omega_1 \omega_2 e^{-\omega_2/\omega_c} \coth \frac{\beta \omega_2}{2} \quad (3.35)
\]

If \( \omega_1 = \omega_2 \), the difference (3.30) is always negative: \( \tilde{\delta} = -4\pi^2 \omega_2^2 e^{-2\omega_2/\omega_c} \); instead, if \( \omega_1 \neq \omega_2 \), \( \tilde{\delta} = D_{(\omega_1)}(\Delta t) D_{(\omega_2)}^{(2)}(\Delta t) > 0 \). Thus, in the latter case, the initial separable state \(|-\rangle \otimes |+\rangle\) cannot get dissipatively entangled by the environment at small times, while it can when \( \omega_1 = \omega_2 \).

Such a sharp dependence of the entanglement capability of the environment on the frequency difference \( 0 < \delta \omega = (\omega_2 - \omega_1)/2 \) can be explained as follows: when the coupling of the qubits to the environment is so weak that effectively \( \lambda \to 0 \), then the dissipative time-evolution of the qubit density matrix occurs over time intervals \( \Delta t \) that are also so long that all off-resonant oscillations depending on \( \delta \omega \) are averaged out. However, this also means that, if \( \lambda \) is small, but not negligibly small, then the qubit density matrix effectively varies over times \( \Delta t < +\infty \); consequently, terms of order \( 1/\Delta t \) like

\[
|D_{(\omega_1)}^{(2)}| = \pi \text{sinc}(\delta \omega \Delta t) \sum_{a=1}^2 \omega_a e^{-\omega_a/\omega_c} \coth(\beta \omega_a/2) \quad (3.36)
\]

can become relevant and can make \( \tilde{\delta} \) become negative even when \( \delta \omega \neq 0 \). Indeed, for high temperatures \( \beta \omega_{1,2} \ll 1 \) and large cut-offs \( \omega_{1,2}/\omega_c \ll 1 \), expanding (3.34) and (3.36) yields

\[
\tilde{\delta} \approx \frac{16\pi^2}{\beta^2} \left( 1 - \beta \delta \omega - \text{sinc}^2(\delta \omega \Delta t) \right). \quad (3.37)
\]

If the qubit frequency difference \( \delta \omega \) and the coupling strength \( \lambda \) are such that \( \delta \omega \Delta t \ll 1 \) then a further expansion of the sinc function yields

\[
\tilde{\delta} \approx -\frac{16\pi^2}{\beta^2} \left( \beta \delta \omega - \frac{(\delta \omega)^2(\Delta t)^2}{3} \right), \quad (3.38)
\]

which is negative when \( \frac{1}{\omega_{1,2}} \gg \beta > \frac{\delta \omega(\Delta t)^2}{3} \).
In conclusion, the fact that the environment may generate two-qubit entanglement only if the qubit frequencies are equal, is a consequence of the weak-coupling limit; in such a case, the coupling constant $\lambda \to 0$ so that the time intervals $\Delta t$ over which the qubit density matrix effectively changes due to the presence of the environment become so large that all off-resonant phenomena are averaged out. By going to a finer time coarse-graining, that is to finite time-resolutions $\Delta t$, one may keep track of finer effects and save the possibility of dissipative entanglement generation. However, in order these effects to be physically accessible, the finite time coarse-graining parameter $\Delta t$ must be compatible with the overall dissipative time-scale which goes as $\lambda^{-2}$. In other words, the experimental visibility of environment-induced entanglement when the two qubits have different frequencies asks for a coupling constant $\lambda$ that is small but not vanishing so that dissipative time-variations of the two-qubit state may occur over times $\Delta t \ll 1/\delta \omega$.

### 3.3 Electromagnetic bath

In this section we shall investigate a more complex case, which models two two-level atoms interacting with an electromagnetic field through a dipole coupling [98]. The quantum fields $\Phi_i(t, \vec{x})$ are taken to be spinless and massless, evolving in time as free relativistic fields with a standard Hamiltonian [12]. A more explicit expression for the generator in (3.12) can be obtained by recalling (3.2) and (3.4). Indeed, after straightforward manipulations, the master equation driving the dissipative dynamics of the two atoms state takes the following Kossakowski-Lindblad form [91, 106, 107]

$$\frac{\partial \rho(t)}{\partial t} = -i[H_{\text{eff}}, \rho(t)] + \mathcal{L}[\rho(t)], \quad (3.39)$$

with

$$H_{\text{eff}} = H_S - \frac{i}{2} \sum_{\alpha, \beta = 1}^{3} \sum_{i, j = 1}^{2} H^{(\alpha \beta)}_{ij} \sigma^{(\alpha)}_i \sigma^{(\beta)}_j, \quad (3.40)$$

and

$$\mathcal{L}[\rho] = \sum_{\alpha, \beta = 1}^{2} \sum_{i, j = 1}^{3} C^{(\alpha \beta)}_{ij} \left[ \sigma^{(\beta)}_j \rho \sigma^{(\alpha)}_i - \frac{1}{2} \{ \sigma^{(\alpha)}_i, \sigma^{(\beta)}_j, \rho \} \right]. \quad (3.41)$$

The coefficients of the Kossakowski matrix $C^{(\alpha \beta)}_{ij}$ and of the effective Hamiltonian $H_{\text{eff}}$ are determined by the field correlation functions in the thermal state $\rho_{\beta}$:

$$G^{(\alpha \beta)}_{ij}(t - t') = \int d^3 x \, d^3 y \, f^{(\alpha)}(\vec{x}) \, f^{(\beta)}(\vec{y}) \, \langle \Phi_i(t', \vec{x}) \Phi_j(t, \vec{y}) \rangle, \quad (3.42)$$
through their Fourier,
\[ G_{ij}^{(a\beta)}(z) = \int_{-\infty}^{\infty} dt \, e^{-izt} G_{ij}^{(a\beta)}(t), \] (3.43)
and Hilbert transform,
\[ K_{ij}^{(a\beta)}(z) = -\int_{-\infty}^{\infty} dt \, \text{sign}(t) e^{-izt} G_{ij}^{(a\beta)}(t) = \frac{P}{\pi i} \int_{-\infty}^{\infty} dw \, \frac{G_{ij}^{(a\beta)}(w)}{w - z}, \] (3.44)
respectively (\(P\) indicates principle value).

More specifically, one finds that the Kossakowski matrix reads:
\[ C_{ij}^{(a\beta)} = \frac{\lambda^2 \Delta t}{2\pi} \sum_{\xi, \xi' = [+,-,0]} \sum_{k,l = 1}^{3} e^{i(\xi \omega_a + \xi' \omega_b)\Delta t/2} \psi_{kl}^{(\xi)} \psi_{ij}^{(\xi')}. \]
\[ \cdot \int_{-\infty}^{\infty} d\omega \, G_{kl}^{(a\beta)}(\omega) \text{sinc}[ (\xi \omega - \omega_a) \Delta t/2 ] \text{sinc}[ (\xi' \omega + \omega_b) \Delta t/2 ], \] (3.45)
where
\[ \psi_{ij}^{(0)} = n_i n_j, \quad \psi_{ij}^{(\pm)} = \frac{1}{2} (\delta_{ij} - n_i n_j \pm i\epsilon_{ijk} n_k), \] (3.46)
are the components of auxiliary three-dimensional tensors, giving the free evolution of the atom operators:
\[ \sigma_i^{(\alpha)}(t) = e^{iH_S t} \sigma_i^{(\alpha)} e^{-iH_S t} = \sum_{\xi = [+,-,0]} \sum_{j=1}^{3} e^{i\xi \omega_a t} \psi_{ij}^{(\xi)} \sigma_j^{(\alpha)}. \]

The \(6 \times 6\) matrix \(C_{ij}^{(a\beta)}\) turns out to be non-negative, since, as already mentioned, the evolution generated by 3.39 is completely positive. On the other hand, let us remark that direct use of the standard second order perturbative approximation (e.g. see [14, 96]) often leads to physically inconsistent results [98, 152, 153], giving a finite time evolution for \(\rho(t)\) that in general does not preserve the positivity of probabilities. An expression similar to the one in (3.45) holds also for \(H_{ij}^{(a\beta)}\) in (3.40), with \(G_{kl}^{(a\beta)}(\omega)\) replaced by \(K_{kl}^{(a\beta)}(\omega)\).

For simplicity, the fields giving rise to the environment are taken to be independent and further assumed to obey a free evolution; in this case, one finds:
\[ \langle \Phi_i(x) \Phi_j(y) \rangle \equiv \text{Tr}[\Phi_i(x)\Phi_j(y)\rho_\beta] = \delta_{ij} G(x - y), \] (3.47)
where \(G(x - y)\) is the standard four-dimensional Wightmann function for a single relativistic scalar field in a state at inverse temperature \(\beta\) [12], that, with the usual \(i\epsilon\) prescription, can be written as:
\[ G(x) = \int \frac{d^4 k}{(2\pi)^3} \theta(k^0) \delta(k^2) \left[ (1 + N(k^0)) e^{-ik \cdot x} + N(k^0) e^{ik \cdot x} \right] e^{-ek^0}, \] (3.48)
where
\[ N(k^0) = \frac{1}{e^{\beta k^0} - 1}. \] (3.49)

Although the \(i\epsilon\) prescription, assuring the convergence of the integral in (3.48), originates from causality requirements, in the present setting it can be related to the finite size of the two atoms. Indeed, the correlations in (3.42) actually involve the Fourier transform \(\hat{f}(\vec{k}) = \int d^3x e^{i\vec{k} \cdot \vec{x}} f(\vec{x})\) of the shape function \(f(\vec{x})\) in (3.3); it can be easily computed to be \(\hat{f}(\vec{k}) = e^{-|\vec{k}|\epsilon/2}\). Inserting it back in (3.42), this contribution can be conveniently attached to the definition of the Wightmann function \(G(x)\), so that the integrand in (3.48) gets an extra \(e^{-\epsilon k^0}\) overall factor.

Using (3.48) and (3.49), the Fourier transform in (3.43) can now be explicitly evaluated; taking for simplicity the limit of pointlike atoms, (the size \(\epsilon\) can be taken to vanish since it does not play any more the role of a regularization parameter), one gets:
\[ G^{(11)}(\omega) = G^{(22)}(\omega) = \frac{\omega}{2\pi} \frac{1 - e^{-\beta\omega}}{1 - e^{-\beta\omega}}, \]
\[ G^{(12)}(\omega) = G^{(21)}(\omega) = \frac{\omega}{2\pi} \frac{\sin(\ell\omega)}{\ell\omega}, \] (3.50)

where \(\ell\) denotes the modulus of the displacement vector \(\vec{\ell}\); then, recalling (3.44), for the Hilbert transform one similarly finds:
\[ K^{(a\beta)}(z) = \delta_{ij} K^{(a\beta)}(z), \quad K^{(a\beta)}(z) = \frac{P}{\pi i} \int_{-\infty}^{\infty} dw \frac{G^{(a\beta)}(w)}{w - z}. \] (3.52)

With these results and taking into account that \(\sum_k \psi^{(\xi)}_{ki} \psi^{(\xi')}_{kj} = \psi^{(-\xi)}_{ij} \delta(\xi + \xi')\), the Kosakowski matrix takes the more explicit form:
\[ C^{(a\beta)}_{ij} = C^{(a\beta)}_+ \delta_{ij} - iC^{(a\beta)}_0 \sum_{k=0}^{3} \epsilon_{ijk} n_k + [C^{(a\beta)}_0 - C^{(a\beta)}_+] n_i n_j, \] (3.53)
where
\[ C^{(a\beta)}_\pm = I^{(a\beta)}_\pm \cos(\omega_{a\beta} \Delta t/2) + i I^{(a\beta)}_\mp \sin(\omega_{a\beta} \Delta t/2), \quad \omega_{a\beta} = \omega_\alpha - \omega_\beta, \] (3.54)

with
\[ I^{(a\beta)}_\pm = \frac{\Delta t}{4\pi} \int_{-\infty}^{\infty} d\omega \left[ G^{(a\beta)}(\omega) \mp G^{(a\beta)}(-\omega) \right] \text{sinc}((\omega - \omega_\alpha)\Delta t/2) \text{sinc}((\omega - \omega_\beta)\Delta t/2), \] (3.55)
while
\[ C^{(\alpha\beta)}_0 \equiv I^{(\alpha\beta)}_0 = \frac{\Delta t}{4\pi} \int_{-\infty}^{\infty} d\omega \left[ G^{(\alpha\beta)}(\omega) + G^{(\alpha\beta)}(-\omega) \right] \left[ \text{sinc}(\omega \Delta t/2) \right]^2. \] (3.56)

Only the following combinations \( G^{(\alpha\beta)}_\pm(\omega) \equiv G^{(\alpha\beta)}(\omega) \pm G^{(\alpha\beta)}(-\omega) \) actually occur in the previous integrals, and from the explicit expressions in (3.51) one obtains:

\[
G^{(11)}_+ = G^{(22)}_+ = \frac{\omega}{2\pi} \left[ 1 + e^{-\beta \omega} \right], \quad G^{(12)}_+ = G^{(21)}_+ = \frac{\omega}{2\pi} \left[ 1 + e^{-\beta \omega} \right] \text{sinc}(\omega \ell), \quad (3.57) \\
G^{(11)}_- = G^{(22)}_- = \frac{\omega}{2\pi}, \quad G^{(12)}_- = G^{(21)}_- = \frac{\omega}{2\pi} \text{sinc}(\omega \ell); \quad (3.58)
\]

they contain the dependence on the bath temperature \( 1/\beta \) and on the separation \( \ell \) between the two atoms. Because of the presence of the Boltzmann factors, the integrals \( I^{(\alpha\beta)}_{\pm,0} \) in (3.55, 3.56) cannot in general be expressed in terms of elementary functions. However, in the case of a bath at high temperature (i.e. for small \( \beta \)), the square bracket in (3.57) behaves as \( 2/\beta \omega \) and the above integrals can be explicitly evaluated (see the Appendix A). In the physical situation for which \( \ell \ll 3\Delta t \), one finds:

\[
I^{(\alpha\beta)}_+ = \frac{1}{\pi \beta \omega_{\alpha\beta} \Delta t} \left( \text{sinc}(\ell \omega_\alpha/2) \sin \left( (\omega_\alpha - \omega_\beta)(1 - \ell/\Delta t) / 2 \right) \right)
\]

\[
+ \sin(\ell \omega_\beta/2) \sin \left( (\omega_\alpha - \omega_\beta)(1 - \ell/\Delta t) / 2 \right), \quad (3.59) \\
I^{(\alpha\beta)}_- = \frac{1}{\pi \ell \omega_{\alpha\beta} \Delta t} \sin \left( \omega_{\alpha\beta}(\Delta t - \ell) / 2 \right) \sin \left( \ell(\omega_\alpha + \omega_\beta) / 2 \right), \quad (3.60) \\
I^{(\alpha\beta)}_0 = \frac{1}{4\pi \beta} \left( 2 - \frac{\ell}{\Delta t} \right). \quad (3.61)
\]

The condition \( \ell \ll 3\Delta t \) assures that the two atoms actually feel the presence of the quantum fields; indeed, due to relativistic causality [12], the fields would not be able to interact with the atoms in the time interval \( \Delta t \) if they were too far apart. Inserting these results back in (3.54) and (3.56), one finally obtains the explicit expression for the Kossakowski matrix \( C^{(\alpha\beta)}_{ij} \), in the large temperature limit. Since this is an approximated result, positivity of the matrix is not a priori guaranteed and should be formally imposed in order to preserve the properties of the exact expression (3.45). In particular, positivity of the two diagonal submatrices \( C^{(\alpha\alpha)}_{ij} \), requires \( \beta \omega_{\alpha} / 2 \ll 1 \), which are satisfied by the requirement of \( \beta \) small.

Coming now to the Hamiltonian contribution to the master equation, one sees that the effective Hamiltonian \( H_{\text{eff}} \) in (3.40) can be split into two parts, \( H_{\text{eff}} = H_S + H_{\text{eff}}^{(12)} \), the
first is just a renormalization of the starting system Hamiltonian, while the second one represents an environment induced direct coupling term for the two atoms. The term $\tilde{H}_S$ has the same form as the Hamiltonian in (3.1) but with redefined frequencies

$$\tilde{\omega}_\alpha = \omega_\alpha - i \frac{\Delta t}{2\pi} \int_{-\infty}^{\infty} d\omega \left[ \mathcal{K}^{(\alpha\alpha)}(\omega) - \mathcal{K}^{(\alpha\alpha)}(-\omega) \right] \left[ \text{sinc}[(\omega - \omega_\alpha)\Delta t/2] \right]^2 . \quad (3.62)$$

Recalling the definition of $\mathcal{K}^{(\alpha\alpha)}(\omega)$ in (3.52), one sees that it can be split as:

$$\mathcal{K}^{(\alpha\alpha)}(\omega) = \frac{1}{2\pi^2 i} P \int_{0}^{\infty} dz \frac{z}{z - \omega} + \frac{1}{2\pi^2 i} P \int_{0}^{\infty} d\omega \left( \frac{1}{1 - e^{i\omega}} \left( 1 - \frac{1}{z + \omega} - \frac{1}{z - \omega} \right) \right) , \quad (3.63)$$

into a vacuum and a temperature-dependent piece. Although not expressible in terms of simple functions, the temperature dependent second term is a finite, odd function of $\omega$; on the contrary, the remaining, vacuum contribution in (3.63) results divergent, and therefore so are the shifted frequencies $\tilde{\omega}_\alpha$. As a consequence, the definition of effective Hamiltonian $H_{\text{eff}}$ requires the introduction of a suitable cutoff and a renormalization procedure. This is not a surprise: the appearance of the divergences is due to the non-relativistic treatment of the two-level atoms, while any sensible calculation of energy shifts would have required the use of quantum field theory techniques [11]. In order to make $H_{\text{eff}}$ well defined we follow a simple prescription: perform a suitable temperature independent subtraction, so that the expressions in (3.62) reproduce the correct quantum field theory result, obtained by considering the external fields in the vacuum state.

The induced two-atom interaction term $H_{\text{eff}}^{(12)}$ can instead be expressed as

$$H_{\text{eff}}^{(12)} = \sum_{i,j=1}^{3} \mathcal{H}_{ij}^{(12)} \sigma_i^{(1)} \otimes \sigma_j^{(2)} , \quad (3.64)$$

where

$$\mathcal{H}_{ij}^{(12)} = \left( \cos \left[ \frac{\omega_{12}\Delta t}{2} \right] \delta_{ij} + \sin \left[ \frac{\omega_{12}\Delta t}{2} \right] \sum_{k=0}^{3} c_{ijk} n_k \right) J_+ + \left( J_0 - \cos \left[ \frac{\omega_{12}\Delta t}{2} \right] J_+ \right) n_i n_j , \quad (3.65)$$

with

$$J_+ = -i \frac{\Delta t}{4\pi} \int_{-\infty}^{\infty} d\omega \left[ \mathcal{K}^{(12)}(\omega) + \mathcal{K}^{(12)}(-\omega) \right] \cdot \text{sinc}[(\omega - \omega_1)\Delta t/2] \text{sinc}[(\omega - \omega_2)\Delta t/2] , \quad (3.66)$$

$$J_0 = -i \frac{\Delta t}{8\pi} \int_{-\infty}^{\infty} d\omega \left[ \mathcal{K}^{(12)}(\omega) + \mathcal{K}^{(12)}(-\omega) \right] \left[ \text{sinc}((\omega\Delta t/2))^2 \right] . \quad (3.67)$$
Also $K^{(12)}(\omega)$ can be split as in (3.63) into a temperature dependent term, odd in $\omega$, and a vacuum piece. Clearly, only this second contribution enters the above integrals $J_{+,0}$; it is finite (for non vanishing atom separation) and with the help of (3.57) can be explicitly computed:

$$K^{(12)}(\omega) + K^{(12)}(-\omega) = \frac{P}{2\pi^2i} \int_{-\infty}^{\infty} \frac{dz}{z + \omega} \frac{\cos \ell z}{\ell}.$$  

Inserting this result in (3.66) and (3.67), one finally obtains, again for $\ell \ll \Delta t$ (see Appendix A):

$$J_+ = -\frac{1}{2\pi \ell \omega_1 \Delta t} \cos \left(\frac{\omega_1 + \omega_2}{2}\ell\right) \sin \left(\frac{\omega_1 (\Delta t - \ell)}{2}\right),$$

$$J_0 = \frac{1}{8\pi} \left(\frac{1}{\Delta t} - \frac{1}{\ell}\right).$$

We are now ready to discuss the entanglement properties of the time evolution generated by the master equation (3.39-3.41).

### 3.3.1 Environment induced entanglement generation

We want to investigate whether entanglement can be created by dissipation at small times. We apply to the case at hand the sufficient condition (2.12) reviewed in the section 2.2 and derived in [138, 155]. In order to obtain a manageable expression for it, we first note that, without loss of generality, the unit vector $\vec{n}$ that defines the atom Hamiltonian in (3.1) can be oriented along the third axis. Further, as initial atom state we shall choose $\rho(0) = |\downarrow \rangle \langle \downarrow | \otimes |\uparrow \rangle \langle \uparrow |$, constructed out of the eigenstates of the single atom Hamiltonian, $\sigma_3 |\uparrow \rangle = \pm |\uparrow \rangle$. As a consequence, recalling (2.11), one finds that the three-dimensional vector $|u\rangle$ has components $u_i = \{1, -i, 0\}$, and further $v_i = u_i$. Then, using the explicit expressions for the elements of the Kossakowski matrix $C_{ij}^{(0)}$ and of the induced interaction Hamiltonian $H_{\text{eff}}^{(12)}$, the inequality (2.12) reduces to

$$\left(1 - \frac{\beta \omega_1}{2}\right)\left(1 + \frac{\beta \omega_2}{2}\right) < \pi^2 \beta^2 \left(4(J_+)^2 + (J_0)^2\right).$$

Notice that the l.h.s. of this expression is positive, since as discussed in the previous section, complete positivity requires $\beta \omega_n/2 \ll 1$.

As already remarked, the parameter $\Delta t$ identifies the time scale over which the presence of the environment is felt by the system of the two atoms; clearly the weaker the coupling with the environment is, the longer one needs to wait for the bath induced effects to become apparent. In the weak coupling limit approximation, one actually let
the coupling constant $\lambda$ to approach zero, so that changes in the two-atom density matrix become visible only for infinitely large $\Delta t$. In this limit however, the two integrals on the r.h.s. of (3.71) become vanishingly small, unless $\omega_1 = \omega_2$. Indeed, in the limit $\Delta t \to 0$ both integrals vanish since, for $\omega_1 \neq \omega_2$, the two functions $\text{sinc}[(\omega - \omega_1)\Delta t/2]$ and $\text{sinc}[(\omega - \omega_2)\Delta t/2]$ have disjoint supports. Thus, for atoms with unequal frequencies, the inequality can never be satisfied, and thus no entanglement is generated.

On the contrary, when the two frequencies coincide, $\omega_1 = \omega_2 = \omega$, the condition (3.71) becomes:

$$1 - \left(\frac{\beta \omega}{2}\right)^2 < \left[\frac{\sin(\omega \ell)}{\omega \ell}\right]^2 + \frac{\beta^2}{4} \left[\frac{\cos(\omega \ell)}{\ell}\right]^2.$$ (3.72)

This result generalizes the one discussed in [144], where the contribution of the environment induced interaction Hamiltonian (the second term in the r.h.s. of (3.71)) was neglected. In particular, one sees that, in this case, for any given (small) inverse temperature $\beta$, there is always an atom separation $\ell$ below which the inequality (3.72) is satisfied, and therefore entanglement created between the two atoms. This phenomenon is forbidden only for infinitely large separation or infinitely large temperature, in which case the environment induced decoherence and noisy effects dominate.

The sharp dependence of the entanglement capability of the environment on the atom frequencies in the weak coupling limit approach is however striking; it originates in the elimination of fast oscillating terms in the reduced two-atom dynamics through an ergodic average, a procedure that is justified only in the limit of a vanishing $\lambda$ and very fast decay of correlations in the environment.

Instead, if the coupling of the atoms to the bath is weak, but not infinitesimally small, environment induced changes in the atom density matrix $\rho(t)$ can be seen on finite time intervals $\Delta t$. In this case, it is the full condition (3.71) that regulates the entanglement capability of the thermal bath. One can check that indeed this inequality can be satisfied even for $\omega_1 \neq \omega_2$, and therefore that a bath made of thermal quantum fields can correlate two unequal atoms.

In order to show this, let us first note that the dissipative and Hamiltonian contributions in the r.h.s. of (2.12) can destructively interfere making the inequality harder to be satisfied and thus reducing the entanglement power of the environment. However, the Hamiltonian contribution in (3.71), being positive, can only enhance entanglement generation; this is the result of the hermiticity of the induced coupling term $H^{(12)}_{\text{eff}}$ in (3.64). One can therefore limit the considerations to a simpler inequality, in which the term $J_+^2$ is neglected; when this reduced condition is satisfied, also the full one in (3.71) will clearly be. Recalling (3.59), and keeping for simplicity only first order terms in $\ell$, the condition
for environment assisted entanglement generation reduces to:

\[
\left( 1 - \frac{\beta \omega_1}{2} \right) \left( 1 + \frac{\beta \omega_2}{2} \right) < \left[ \frac{\sin (\omega_{12} \Delta t / 2)}{\omega_{12} \Delta t / 2} \right]^2 - \left( \frac{\ell}{\Delta t} \right) \frac{\sin (\omega_{12} \Delta t)}{\omega_{12} \Delta t}. \tag{3.73}
\]

For given bath temperature and atom frequencies, this condition is satisfied provided a sufficiently small time interval \(\Delta t\) results from the coupling with the environment. Further, the smaller the atom separation is, the easier the condition of (3.73) will be met.

In the high temperature case (i.e. \(\beta\) small) and arbitrary \(\Delta t\), we have explicitly shown that this conclusion holds because of the condition (3.73). Similarly, in situations allowing a large but finite \(\Delta t\), a different approximation of the full entanglement condition (2.12) can be given; it can be obtained using techniques and procedures analogous to the ones discussed in the previous sections. Neglecting again the Hamiltonian contribution, one explicitly finds:

\[
\left( 1 - R_1 \right) \left( 1 + R_2 \right) < \frac{1}{4} \left[ \frac{\sin (\omega_{12} \Delta t / 2)}{\omega_{12} \Delta t / 2} \right]^2 \left[ \left( \frac{\omega_1}{\omega_2} \frac{R_2}{R_1} \right)^{1/2} S_1 + \left( \frac{\omega_2}{\omega_1} \frac{R_1}{R_2} \right)^{1/2} S_2 \right]^2, \tag{3.74}
\]

where

\[
R_\alpha = \frac{1 - e^{-\beta \omega_\alpha}}{1 + e^{-\beta \omega_\alpha}}, \quad S_\alpha = \text{sinc} (\omega_\alpha \ell), \quad \alpha = 1, 2. \tag{3.75}
\]

It is a further generalization of the condition discussed in [144] in the case of identical atoms, to which it reduces for \(\omega_1 = \omega_2\) and \(\Delta t\) infinite. Although valid only for large (but finite) \(\Delta t\), it can always be satisfied with suitably chosen \(\beta\) and \(\ell\). In particular, (3.74) is always true in the zero temperature case, i.e. in the limit \(\beta \to \infty\); in other words, a bath made of quantum fields in the vacuum state is always able to generate entanglement, for any finite spatial separation of the two atoms.

Finally, note that, in contrast to the situation encountered in the weak coupling limit approximation, here there is no sharp change between the regime of entanglement generation and the one of solely decoherence; the transition is smoothly regulated by the coarse graining parameter \(\Delta t\), i.e. ultimately by the strength of the coupling of the atoms to the environment.
Reconstruction of master equation parameters

This chapter is a revision of the results discussed in [163, 168, 169]. The dissipative evolution of a quantum system interacting with an environment represents a phenomenon of paramount importance in quantum information science and beyond, as it addresses a fundamental issue in quantum theory. In general a complete microscopic description of the dynamical evolution of a system coupled to the environment (or bath) is a complex many-body problem which requires the solution of a potentially infinite number of coupled dynamical equations. According to an open system approach, this issue is tackled by retaining only basic information about the environment and describing the system dynamics in terms of a master equation [85, 87]. The basic information is given by the Hamiltonian pertaining to the environment and the interaction between the environment and the system, via the spectral density [87, 102] or the correlation functions [87, 98] and the scattering matrix [87, 89], and by the initial state, e. g. via the temperature for a Gibbs state for the environment. The lack of a complete knowledge about the bath leads to master equations coefficients (MECs) which may be either unknown, or obtained from a microscopical derivation carried out within some approximation scheme. Recent investigations [132, 156, 162, 166] provide a more accurate approximation than the weak coupling limit, due to a more fine coarse grained dynamics. This approximation gives a family of Markovian master equations, parametrized by a quantity that represents the time coarse-graining that is the largest time interval unaccessible within the approximation. Again we have a phenomenological master equation with unknown coefficients. As a matter of fact it would then be highly appealing to devise a procedure allowing to retrieve the MECs starting from experimentally accessible quantities. This would in fact
both give access to otherwise unknown quantities and provide a strong indication about the validity of the adopted theoretical framework.

So far two main dynamical regimes, Markovian and non-Markovian, can usually be distinguished according to the timescale of environment dynamics (respectively shorter or longer than that of the system). We present some experimentally feasible procedures that exploit symplectic tomography and which, under the assumption of Gaussian noise, allows to reconstruct the unknown MECs. Thus, our key ingredient are Gaussian shape preserving (GSP) master equations and Gaussian states as probes. Even though the assumption of Gaussian noise might be seen as an idealization, it is actually well fitted for a significant number of models [85, 87]. Also, small deviations from Gaussianity would introduce small and controllable errors. We also note that Gaussian probes are quite straightforward to produce [52]. The advantage of using Gaussian probes to investigate a dissipative dynamics arises also within a statistical perspective. One could in fact wonder whether, due to experimental errors, a violation of the uncertainty principle might be observed. This may happen if measurements are performed on states almost saturating the Robertson-Schrödinger inequality, i.e. on the minimum uncertainty states which are pure. However, our measurements are performed on states undergoing a dissipative evolution i.e. on states typically far from being pure hence from saturating the inequality. Furthermore any additional noise of statistical origin will have the effect of moving the reconstructed state further away from the boundary, as noted in [35].

We then focus on the time evolution of the first and second cumulants of a Gaussian state, which completely determine its dynamics. Given a master equation governing the evolution of the density matrix of the system $\rho(t)$, the dynamical equations for the first two cumulants formally read

$$\langle q \rangle_t = \text{Tr}(\rho(t)q),$$
$$\langle p \rangle_t = \text{Tr}(\rho(t)p),$$
$$\Delta q^2_t = \text{Tr}(\rho(t)q^2) - \langle q \rangle_t^2,$$
$$\Delta p^2_t = \text{Tr}(\rho(t)p^2) - \langle p \rangle_t^2,$$
$$\sigma(q, p)_t = \text{Tr}\left(\rho(t)\frac{qp + pq}{2}\right) - \langle q \rangle_t\langle p \rangle_t. \quad (4.1)$$

The explicit form of these equations depends on the adopted master equation whose coefficients, in general, are either unknown or derived by means of phenomenological assumptions. Inserting into equation (4.1) the explicit expression of $\rho(t)$ and then solving for the MECs, allows to write these coefficients (or the differential equations they satisfy) as a function of the first two cumulants of a Gaussian probe. Hence, by measuring these two quantities, one can gain indirect experimental information about the MECs. To this purpose, symplectic quantum tomography arises naturally as a key tool to perform the
required measurements. In particular we will use the symplectic transform [18], that finds its natural implementation in experiments with massive particles, as for example those to detect the longitudinal motion of neutrons [32] and to reconstruct the transverse motional states of helium atoms [27]. We also note that the symplectic transform is equivalent to the Radon transform [40] which is experimentally implemented by homodyne detection in the context of quantum optics [34].

The tomographic analysis is based on a probabilistic approach towards physical system investigation, allowing to reconstruct the state or some other properties of classical and quantum physical systems [18]. In particular, its key ingredient is the Radon transform [19]. Given the phase-space of the system, this invertible integral transform allows to retrieve the marginal probability densities of the system, i.e. the probability density along straight lines. However, while in the classical regime the state of the system can be fully described by means of a probability distribution on its phase space, this is no longer the case of quantum systems. Indeed, due to the Heisenberg uncertainty relation, it is not possible to write a probability distribution as a function of both momentum and position. In this case, the Wigner function [21, 25] can be employed as a quantum generalization of a classical probability distribution. This function is a map between phase-space functions and density matrices. Even if the Wigner function can take on negative values, by integrating out either the position or the momentum degrees of freedom, one obtains a bona fide probability distribution for the conjugated variables. From this point of view, the Wigner function corresponding to a quantum state can be regarded as a quasi-probability distribution and interpreted as a joint probability density in the phase space [29]. See appendix B for some details.

4.1 Cumulants reconstruction through tomography

In this section we introduce a procedure based on symplectic tomography in order to measure the first and second cumulants of a Gaussian wave packet at an arbitrary time \( t \). This will allow us to indirectly measure the MECs, them being functions of the evolved cumulants at an arbitrary time (see next sections). The tomographic approach is very useful when dealing with phenomenological GSP master equations, as the dependence of the MECs from the physical parameters may be unknown. In fact, the dynamical evolution of a Gaussian state is completely determined by the evolution of its first and second order cumulants, which are measurable quantities. The unknown master equation coefficients enter the dynamical equations of the cumulants, hence can be retrieved by simple inversion, once the latter are measured. The cumulants can be obtained by using symplectic tomography.
Indeed our aim is further supported by recent work [33, 38, 39], in which it has been proved that it is in principle possible to make tomographic measurements of the probability densities associated to every quadrature in phase space (for example in quantum optics it could be realized by means of homodyne detection). Other methods to measure the covariance matrix of Gaussian states have been discussed in [35]. However in this case the amount of required measurements is much higher, the focus being on the reduction of experimental errors.

We now introduced a procedure that allows to relate the cumulants to points on tomograms, via a small number of detections. Tomograms \( \varpi(X, \mu, \nu) \) are the integrals of the Wigner function of a quantum state along one direction \( X - \mu q - \nu p = 0 \) of the quantum phase-space \((q, p)\). See appendix B for some details on the Wigner function and the symplectic tomography. In the following, we will refer to the mentioned procedure as the tomograms-cumulants (T-C) procedure. Let us consider the tomograms corresponding to a Gaussian state and two different directions in phase space, i.e. to two different couples of parameters \((\mu, \nu)\), e.g. \( X = q \) and \( X = p \). These lines in phase-space are associated respectively to the position and momentum probability distribution functions:

\[
\varpi(X, 1, 0) = \frac{1}{\Delta q_t \sqrt{2\pi}} \exp \left[ -\frac{(X - \langle q \rangle_t)^2}{2\Delta q_t^2} \right],
\]

\[
\varpi(X, 0, 1) = \frac{1}{\Delta p_t \sqrt{2\pi}} \exp \left[ -\frac{(X - \langle p \rangle_t)^2}{2\Delta p_t^2} \right].
\]

From equations (4.2)-(4.3) we see that the tomographic map depends only on a single parameter \( X \). This reduces the dimensionality of the problem with respect to the Wigner function, that is a function of both \( p \) and \( q \). The lines selected by the choices \((\mu, \nu) = (1, 0)\) and \((\mu, \nu) = (0, 1)\) correspond to tomograms depending on the time average and variance respectively of position and momentum. In order to determine the latter quantities we have to invert equations (4.2) and (4.3) for different values of \( X \), i.e. for a given number of points to measure along a tomogram. Thus, our first goal is to determine the number of tomograms required to measure the cumulants of our Gaussian state.

To answer this question, we first focus on the direction \( \mu = 1, \nu = 0 \). In figure 4.1 we plot the Wigner function of our system at a generic time \( t \) and some straight lines along the considered direction. In figure 4.2 we plot the GSP tomogram defined by equation (4.2). Inverting equation (4.2), we obtain:

\[
(X - \langle q \rangle_t)^2 = 2\Delta q_t^2 \ln \frac{1}{\varpi(X, 1, 0) \Delta q_t \sqrt{2\pi}}.
\]
Using the value of the tomogram $\varpi(0, 1, 0)$ we can get $\langle q \rangle_t$ as a function of $\Delta q_t$:

$$
\langle q \rangle_t = \pm \Delta q_t \sqrt{\frac{2 \ln 1}{\varpi(0, 1, 0) \Delta q_t} \sqrt{2\pi}}.
$$

(4.5)

If we know the sign of $\langle q \rangle_t$, then we need only the value of the tomogram $\varpi(0, 1, 0)$ to get $\langle q \rangle_t$, otherwise we need another point. Using equation (4.5), equation (4.2) becomes an equation for $\Delta q_t$ only, and it can be rewritten as

$$
2\Delta q_t^2 \ln \frac{1}{\varpi(X, 1, 0) \Delta q_t} \sqrt{2\pi} = \left( X \mp \Delta q_t \sqrt{2 \ln \frac{1}{\varpi(0, 1, 0) \Delta q_t} \sqrt{2\pi}} \right)^2.
$$

(4.6)

This equation is transcendental, therefore we will solve it numerically. We can graphically note in figure 4.3 that for each $X$ and corresponding $\varpi(X, 1, 0)$ there may be two values of $\Delta q_t$ satisfying the previous equation. In order to identify one of the two solutions, it is enough to consider two points, $\{(X_1, \varpi(X_1, 1, 0))\}$ and $\{(X_2, \varpi(X_2, 1, 0))\}$, and to choose the common solution for the variance. This is made clear by figure 4.3, where the ratio between right and left side of equation (4.6) for two different values of $X$ is plotted. The common solution (i.e. when both ratios are equal to 1) is labeled $\overline{\Delta q_t}$. As a consequence,

![Figure 4.1: Wigner function, $W(q, p, t)$, of equation (B.8) and some straight lines along the direction $\mu = 1$ and $\nu = 0$ on the plane $qp$. $\Delta q_t^2 \Delta p_t^2 - \sigma(q, p)_t^2 = 0.64 \Delta q_t^2 \Delta p_t^2$. $W_{\mathcal{M}} = \frac{1}{2\pi \Delta q_t^2 \Delta p_t^2 - \sigma(q, p)_t^2}$.

whether we know or not the sign of the average $\langle q \rangle_t$, we need three or four points to determine $\langle q \rangle_t$ and $\Delta q_t$ in equation (4.2). Analogously, we need other three or four points for $\langle p \rangle_t$ and $\Delta p_t$ in equation (4.3).
4.1 - Cumulants reconstruction through tomography

Figure 4.2: Tomogram, $\varpi(X, 1, 0)$, of equation (4.2) for the direction $\mu = 1$ and $\nu = 0$.

Figure 4.3: The ratio between right and left side of equation (4.6) for two different values of $X$ with $\mu = 1$ and $\nu = 0$ is plotted as a function of $\Delta q_t / \langle q \rangle_t$. Values used: $\langle q \rangle_t = 3$ and $X_1 = 4.5$ (continuous line) and $X_2 = 2.5$ (dashed line). The values of $\varpi(X, 1, 0)$ are computed using $\Delta q_t = 1$ to simulate what one would get experimentally. Continuous line shows how equation (4.6) with $X_1 = 4.5$ and $\varpi(4.5, 1, 0)$ can be satisfied (ratio=1) by two values of $\Delta q_t$. The comparison with a second case with $X_2 = 2.5$ allows to determine which value of $\Delta q_t$ is the right one.
Let us now compute the covariance $\sigma(q, p)_t$. To this purpose, we consider the tomogram:

$$\varpi\left(X, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right) = \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{\Delta q_t^2 + \Delta p_t^2 + 2\sigma(q, p)_t}} \exp\left[-\frac{\left(X - \langle q_t \rangle + \langle p_t \rangle\right)^2}{\Delta q_t^2 + \Delta p_t^2 + 2\sigma(q, p)_t}\right].$$

(4.7)

This is a Gaussian whose average value is already determined. Indeed, according to the previous steps, we need two more points of this tomograms to determine the spread $(\Delta q_t^2 + \Delta p_t^2)/2 + \sigma(q, p)_t$, from which we can retrieve $\sigma(q, p)_t$.

Hence, we have shown that by means of eight or at most ten points belonging to three tomograms, the first and second order momenta of a Gaussian state can be measured at an arbitrary time $t$. One can then use these measured cumulants in order to infer the master equation parameters describing the system under investigation. We note also that we can reasonably infer that the number of tomograms needed to reconstruct the system density operator is minimized by employing Gaussian wave packets as a probe. Indeed these states have minimum uncertainty, and are the only states having positive Wigner function [2].

### 4.1.1 An alternative procedure

Here we propose an alternative time-dependent procedure to compute the second cumulants of a Gaussian state, by means of tomograms, given the knowledge of the first cumulants time evolution. To this purpose we need to consider the following three tomograms:

$$\varpi_1 = \varpi(\langle p \rangle_t, 0, 1) = \frac{1}{\sqrt{2\pi}\Delta p_t},$$

$$\varpi_2 = \varpi(\langle q \rangle_t, 1, 0) = \frac{1}{\sqrt{2\pi}\Delta q_t},$$

$$\varpi_3 = \varpi\left(\frac{\langle p \rangle_t + \langle q \rangle_t}{\sqrt{2}}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right) = \frac{1}{\sqrt{2\pi} \sqrt{\Delta q_t^2/2 + \Delta p_t^2/2 + \sigma(q, p)_t}}.$$  

(4.8)

Inverting the previous equations one can infer $\Delta q_t$, $\Delta p_t$, and $\sigma(q, p)_t$, from the knowledge of $\varpi_1$, $\varpi_2$ and $\varpi_3$. However, this procedure presents two drawbacks. In fact, the evolved
averaged values $\langle q \rangle_t$ and $\langle p \rangle_t$ are required and we need tomograms evaluated on time-dependent variables. These problems do not arise in the time-independent procedure, based only on tomograms for which no a priori knowledge on the Gaussian state is required. Nevertheless, in this alternative time-dependent scheme only three tomograms are required.

4.2 Markovian master equations

In this section, we will focus on the class of Markovian, time-independent, GSP master equations. Equation (1.23) reads \[95, 116, 117\]

\[
\frac{d\rho(t)}{dt} = -\frac{i}{\hbar} [H_0, \rho(t)] - \frac{i(\lambda + \delta)}{2\hbar} [q, \rho(t)p + p\rho(t)] + \\
\frac{i(\lambda - \delta)}{2\hbar} [p, \rho(t)q + q\rho(t)] - \frac{D_{pp}}{\hbar^2} [q, [q, \rho]] - \frac{D_{qq}}{\hbar^2} [p, [p, \rho]] + \\
+ \frac{D_{qp}}{\hbar^2} ([q, [p, \rho]] + [p, [q, \rho]]).
\]

(4.9)

The time-evolved cumulants (1.33)-(1.38) can be straightforwardly derived \[95, 116\], allowing to obtain them as a function of the MECs $\lambda, D_{qq}, D_{pp}, D_{qp}$. We now show how to invert these relations in order to express the parameters $\lambda, D_{qq}, D_{pp}, D_{qp}$ as a function of the evolved cumulants at an arbitrary time. The equations (1.33) now read

\[
\begin{align*}
\langle q \rangle_t &= e^{-\lambda t} \left[ \langle q \rangle_0 \left( \cosh \eta t + \frac{\delta}{\eta} \sinh \eta t \right) + \langle p \rangle_0 \frac{1}{m \eta} \sinh \eta t \right] \\
\langle p \rangle_t &= e^{-\lambda t} \left[ -\langle q \rangle_0 \frac{m \omega^2}{\eta} \sinh \eta t + \langle p \rangle_0 \left( \cosh \eta t - \frac{\delta}{\eta} \sinh \eta t \right) \right].
\end{align*}
\]

(4.10)

where $\eta^2 = \delta^2 - \omega^2$. If $\eta^2 < 0$ we can set $\eta = i\Omega$ and the previous equations hold again with trigonometric instead of hyperbolic functions. The coefficient $\lambda$ can then be obtained by inverting equations (4.10). The diffusion coefficients can be retrieved from the second cumulants (1.38)

\[
X(t) = (Te^{K^t}T)X(0) + TK^{-1}(e^{K^t} - 1)TD,
\]

(4.11)

where
\[ T = \frac{1}{2\eta} \begin{pmatrix} \delta + \eta & \delta - \eta & 2\omega \\ \delta - \eta & \delta + \eta & 2\omega \\ -\omega & -\omega & -2\delta \end{pmatrix}, \]
\[ K = \begin{pmatrix} -2(\lambda - \eta) & 0 & 0 \\ 0 & -2(\lambda + \eta) & 0 \\ 0 & 0 & -2\lambda \end{pmatrix}. \quad (4.12) \]

From the invertibility of matrices \( T \) \((T^2 = 1)\) and \( \tilde{K} = K^{-1}(e^{Kt} - 1) \) (invertible for bounded \( K \) also if some of its eigenvalues are 0), we can derive the expression of \( D_{qq} \), \( D_{pp} \) and \( D_{qp} \) using the equation (4.11):

\[ D = T\tilde{K}^{-1}T \left( X(t) - (Te^{Kt})X(0) \right), \]

\[ \tilde{K} = K^{-1}(e^{Kt} - 1) = \]
\[ = \begin{pmatrix} \frac{1 - e^{-2(\lambda - \eta)}}{2(\lambda - \eta)} & 0 & 0 \\ 0 & \frac{1 - e^{-2(\lambda + \eta)}}{2(\lambda + \eta)} & 0 \\ 0 & 0 & \frac{1 - e^{-2\lambda}}{2\lambda} \end{pmatrix}. \quad (4.14) \]

We emphasize that the time \( t \) at which we are considering the cumulants is completely arbitrary. For instance, the expression of the coefficients \( D_{qq}, D_{pp}, D_{qp} \) in terms of the asymptotic second cumulants and the parameter \( \lambda \) reads:

\[ D_{qq} = (\lambda - \delta)\Delta q_\infty^2 - \frac{1}{m}\sigma(q, p)_\infty, \]
\[ D_{pp} = (\lambda + \delta)\Delta p_\infty^2 + m\omega^2\sigma(q, p)_\infty, \]
\[ D_{qp} = \frac{1}{2} \left( m\omega^2\Delta q_\infty^2 - \frac{1}{m}\Delta p_\infty^2 + 2\lambda\sigma(q, p)_\infty \right). \quad (4.15) \]

Equations (4.10) and (4.11) give the MECs in terms of the cumulants at time \( t \). Applying the T-C procedure we can measure all the cumulants at the same time with at most ten tomographic detections, reconstructing the MECs. We should strongly stress the very small number of needed detections.
4.3 Convolutionless non-Markovian master equations

This result leads to some interesting applications. Once retrieved the unknown master equation coefficients, it is possible to compute the dynamical evolution of any physical quantity whose analytical expression is known. The indirect-measurement scheme we propose could be then employed to make predictions on system loss of coherence due to the external environment. In order to perform this kind of analysis one can consider some quantities such as the spread and the coherence length in both position and momentum [133], provided their analytical expressions are available for an arbitrary time $t$ (e.g. see [154]). Working in the coherent state representation, the evolution of the system of interest from an arbitrary initial state can be in principle predicted. Therefore, it is possible to perform the proposed indirect analysis of the decoherence processes. For example, if we consider an initial Schrödinger-cat state, highly interesting due to its potentially long-range coherence properties and its extreme sensitivity to environmental decoherence [127], we can re-write it as a combination of four Gaussian functions. Therefore, due to the linearity of the master equation, it can be possible to derive analytically the state evolution and to analyze its loss of coherence by means of the procedure we propose.

4.3 Convolutionless non-Markovian master equations

When dealing with a time-dependent generator one can face two, in principle distinct, kinds of problems. On one hand, taking for granted the functional form of the dissipative generator, one might be interested in retrieving the time-independent parameters (TIPs) which characterize it, as for example the system-bath coupling, temperature and bath frequency cut-off. On the other hand, one might be interested in the more general problem of reconstructing the functional form of the dissipative generator itself. This might be the case either because the time-dependence of the dissipative generator is completely unknown or because one wants to test the validity of the theoretical assumptions at the basis of the dissipative model. Indeed, even if we assumed a wrong time-dependence for the MECs, we could find numerical values for the TIPs that almost fit with the experimental data. A complete reconstruction is more accurate. Moreover, it may serve as a check for the assumed time-dependence, once we have determined the TIPs consecutively implementing the two reconstructions. We propose two alternative procedures aiming at reconstructing the TIPs or the MECs by means of symplectic tomography.

**Integral approach** Here we introduce an approach based on formal integration of the dynamical equations (1.33) and (1.38). We can rewrite the latter equations as
\[ \Lambda(t) \equiv \int_0^t dt' \lambda(t') = \ln \left( \frac{\tilde{S}_j(0)}{\tilde{S}_j(t)} \right), \]  
(4.16)

where the suffix \( j = 1, 2 \) labels the two components of the vector \( \tilde{S}(t) \), and

\[ \int_0^t dt' e^{-2\Lambda(t,t')} e^{i(t-t')\mathcal{R}} D(t') = X(t) - e^{i\mathcal{R}} e^{-2\Lambda(t)} X(0), \]  
(4.17)

where \( \Lambda(t, t') = \int_{t'}^t dt'' \lambda(t'') \).

The right hand side of both equations involves experimental inputs (\( \tilde{S}(t) \) and \( X(t) \)) and known Hamiltonian parameters (\( M \) and \( R \)). The left hand sides can be regarded as functions of the MECs we want to reconstruct. Hence the set of MECs can be in principle obtained by inverting these relations. From equation (4.16) the friction coefficient can be retrieved. Afterward, we exploit this reconstruction to get the diffusion coefficients from equation (4.17). Unfortunately, in general, an analytical inversion of (4.16) and (4.17) may represent a highly involved task. In facts, even if we assume a known MECs time-dependence, we could be unable to either compute analytically the integrals on the right hand side of (4.16) and (4.17), or to invert the equations or even both. All these problems can be anyway overcome by resorting to numerical computation.

We note that the integral approach is also feasible in case of time-dependent Hamiltonian parameters (i.e. \( m(t) \), \( \omega(t) \), \( \delta(t) \)) as long as the generator remains GSP. In general this kind of generators requires a numerical evaluation of the integrals in equations (1.28) and (1.29).

**Differential approach** The tomographic T-C procedure allows us to measure not only the cumulants of a given Gaussian state but also their first time derivatives. Indeed, we can estimate the derivative through the incremental ratio by measuring each cumulant at two different times \( t \) and \( t + \delta t \). For instance

\[ \frac{d}{dt} \Delta q_t^2 \sim \frac{\Delta q_{t+\delta t}^2 - \Delta q_t^2}{\delta t}, \]  
(4.18)

where the amount of time \( \delta t \) is defined as the smallest time interval which allows to experimentally distinguish two different values of the given cumulant. Once we substitute derivatives with their approximations, the two sets of equations (1.28) and (1.29) are not differential anymore. Being the cumulants and their approximate derivatives at given times experimental inputs, the two sets of equations (1.28) and (1.29) reduce to algebraic equations which can always be solved, at least numerically, for retrieving the MECs \( \lambda(t) \).
and $D(t)$ (and in case $m(t)$, $\omega(t)$, $\delta(t)$) or the TIPs. Hence from equations (1.28) and (1.29) we obtain the desired experimentally accessible estimations for the MECs

$$\lambda_{\text{ex}}(t) \approx \delta + \frac{1}{\langle q \rangle_t} \left( \frac{1}{m} \langle p \rangle_t - \frac{\langle q \rangle_{t+\delta t}^2 - \langle q \rangle_t^2}{\delta t} \right) \approx$$

$$\approx -\delta - \frac{1}{\langle p \rangle_t} \left( m \omega^2 \langle q \rangle_t + \frac{\langle p \rangle_{t+\delta t}^2 - \langle p \rangle_t^2}{\delta t} \right).$$

(4.19)

$$D_{qq}^{\text{ex}}(t) \approx (\lambda(t) - \delta) \Delta q_t^2 - \frac{1}{m} \sigma(q, p)_t + \frac{\Delta q^2_{t+\delta t} - \Delta q_t^2}{2\delta t},$$

(4.20)

$$D_{pp}^{\text{ex}}(t) \approx (\lambda(t) + \delta) \Delta p_t^2 + m \omega^2 \sigma(q, p)_t + \frac{\Delta p^2_{t+\delta t} - \Delta p_t^2}{2\delta t},$$

(4.21)

$$D_{qp}^{\text{ex}}(t) \approx \frac{m}{2} \omega^2 \Delta q_t^2 - \frac{1}{2m} \Delta p_t^2 + \lambda(t) \sigma(q, p)_t + \frac{\sigma(q, p)_{t+\delta t}^2 - \sigma(q, p)_t^2}{2\delta t}.$$ 

(4.22)

Due to this simplification, this approach is also suitable when dealing with more complicated generators than the one considered here in equation (1.23), e.g. when the Lamb shift contribution is explicitly taken into account such that the Hamiltonian parameters become time-dependent ($m(t)$, $\omega(t)$, $\delta(t)$), as long as the generator remains GSP. We note that the two sets (1.28) and (1.29) consist of five equations which must be fulfilled at any chosen time. Therefore, considering them at different times, we can derive a system made up of an arbitrary number of equations. Otherwise, we can consider the evolution equations for higher order cumulants, e.g. $\text{Tr}(\rho(t)q^3)$ and $\text{Tr}(\rho(t)p^3)$. This would not increase the number of experimental measurements, since the higher order moments and cumulants of Gaussian states are completely determined by the first and the second cumulants. The number of equations must then be chosen as the minimum amount of equations needed to uniquely determine the MECs or the TIPs.

In the following, we will show how to apply the two procedures to a benchmark model to reconstruct either MECs and TIPs and we will discuss the differences and their different advantages.

### 4.3.1 A benchmark model

Here we refer to a specific model of a quantum Brownian particle discussed in [143]. We will show how to apply in this specific case the two general procedures presented in the previous section. The model consists of an Ohmic reservoir made of harmonic oscillators, linearly coupled to a single harmonic oscillator of frequency $\omega$ (our system particle) through the coupling constant $\alpha$, with a Lorentz-Drude cut-off [87] $\omega_c$ and at temperature $T$. Starting from a superoperatorial version of the Hu-Paz-Zhang master
equation [122], in the weak-coupling limit (up to the second order in $\alpha$) and using a secular approximation (also called rotating wave approximation or ergodic average, i.e. an average over the rapidly oscillating terms), a generator of the form of equation (1.23) can be obtained [143] with the following coefficients:

$$\begin{align*}
\delta &= 0, \quad D_{qp} = 0, \quad \frac{m\omega D_{qq}}{\hbar} = \frac{D_{pp}}{\hbar m\omega} = \frac{\Lambda(t)}{2}, \\
\lambda(t) &= \frac{\alpha^2 \omega^2 \omega}{\omega_c^2 + \omega^2} \left( 1 - e^{-\omega_c t} \left[ \cos(\omega t) + \frac{\omega_c}{\omega} \sin(\omega t) \right] \right), \\
\Lambda(t) &= \frac{2\alpha^2 \omega^2}{\omega_c^2 + \omega^2} \frac{kT}{\hbar} \left( 1 - e^{-\omega_c t} \left[ \cos(\omega t) - \frac{\omega}{\omega_c \omega} \sin(\omega t) \right] \right),
\end{align*}$$

the last having this form for high temperatures $T$. This master equation is of Lindblad-type when the coefficients $\Lambda(t) \pm \lambda(t)$ are positive at all times. The border between the Lindblad-type and the non-Lindblad-type master equations as a function of the temperature $T$ and the frequency cutoff $\omega_c$ has been analyzed in [143]. As Gaussianity is preserved, by choosing a Brownian particle initially in a Gaussian state, the T-C procedure can be employed at any time. The coefficients $\lambda(t)$ and $\Lambda(t)$ reach stationary values for $t \gg 1/\omega_c$:

$$\lambda(t) \rightarrow \frac{\alpha^2 \omega^2 \omega}{\omega_c^2 + \omega^2}, \quad \Lambda(t) \rightarrow \frac{2\alpha^2 \omega^2}{\omega_c^2 + \omega^2} \frac{kT}{\hbar}. \quad (4.25)$$

In this specific model, the unknown TIPs are the coupling constant $\alpha$, the temperature $T$ and the frequency cut-off $\omega_c$. Usually, when studying quantum Brownian motion, one assumes $\omega_c/\omega \gg 1$, corresponding to a Markovian reservoir, with $\omega_c \rightarrow \infty$. In this limit, the thermalization time [143] is inversely proportional to the coupling strength, while for an out-of-resonance engineered reservoir with $\omega_c/\omega \ll 1$ (i.e. highly non Markovian), the thermalization process is slowed down. Microscopic derivations of Master Equations usually give a time dependent renormalization of Hamiltonian parameters ($m$, $\omega$, $\delta$). However, they are negligible for this benchmark model in the considered limits.

### 4.3.2 Time independent coefficients

In this section, we assume that the MECs $\lambda(t)$, $D_{qq}(t)$, $D_{pp}(t)$ and $D_{qp}(t)$ have a known functional form. This implies that the non-Markovian master equation with certain expressions for the MECs has been previously derived within some approximation scheme (e.g. by means of a microscopic derivation and subsequent dynamical assumptions). The time-dependent MECs are thus function of a set of time-independent parameters (TIPs) whose value is a priori unknown.
We now apply the integral and the differential approaches previously introduced to the benchmark model discussed in 4.3.1.

**Integral approach: benchmark model** Here we apply the integral procedure to the benchmark model. In this case the left hand side of (1.32) is not simply analytically computable. Thus we must use (4.16) to reconstruct all the TIPs it involves, and then numerically integrate the left hand side of (1.32).

The left hand side of (4.16) is given by the theoretical value

\[
\Lambda(t) = \frac{\alpha^2 \omega_c^2 \omega^2}{(\omega_c^2 + \omega^2)^2} \left\{ \frac{\omega^2}{\omega^2} + \frac{\omega^2}{\omega^2} - \frac{2 \omega_c}{\omega} \right. \\
\left. + e^{-\omega_c t} \left[ 2 \frac{\omega_c}{\omega} \cos(\omega t) + \frac{\omega_c^2 - \omega^2}{\omega^2} \sin(\omega t) \right] \right\}. \tag{4.26}
\]

By using (4.16) and (4.26) we obtain the coupling strength \(\alpha\) as a transcendental function of the cutoff \(\omega_c\):

\[
\alpha^2 = \ln \left( \frac{\hat{S}_j(0)}{\hat{S}_j(t)} \right) \left( \frac{\omega_c^2 + \omega^2}{\omega_c^2 \omega^2} \right)^2 \left\{ \frac{\omega^2}{\omega^2} + \frac{\omega^2}{\omega^2} - \frac{2 \omega_c}{\omega} \right. \\
\left. + e^{-\omega_c t} \left[ 2 \frac{\omega_c}{\omega} \cos(\omega t) + \frac{\omega_c^2 - \omega^2}{\omega^2} \sin(\omega t) \right] \right\}^{-1}, \tag{4.27}
\]

where the ratio \(\hat{S}_j(0)/\hat{S}_j(t)\) is the experimentally measurable quantity. Hence, by performing two distinct measurements of this ratio we can evaluate (4.27) at two different times. We thus obtain a system of two numerically solvable equations, which allows us to retrieve the time-independent parameters \(\alpha\) and \(\omega_c\). To provide a concrete evidence of the validity of this procedure, we show two numerical examples in figure 4.4. Indeed we retrieve the TIP \(\alpha^2 = 0.01\) in two different dynamical regimes, respectively close to the Markovian (figure 4.4(a)) and non-Markovian (figure 4.4(b)) limit.

The last missing parameter is the temperature \(T\) entering the coefficient \(\Delta(t)\). By using (1.32), we obtain the following equation:

\[
\frac{kT}{\hbar \omega} = \left[ X_j(t) - e^{-2 \int_0^t \lambda(t') \, dt'} \right] \left( e^{\lambda(t)} X(0) \right) \frac{\omega_c^2 + \omega^2}{2 \alpha^2 \omega^3} \left( \int_0^t dt' e^{-2 \int_0^{t'} \lambda(t'')} \right) \cdot \sum_{l=1}^2 \left( e^{l(t-t')} \right)_{j,l} \left( 1 - e^{-\omega_c t} \left[ \cos(\omega t') - \frac{\omega}{\omega_c} \sin(\omega t') \right] \right)^{-1}. \tag{4.28}
\]
Figure 4.4: We show how to indirectly measure the time independent parameters $\omega_c$ and $\alpha^2$, in two different regimes respectively close to the Markovian (figure 4.4(a)) and non-Markovian dynamics (figure 4.4(b)). Each line refers to an experimental measure of $\ln \left( \tilde{S}_j(0)/\tilde{S}_j(t) \right)$ at a specific time $\omega t$. In both regimes, the time independent parameter values are found at the intersection of the two lines. In the example close to the Markovian regime (figure 4.4(a)) if we measure $3.03 \cdot 10^{-3}$ at $\omega t_1 = 0.5$ (solid line) and $9.70 \cdot 10^{-2}$ at $\omega t_2 = 10$ (dashed line), we retrieve $\alpha^2 = 0.01$ and $\omega_c/\omega = 10$. Analogously, for the example close to the non Markovian regime (figure 4.4(b)) if we measure $4.55 \cdot 10^{-5}$ at $\omega t_1 = 0.5$ (solid line) and $1.84 \cdot 10^{-2}$ at $\omega t_2 = 10$ (dashed line), we retrieve $\alpha^2 = 0.01$ and $\omega_c/\omega = 0.5$.

where $j = 1, 2, 3$ denotes the vector components, and $(e^{(t-t')R})_{jj}$ are the matrix elements of the matrix $e^{(t-t')R}$. The explicit expression of the integral appearing on the first line of (4.28) is provided in (4.26). In general, the remaining integrals are not analytically computable. However, since all the parameters involved have been previously reconstructed, these integrals can be computed numerically.

**Number of tomographic measurements** Let us now explicitly compute the number of tomograms needed to apply the integral approach to the benchmark model. To reconstruct $\alpha$ and $\omega_c$ each of the quantities $\tilde{S}_{1,2}(t) = (e^{-tM}\mathcal{S}_{jj})_{1,2}(t)$ must be measured once but not at the same time, as shown by (4.27) and figure 4.4. Each $\tilde{S}_{1,2}(t)$ is a function of the first cumulants of both position and momentum. According to the T-C procedure, the reconstruction of a first cumulant involves at most four tomographic points. Thus $\alpha$ and $\omega_c$ can be obtained via, in the worst case, sixteen measures. Furthermore, being $e^{-tM}$ an orthogonal transformation, $e^{-tM}\mathcal{S}_{jj}(t)$ is by itself a first cumulant along a time-dependent direction in phase-space. Hence, if time-dependent tomographic measurements (i.e. measurements in a frame rotating as $e^{-tM}$) are allowed, the number of required tomograms decreases to eight, as we would only need a single first cumulant ($\tilde{S}_1(t)$ or $\tilde{S}_2(t)$).

To measure $T$ we should evaluate one of the second cumulants at a given time. Following the T-C procedure this amounts to two tomographic points. However, the required
second cumulant has been already obtained when reconstructing the corresponding first cumulant, hence the temperature can be retrieved without further effort. This argument also holds for time-dependent measurements. In fact, the reconstruction formula (4.28) has been derived from (1.32), which can be recast in terms of the variances in the rotating frame. The temperature can be then obtained using the variance along the same time-dependent direction of the measured first cumulant.

In conclusion, in order to implement the integral approach in the benchmark model, according to whether we can perform time-dependent measurements or not, we need eight or at most sixteen tomographic points.

**Differential approach: benchmark model** We now skip to the differential procedure. In (4.23) the dependence on $\alpha^2$ and $\omega_c$ is factorized, hence using (1.28) one gets

$$
\alpha^2 \sim \frac{1}{\langle q \rangle_t} \left( \frac{\langle p \rangle_t - \langle q \rangle_t}{\delta t} \right) \frac{\omega_c}{\omega} \left( 1 - e^{-\omega_c t} \left[ \cos(\omega t) + \frac{\omega_c}{\omega} \sin(\omega t) \right] \right)^{-1}.
$$

(4.29)

Since $\alpha^2$ and $\omega_c$ are time-independent, they can be determined by solving (4.29) for two different times $t_1$ and $t_2$, and looking at the intersection of the two different solutions. This procedure requires to measure the cumulants $\langle q \rangle_t$, $\langle q \rangle_{t+\delta t}$, and $\langle p \rangle_t$ at $t = t_1, t_2$ and to solve (4.29) numerically, as shown in figure 4.5. In other words, the first two TIPs, $\alpha^2$ and $\omega_c$, can be determined by measuring six quantities. As for the integral procedure, we retrieve the TIP $\alpha^2 = 0.01$ in two cases, corresponding to the extreme dynamical regimes, Markovian $\omega_c/\omega \gg 1$ in figure 4.5(a), and the highly non-Markovian, $\omega_c/\omega \ll 1$, in figure 4.5(b).

Again, we are left with determining the temperature $T$ appearing in (4.23). To this end, we consider one of the equations of system (1.32), e.g. that for $\langle \Sigma \rangle_m$ we reformulate as:

$$
\frac{kT}{\hbar \omega} \sim \frac{1}{\hbar} \left[ m \left( \frac{\Delta q^2_{t+\delta t} - \Delta q^2_t}{\delta t} + 2\lambda(t)\Delta q_t^2 \right) - 2\sigma(q, p) \right].
$$

$$
\frac{\omega^2 t + \omega^2}{2\alpha^2 \omega_c^2} \left( 1 - e^{-\omega_c t} \left[ \cos(\omega t) - \frac{\omega_c}{\omega} \sin(\omega t) \right] \right)^{-1}. \tag{4.30}
$$

Equation (4.30) allows to retrieve $T$ once the cumulants $\Delta q^2_t, \Delta q^2_{t+\delta t}$ and $\sigma(q, p)_t$ are measured and both $\alpha^2$ and $\omega_c$ are known from the previous steps. As an example, at time $\omega t = 1$ the same value of temperature, $kT = 10\hbar \omega$ may correspond to different measured values of the quantity
Figure 4.5: As for the integral approach we obtain an indirect measure of the time-independent parameters $\omega_c$ and $\alpha^2$, both in the almost Markovian (figure 4.5(a)) and in the almost non-Markovian regime (figure 4.5(b)). Each line refers to an experimental measure of $\langle q(t) - q(t-\delta t) \rangle$ at a specific time $\omega t$. In the almost Markovian example shown in figure 4.5(a), if we obtain $9.52 \cdot 10^{-3}$ at $\omega t_1 = 0.5$ (solid line) and $9.90 \cdot 10^{-3}$ at $\omega t_2 = 10$ (dashed line), we retrieve $\alpha^2 = 0.01$ and $\omega_c/\omega = 10$. Analogously, for the almost non-Markovian case in figure 4.5(b), if we measure $2.59 \cdot 10^{-4}$ at $\omega t_1 = 0.5$ (solid line) and $2.01 \cdot 10^{-3}$ at $\omega t_2 = 10$ (dashed line), we retrieve $\alpha^2 = 0.01$ and $\omega_c/\omega = 0.5$.

\[
\frac{1}{\hbar} \left[ m \left( \frac{\Delta q_i^2}{\delta t} - \frac{\partial}{\partial t} \langle q_i \rangle \right) + 2\lambda(t)\Delta q_i^2 - 2\sigma(q, p) \right], \quad (4.31)
\]

according to different dynamical regimes. For instance, by setting $\omega_c/\omega = 10$ close to the Markovian regime one would measure 0.198 as output whereas, setting $\omega_c/\omega = 0.5$ close to the non-Markovian case, the output corresponding to the same $T$ is 0.067.

**Number of tomographic measurements** We now count the number of tomographic measurements to apply the differential approach to this example. The reconstruction of both $\alpha$ and $\omega_c$ is based on (4.29), which must then be evaluated at two different times $t_1$ and $t_2$, see figure 4.5. Each evaluation of (4.29) requires two measurements of the average position, at times $t_i$ and $t_i + \delta t$, and one of the average momentum at time $t_i$, where $i = 1, 2$. This implies reconstructing six first cumulants. As each first cumulant requires four tomographic points, the total amount of needed tomographic points amounts to twenty-four.

The reconstruction of temperature $T$ is based on equation (4.30). We need the variance of the position at time $t$ and at time $t + \delta t$, and the covariance of $q$ and $p$ at time $t$. However, according to the T-C procedure, the variance is required to obtain the position average. This implies that the second cumulant has been already measured during the previous
reconstruction, and there is no need to measure it again. Retrieving the covariance requires two more tomographic points.

In conclusion, in order to implement the differential approach in the benchmark model, we need twenty-six tomograms.

Comparison between the two approaches Let us now briefly compare the two procedures described in this section. On one hand the differential approach requires more experimental measurements compared to the integral one while, on the other, the latter procedure is more involved from a computational point of view. Indeed, it may happen that to compute the first members of equations (4.16) and (4.17) some numerical or analytical approximations are needed, thus reducing the accuracy of the reconstruction. In this case, the differential approach should be preferred as it is very simple from the point of view of analytical computation. Clearly, if the computation of the integral functions in equations (4.16) and (4.17) does not present remarkable difficulties, the integral procedure proves better as, requiring less measurements, it involves a lower number of interactions with the physical system. For example, in our benchmark model, the differential approach requires twenty-six measurements, while the integral approach requires sixteen time-independent measurements or only eight time-dependent measurements.

One could summarize by saying that the integral procedure is more advantageous in terms of number of measurements, but requires the ability of solving potentially involved analytical expressions. The differential approach, instead, is more advantageous from the point of view of versatility, as it allows to deal in a straightforward way with complex generators, at the expenses of a higher number of measurements.

In conclusion, the choice between the two strategies strictly depends on the specific model under investigation.

4.3.3 Master equation parameters

We now discuss the full reconstruction of the MECs in equation (1.23). Our strategy is made up of three main steps:

1. use the T-C procedure to get indirect measurements of the evolved cumulants at different times;

2. use these measurements to retrieve the values of the MECs (or functions of them) at those times exploiting the connection between MECs and first cumulants of a Gaussian probe, obtained by employing the dynamical equations (4.1);
3. starting from the obtained discrete and finite set of values, reconstruct the full expression for the MECs by applying proper sampling theorems.

In particular, useful for our purposes will be the Nyquist-Shannon theorem [4, 5] and one of its more sophisticated generalizations involving an additive random sampling [4, 6, 8]. In principle we can distinguish two different applications of the reconstruction procedure: check of the a priori assumed time-dependence of MECs (Case I) or complete reconstruction of MECs with no a priori assumptions (Case II).

**Case I:** we assume a priori a certain time dependence of the MECs as a consequence, for example, of a microscopical derivation of the master equation. In this perspective, we are interested in experimentally reconstructing the MECs to check the validity of the approximations made. A mismatch between the assumed and the measured MECs would in fact provide a strong evidence of the breakdown of the adopted approximation scheme. In this case a full knowledge of the MECs is assumed, including that of the TIPs involved, such as the bath frequency cut-off, system-bath coupling, etc. The TIPs can be either assumed or previously reconstructed. In this case, given the prior knowledge of the bandwidth associated to the function to be reconstructed (i.e. the width of its Fourier transform), the suitable sampling theorem can be chosen accordingly. If the function is band-limited then to obtain an exact reconstruction it is enough to apply the simplest sampling theorem, i.e. the Nyquist-Shannon theorem (see the appendix C). The function can hence be reconstructed starting from a discrete set of values spaced according to the width of its Fourier transform. If the bandwidth is not limited one could truncate it and still apply the same procedure, which would then be affected by the so-called aliasing error. To minimize it one can perform a proper truncation. Alternatively a more general additive random sampling, that avoids the aliasing error (see the appendix C), can be employed.

**Case II:** here we want to fully reconstruct the MECs, or derived functions, with no previous assumption on the dynamics, i.e. the MECs are fully unknown. In general, this implies no prior knowledge of the bandwidth associated to the function to be reconstructed. In this case we must resort to an additive random sampling (see the appendix C). If on one hand this procedure involves function averages with respect to the probability of drawing $n$ sampling times (i.e. more involved measurements), on the other it does not require prior knowledge of the bandwidth and is an alias-free sampling. To obtain the averages of the function we should in principle perform measurements over a continuous interval of time, as the reconstruction is proposed with continuous random processes. In practice, every experimental apparatus employed to record and process the data has a dead working time, such that the random process will be discrete in time, no matter how dense, thus introducing an intrinsic source of error in the procedure.

We note that in both cases the set of measurements required turns out to be discrete but in principle infinite, as the reconstruction should be performed over the whole real axis.
This number can be made finite by invoking the largely reasonable physical condition of a finite observation time.

To provide an example of how to implement the proposed integral and differential procedures, we apply both to the benchmark model introduced in 4.3.1 i.e. within the perspective of Case I.

**Integral approach: benchmark model** Following the steps of the integral approach we solve equation (4.16) using equations (4.23) and we get the theoretical value (4.26). The obtained function does not belong to the functional space $L^2(R)$ thus not matching the condition for the applicability of the Nyquist-Shannon theorem (see the appendix C). However, as we are interested in a finite time interval, we can restrict the support of $\Lambda^\text{th}(t)$ to $[0, \bar{t}]$ and define:

$$\tilde{\Lambda}^\text{th}(t) \equiv \begin{cases} 
\Lambda^\text{th}(t) & t \in [0, \bar{t}] \\
0 & \text{else}
\end{cases}.$$  \hspace{1cm} (4.32)

The function $\tilde{\Lambda}^\text{th}(t)$ is in $L_2(\mathbb{R})$ thus can be reconstructed by the Nyquist-Shannon theorem. The discontinuity at $\bar{t}$, by inducing the Gibbs phenomenon (i.e. a finite Fourier sum overshoots at the jump), might at this point constitute a source of error. This problem can be anyway overcome by slightly restricting the domain in which the reconstruction of $\tilde{\Lambda}^\text{th}(t)$ can be trusted to $[0, \bar{t} - \xi]$ with $\xi > 0$.

![Figure 4.6](image-url)

**Figure 4.6:** Comparison $\tilde{\Lambda}^\text{th}(t)$ (dotted) and $i\tilde{\Lambda}^\text{th}(t)$ (continuous), in the Markovian regime, i.e. $\omega_c/\omega = 10$. The support of $\tilde{\Lambda}^\text{th}(t)$ is $[0, 12/\omega_c]$ and the reconstruction is trusted in $[0, 10/\omega_c]$, with $\alpha = 0.1$ and $T = 10(\hbar \omega)/k_B$. In figure 4.6(a), contributions smaller than 0.1% of the maximum value of the Fourier transform are neglected (bandwidth $W = 19.4/2\pi$, 7 reconstruction points) while in figure 4.6(b), those below 0.01% (bandwidth $W = 196/2\pi$, 74 reconstruction points).
Performing the Fourier transform of $\hat{\Lambda}_{\text{th}}(t)$ we obtain

$$
\mathcal{F}[\hat{\Lambda}_{\text{th}}](s) = \frac{\alpha^2 \omega \omega_c}{s^2[\omega^2 - (s + i\omega_c)^2](\omega_c^2 + \omega^2)^2} \left\{ -\left(\omega_c^2 + \omega^2\right)^2 + i e^{i(s-\omega_c)} \left[ (s + i\omega_c)^2 - \omega^2 \right] \left[ i\omega^2 + \omega^2 s i + i\omega_c^2 + \omega_c^2 s i - 2\omega_c s \right] + e^{i(s-\omega_c)} s^2 \left[ \omega^2 + 2i\omega_c s - 3\omega_c^2 \right] \cos(\omega t) + e^{i(s-\omega_c)} s^2 \left[ 3\omega \omega_c - \frac{\omega_c^3}{\omega} + i \frac{\omega_c^2 - \omega^2}{\omega} - 3 \right] \sin(\omega t) \right\}.
$$

(4.33)

From the above equation we note that $\hat{\Lambda}_{\text{th}}(t)$ is not band limited, i.e. $\mathcal{F}[\hat{\Lambda}_{\text{th}}](s)$ is not defined on a compact support. Nevertheless, since it is symmetrically decreasing around $s = 0$ (modulo a negligible oscillating behavior for higher frequencies), we can define an effective limited bandwidth and apply the Nyquist-Shannon theorem by truncating its support to a symmetric interval around zero. In figures 4.6 and 4.7 we compare $\hat{\Lambda}_{\text{th}}(t)$ and the experimental estimation $\hat{\Lambda}_{\text{ex}}(t)$ (obtained by applying the reconstruction formula (C.1)) in both the Markovian ($\omega_c/\omega = 10$) and the non-Markovian ($\omega_c/\omega = 0.1$) limit. To respect the conditions of weak coupling and high temperature, in both plots $\alpha$ is set to 0.1 and $T$ to $10(h\omega)/k_B$. The reconstruction of $\hat{\Lambda}_{\text{ex}}(t)$ is trusted in $[0, t - \xi = 10/\omega_c]$. As already mentioned, the truncation of the Fourier transform required by the Nyquist-Shannon theorem is the source of the so-called aliasing error in the reconstruction. In order to provide

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Figure 4.7: Comparison between $\hat{\Lambda}_{\text{ex}}(t)$ (dotted) and $\hat{\Lambda}_{\text{th}}(t)$ (continuous) in the non-Markovian regime, i.e. $\omega_c/\omega = 0.1$. The support of $\hat{\Lambda}_{\text{th}}(t)$ is $[0, 12/\omega_c]$, with $\omega_c/\omega = 0.1$, and the reconstruction is trusted in $[0, 10/\omega_c]$, with $\alpha = 0.1$ and $T = 10(h\omega)/k_B$. In figure 4.7(a), contributions smaller than 0.01% of the maximum value of the Fourier transform are neglected (bandwidth $W = 0.16/2\pi$, 6 reconstruction points) while in figure 4.7(b), those below 0.01% (bandwidth $W = 1.66/2\pi$, 64 reconstruction points).
evidence of this phenomenon we compare the results obtained for two different effective supports of the Fourier transform: in figures 4.6(a) and 4.7(a) we consider only contributions higher than 0.1% of the maximum value, whereas in figures 4.6(b) and 4.7(b) those higher than the 0.01%. As expected, the second case returns a better approximation and the aliasing error becomes negligible, thus not requiring the application of additive random sampling. For more involved Fourier transforms, a more general truncation criterion would be taking as effective support the region where the integral of the Fourier transform is greater than a chosen threshold value. We skip the reconstruction of the remaining MECs as the procedure is analogous, the only difference being that the integrals on the left hand side of equation (4.17) require a numerical evaluation.

**Differential approach: benchmark model** Let us now apply the differential procedure to our model. We note that in this specific example, as the four MECs to be reconstructed effectively reduce to two \((\lambda(t), \Delta(t))\), we could in principle allow for time dependent Hamiltonian parameters \((m(t), \omega(t))\) without increasing the number of equations. However, to be consistent with the previous sections and with Ref. [143], we will consider time-independent Hamiltonian parameters. For our model, equations (4.19) and (4.22) read

\[
\lambda^{ex}(t) = \frac{1}{\langle q \rangle_t} \left( \frac{1}{m} \langle p \rangle_t - \frac{\langle q \rangle^2 + \langle q \rangle^2 - \langle q \rangle^2 t_{i\rightarrow t}}{\delta t} \right),
\]

\[
\Delta^{ex}(t) = 2 \hbar m \omega \lambda(t) \Delta q^2_t - 2 \hbar \omega \Delta(q, p)_t + \hbar m \omega \frac{\Delta q^2_{i\rightarrow t} - \Delta q^2_t}{\delta t} \equiv \frac{2 \hbar m \omega \lambda(t)}{\hbar} \Delta p^2_t + \frac{2 \hbar \Delta(q, p)_t}{\hbar} + \frac{1}{\hbar m \omega} \frac{\Delta p^2_{i\rightarrow t} - \Delta p^2_t}{\delta t}. \tag{4.35}
\]

Once again we restrict ourselves to a compact support \([0, \bar{t}]\) (trusting the reconstruction in \([0, \bar{t} - \xi]\)) by defining

\[
\tilde{\lambda}^{ex}(t) \equiv \begin{cases} \lambda^{ex}(t) & t \in [0, \bar{t}] \\ 0 & \text{else} \end{cases}, \quad \tilde{\Delta}^{ex}(t) \equiv \begin{cases} \Delta^{ex}(t) & t \in [0, \bar{t}] \\ 0 & \text{else} \end{cases}. \tag{4.36}
\]

The Fourier transforms of the restricted functions read:

\[
\mathcal{F}[\tilde{\lambda}^{ex}](s) = \frac{\alpha^2 \omega^2}{k \left( \omega^2 - (s + i \omega_c)^2 \right) \left( \omega^2 + \omega_c^2 \right)}.
\]
As in the previous section, the supports of both $\mathcal{F}[\xi s](s)$ and $\mathcal{F}[\Delta s](s)$ are not compact, such that we need to truncate them. Having already reconstructed $\xi s(t)$ in the previous section, we focus here on the remaining MEC. In figures 4.8 (Markovian regime) and 4.9 (non-Markovian regime) the reconstructed function, $\xi s(t)$, (obtained by applying the reconstruction formula (C.1)) is compared with the theoretical curve $\xi s(t)$ (equation (4.24)) within the time interval $[0, \xi t - \xi = 10/\omega c]$. As in the previous section, the coupling constant and the temperature are set to $\alpha = 0.1$ and $T = 10(\hbar \omega)/k_B$. Again, in order to provide an indication of the sensitivity of the differential procedure to different truncations of the Fourier transform (aliasing error), in figures 4.8(a) and 4.9(a) the contributions smaller than $0.1\%$ of its maximum value have been neglected, whereas in figures 4.8(b) and 4.9(b) those smaller than the $0.01\%$. Analogously to what happened for the integral procedure, the truncation to $0.01\%$ returns a better reconstruction and the aliasing error becomes almost negligible (thus not requiring additive random sampling).

**Comparison between the two approaches** Let us now briefly compare the two procedures described in this section. The differential approach requires more experimental measurements compared to the integral approach, whereas the latter might result more involved from a computational point of view. For example, within the frame of Case I, the computation of the first member of equations (4.16) and (4.17) might require some numerical or analytical approximations. As any kind of approximation in principle reduces the accuracy of the reconstruction, the differential approach would be a better choice. On the other hand, if the computation of the integral functions in equations (4.16) and (4.17) does not exhibit remarkable difficulties, the integral procedure should be preferred, since it requires a lower number of interactions with the physical system.

In Case II, the integral approach could be employed to reconstruct the left hand sides of equations (4.16) and (4.17), which are functionals of the unknown MECs. By means
4.3 - Convolutionless non-Markovian master equations

Figure 4.8: Comparison between $\tilde{\Delta}^e(t)$ (dotted) and $\tilde{\Delta}^h(t)$ (continuous) in the Markovian regime, i.e. $\omega_c/\omega = 10$. The support of $\tilde{\Delta}^e(t)$ is $[0, 12/\omega_c]$ and the trusted interval is $[0, 10/\omega_c]$ with $\alpha = 0.1$ and $T = 10(\hbar\omega)/k_B$. In figure 4.8(a), contributions smaller than 0.1% of the maximum value of the Fourier transform are neglected (bandwidth $W = 19.5/2\pi$, 7 reconstruction points) while in figure 4.8(b), those below 0.01% (bandwidth $W = 73/2\pi$, 34 reconstruction points).

Figure 4.9: Comparison between the reconstructed function $\tilde{\Delta}^e(t)$ (dotted) and its theoretical behavior $\tilde{\Delta}^h(t)$ (continuous) in non-Markovian regime, i.e. $\omega_c/\omega = 0.1$. The support of $\tilde{\Delta}^e(t)$ is $[0, 12/\omega_c]$ and the trusted interval is $[0, 10/\omega_c]$ with $\alpha = 0.1$ and $T = 10(\hbar\omega)/k_B$. In figure 4.9(a), contributions smaller than 0.1% of the maximum value of the Fourier transform are neglected (bandwidth $W = 1.32/2\pi$, 50 reconstruction points) while in figures 4.9(b), those below 0.01% (bandwidth $W = 3/2\pi$, 114 reconstruction points.)
of time derivatives and linear operations on the reconstructed functions, the MECs can finally be retrieved. However, the time derivatives may amplify the error of the reconstruction. For instance, the Nyquist-Shannon theorem requires a truncation of the Fourier’s frequencies, thus inducing an oscillating behavior of the reconstructed functions, i.e. introducing the so-called aliasing error (see the appendix C). Even if the oscillations around the mean (true) functions are small, the time derivative may increase them. Hence, either one performs a better reconstruction (e.g. a larger truncation or a random additive sampling requiring a larger number of measurements) or one adopts the differential approach, thus directly reconstructing the MECs.

In general, one could say that the integral procedure is more advantageous in terms of number of measurements, but requires the ability of solving potentially involved analytical expressions. The differential approach, instead, is more advantageous from the point of view of versatility, as it allows to deal in a straightforward way with complex generators (i.e. exhibiting time-dependent Hamiltonian parameters), at the expenses of a higher number of measurements. Therefore, which of the two proposed approaches proves better, strictly depends on the specific case under investigation.
Quantum metrology

In the following, we discuss and enlarge the results presented in [196, 197]. Quantum interferometry is one of the most useful measurement techniques used in quantum metrology: it exploits the high sensitivity of certain quantum systems to small changes of external conditions, due to their intrinsic quantum coherence. Although various implementations of this general measurement procedure have been realized, the aim is always that of estimating the relative phase between the two arms of the interferometer and great efforts have been pursued to enhance the accuracy of this phase determination [53, 54].

The accuracy of the whole estimation procedure [177, 178, 57, 179, 180] depends on the number of resources at disposal, i.e. on the total number $N$ of particles involved in the interferometric measure. It turns out that the minimum uncertainty in the phase estimation that can be achieved by feeding the interferometer with “classical” states can not exceed the shot noise limit, also called the standard quantum limit, where the precision scales as $1/\sqrt{N}$.

Various strategies have been devised in order to beat this limit, typically adopting non-standard measurement protocols that make use of quantum correlated (entangled), non-classical states. In this way, at least in line of principle, the so called Heisenberg limit can be reached, where the uncertainty in the phase estimation scales as $1/N$ rather than $1/\sqrt{N}$.

A particularly promising implementation of an interferometer that could reach such a high sensitivity is that based on a Bose-Einstein condensate (BEC) [43, 46, 47, 48, 49, 51] trapped in a double-well optical potential. Although similar to more traditional constructions that use beams of particles travelling along separate paths, this new realization of the interferometry paradigm allows a precise control on the preparation and dynamics of the system.
The clear advantage in using BEC-based interferometers is that all particles in the apparatus, being in a condensed phase, share the same quantum state; this fact, together with the possibility of preparing them in a suitably entangled state, have been shown to lead to the possibility of phase estimation with sub-shot-noise accuracy [181, 184, 185, 69, 70, 77, 78, 193]. However, these particles, being spatially confined Bosons, behave as identical particles, a fact that seems to have not been properly taken into account in the derivation of the above mentioned results.

Purpose of the present investigation is to study the effects of particle indistinguishability in relation to the metrological use of BEC-based interferometers for phase estimation. Since entanglement appears to be a fundamental resource in reaching sub-shot-noise accuracies, we shall apply the generalized algebraic notion of entanglement discussed in section 2.3 to states describing identical particles in the case of a BEC confined in a double-well trap (see the discussion and the notation in subsections 2.3.2 and 2.3.4). In the light of this discussion, we shall critically re-examine the theoretical results concerning the use of the notion of spin squeezing and quantum Fisher information in getting sub-shot-noise accuracies in quantum metrological phase estimation. In appendix E, some basic introduction on estimation theory and Fisher information is presented.

5.1 Interferometry

Ultracold atoms trapped in a double-well optical potential realize a very accurate interferometric device: indeed, state preparation and beam splitting can be precisely achieved by tuning the interatomic interaction and by acting on the height of the potential barrier. The combination of standard Mach-Zhender type interferometric operations, i.e. state preparation, beam splitting, phase shift and subsequent beam recombination, can be effectively described as a suitable rotation of the initial state $\rho_0$ by a unitary transformation [183, 187]:

$$\rho_0 \rightarrow \rho_\theta = U_\theta \rho_0 U_\theta^\dagger \quad U_\theta = e^{i\theta J_\theta}.$$  

The phase change is induced by the generator

$$J_\theta \equiv n_x J_x + n_y J_y + n_z J_z , \quad n_x^2 + n_y^2 + n_z^2 = 1 ,$$

i.e. by a general combination of the following collective bilinear operators

$$J_x = \frac{1}{2}(a_1^\dagger a_2 + a_1 a_2^\dagger) , \quad J_y = \frac{1}{2i}(a_1^\dagger a_2 - a_1 a_2^\dagger) , \quad J_z = \frac{1}{2}(a_1^\dagger a_1 - a_2^\dagger a_2) ,$$

satisfying the $SU(2)$ algebraic relations:

$$[J_x, J_y] = iJ_z , \quad [J_y, J_z] = iJ_x , \quad [J_z, J_x] = iJ_y .$$
In practice, the state transformation $\rho_0 \mapsto \rho_0$ inside the interferometer can be effectively modeled as a pseudo-spin rotation along the unit vector $\vec{n} = (n_x, n_y, n_z)$, whose choice depends on the specific realization of the interferometric apparatus and of the adopted measurement procedure.

We consider the commuting subalgebras $\mathcal{A}_1$ and $\mathcal{A}_2$, $[\mathcal{A}_1, \mathcal{A}_2] = 0$, consisting of all polynomials in $a_1, a_1^\dagger$, and $a_2, a_2^\dagger$ respectively. It is interesting to notice that, although the operators in (5.3), being linear combinations of both $a_i$ and $a_i^\dagger$, are clearly non-local with respect to the bipartition ($\mathcal{A}_1, \mathcal{A}_2$), their exponentials are not all so. While $e^{i\theta J}$ and $e^{i\theta J}$, $\theta \in [0, 2\pi]$, are non-local, the exponential of $J_z$ turns out to be local:

$$e^{i\theta J_z} = e^{i\theta a_1^\dagger a_1/2} \cdot e^{-i\theta a_2^\dagger a_2/2}, \quad e^{i\theta a_1^\dagger a_1/2} \in \mathcal{A}_1, \quad e^{-i\theta a_2^\dagger a_2/2} \in \mathcal{A}_2. \quad (5.5)$$

Further, by changing the bipartition of the algebra of all operators, one can transfer this property to another of the operators in (5.3). For instance, let us introduce a new set of creation and annihilation operators $b_i^\dagger$, $b_i$, $i = 1, 2$ through the following Bogolubov transformation:

$$b_1 = \frac{a_1 + a_2}{\sqrt{2}}, \quad b_2 = \frac{a_1 - a_2}{\sqrt{2}}, \quad (5.6)$$

and their hermitian conjugates. Correspondingly, the three operators in (5.3) can be equivalently rewritten as:

$$J_x = \frac{1}{2}(b_1^\dagger b_1 - b_2^\dagger b_2), \quad J_y = \frac{1}{2i}(b_1 b_2^\dagger - b_1^\dagger b_2), \quad J_z = \frac{1}{2}(b_1 b_2^\dagger + b_1^\dagger b_2). \quad (5.7)$$

In analogy with what has been done before, one can now define a bipartition ($\mathcal{B}_1, \mathcal{B}_2$) of the full algebra using the mode operators $b_1^\dagger$, $b_i$ instead of $a_i^\dagger$, $a_i$. In this case, it is the exponential of the operator $J_z$ that now turns out to be local:

$$e^{i\theta J_z} = e^{i\theta b_1^\dagger b_1}, \quad e^{-i\theta b_1^\dagger b_1} \in \mathcal{B}_1, \quad e^{-i\theta b_2^\dagger b_2} \in \mathcal{B}_2. \quad (5.8)$$

This explicitly shows that an operator, local with respect to a given bipartition, can result non-local if a different algebraic bipartition is chosen.

From the point of view of the states, the above Bogolubov transformation corresponds to a change of basis in the Hilbert space, from the one consisting of spatially localized states ($a_i^\dagger$ and $a_i$ create and destroy particles in the two wells), to the one spanned by their (spatially non-local) superpositions, as, for instance, $b_1^\dagger |0\rangle = [a_1^\dagger |0\rangle + a_2^\dagger |0\rangle]/\sqrt{2}$ and $b_2^\dagger |0\rangle = [a_1^\dagger |0\rangle - a_2^\dagger |0\rangle]/\sqrt{2}$, which are energy eigenstates of the Bose-Hubbard Hamiltonian in the limit of a highly penetrable barrier. As a consequence, the Fock states in (2.28) results entangled with respect to this new bipartition ($\mathcal{B}_1, \mathcal{B}_2$); indeed, one finds:

$$|k, N - k\rangle = \frac{1}{2^{N/2}} \frac{1}{\sqrt{k!(N-k)!}} \sum_{r=0}^k \sum_{s=0}^{N-k} \binom{k}{r} \binom{N-k}{s} (-1)^{N-k-s} (b_1^\dagger)^r (b_2^\dagger)^s |0\rangle, \quad (5.9)$$
so that $|k, N-k\rangle$ is a combination of $(B_1, B_2)$-separable states. A similar conclusion applies to the mixed states (2.33). This explicitly shows that in the case of systems of identical particles, the notion of separability can not be given abstractly, but must be associated to a specific bipartition of the full algebra of operators. Because of their physical meaning, in the following we shall refer to the $(B_1, B_2)$ bipartition as the energy bipartition, and call spatial bipartition the original $(A_1, A_2)$ one. We shall now apply these considerations to the problem of phase estimation in quantum interferometry with systems of identical particles.

If the particles were distinguishable, then the operators $J_{x,y,z}$ and the corresponding rotations are sums of single particle spin operators, $J_{x,y,z}(j)$, i.e.

$$J_{x,y,z} = \sum_{j=1}^{N} J_{x,y,z}(j), \quad e^{i\theta_{x,y,z} J_{x,y,z}} = \bigotimes_{j=1}^{N} e^{i\theta_{x,y,z} J_{x,y,z}(j)}. \quad (5.10)$$

The latter are local operators with respect to tensor product structure in (2.2).

### 5.2 Spin inequalities

In this section, we show that spin-squeezing inequalities that are derived for distinguishable qubits can not directly be used as entanglement witnesses in the context of identical qubits. Since the use of spin-squeezed states for metrological purposes have recently become the focus of much theoretical [181, 184, 185, 69, 70, 193] and experimental [192, 194, 195] investigations, we now discuss the impact of particle indistinguishability on such an issue.

#### 5.2.1 Collective spin inequalities and entanglement

Based on (5.10), the variance $\Delta^2 J_{\vec{n}}$ of the collective spin $J_{\vec{n}} = n_x J_x + n_y J_y + n_z J_z$ along the unit spatial direction $\vec{n} = (n_x, n_y, n_z)$, with respect to separable vector states $|\Psi\rangle = \bigotimes_{j=1}^{N} |\psi_j\rangle$ results

$$\Delta^2 J_{\vec{n}} = \langle \Sigma_{j=1}^{N} (J_{x,y,z}(j) \otimes |\psi_j\rangle | \otimes |\psi_j\rangle - \sum_{j=1}^{N} \langle \psi_j | J_{x,y,z}(j) | \psi_j\rangle \otimes |\psi_j\rangle = \sum_{j=1}^{N} \langle \psi_j | (J_{x,y,z}(j)^2 | \psi_j\rangle - \sum_{j=1}^{N} (\langle \psi_j | J_{x,y,z}(j) | \psi_j\rangle)^2.$$
5.2 - Spin inequalities

\[ \Delta^2 J_{\vec{n}} = \langle k, N-k | J_{\vec{n}}^2 | k, N-k \rangle - \langle k, N-k | J_{\vec{n}} | k, N-k \rangle^2 = \frac{1 - n_z^2}{4} (N + 2k(N-k)) . \]  

(5.14)

Therefore, if \( k \neq 0, N \), for all \( \vec{n} \) that satisfy

\[ n_z^2 < \frac{2k(N-k)}{N+2k(N-k)} \leq 1 , \]

the states \( |k\rangle \), though \((\mathcal{A}_1, \mathcal{A}_2)\)-separable, nevertheless yield \( \Delta^2 J_{\vec{n}} > N/4 \); therefore, \( \Delta^2 J_{\vec{n}} \) is not an entanglement witness for pure states of Bosonic qubits.

In greater generality, inequalities for mean values and variances of collective spin operators with respect to any (mixed) separable state of distinguishable qubits (2.2) have been derived in [77, 78]; these are called spin squeezing inequalities and read

\[ \langle J_{\vec{n}_1}^2 \rangle + \langle J_{\vec{n}_2}^2 \rangle + \langle J_{\vec{n}_3}^2 \rangle - \frac{N(N+2)}{4} \leq 0 , \]  

(5.15)

\[ \Delta^2 J_{\vec{n}_1} + \Delta^2 J_{\vec{n}_2} + \Delta^2 J_{\vec{n}_3} - \frac{N}{2} \geq 0 , \]  

(5.16)

\[ \langle J_{\vec{n}_1}^2 \rangle + \langle J_{\vec{n}_2}^2 \rangle - \frac{N}{2} - (N-1)\Delta^2 J_{\vec{n}_3} \leq 0 , \]  

(5.17)

\[ (N-1)(\Delta^2 J_{\vec{n}_1} + \Delta^2 J_{\vec{n}_2}) - \langle J_{\vec{n}_3}^2 \rangle - \frac{N(N-2)}{4} \geq 0 , \]  

(5.18)

where \( \vec{n}_{1,2,3} \) denotes any triplet of unit vectors corresponding to orthogonal spatial directions and \( \langle X \rangle \) the mean value of an operator \( X \). In [77, 78], these inequalities are derived
with respect to the standard triplet \( \vec{n}_1 = \hat{x}, \vec{n}_2 = \hat{y}, \vec{n}_3 = \hat{z} \). The result easily extends to more general triplets.

Moreover, almost all the values of the first and the second moments of the total spin satisfying the inequalities correspond to separable states. The number of entangled states satisfying the inequalities is negligible for large \( N \) and is exactly zero under some special conditions. In this sense these inequalities are said to be complete. Indeed, for large \( N \), the first and the second moments of the total spin do not suffice to prove entanglement.

Indeed, the inequalities (5.11, 5.15-5.18) have been proved by using the decomposition of the collective operators \( J_\alpha, \alpha = x, y, z \), in terms of single-particle pseudo-spin: \( J_\alpha = \sum_i J_\alpha^{(i)} \), where \( J_\alpha^{(i)} \) refers to the \( i \)-th particle inside the trap. This is possible only if the particles are distinguishable. In the case of identical particles, single-particle operators like \( J_\alpha^{(i)} \) are not addressable, otherwise one would be able to distinguish the particles by means of them: only observables that are symmetric with respect to all permutations of the \( N \) Bosons, like the \( J_\alpha \)'s, are in fact permitted.

It is thus interesting to study whether these inequalities are also satisfied by \((\mathcal{A}_1, \mathcal{A}_2)\)-separable states (2.33) of \( N \) identical qubits. Let \( \bar{k} \equiv \sum_{k=0}^N k \pi_k \), \( a = 1, 2 \), denote first and second moments of the \( N + 1 \)-valued stochastic variable \( k \) with respect to the probability distribution \( \pi = \{p_k\}_{k=0}^N \). Using (5.12-5.14), mean-values and variances of collective spin operators \( J_\vec{n} \) with respect to the states in (2.33) read

\[
\langle J_\vec{n} \rangle = \frac{n_z}{2}(2\bar{k} - N) \quad (5.19)
\]
\[
\langle J_\vec{n}^2 \rangle = \frac{N(1 + 2\bar{k}) - 2k^2}{4} + \frac{n_z^2}{4}(N(N - 1) - 6N\bar{k} + 6\bar{k}^2) \quad (5.20)
\]
\[
\Delta^2 J_\vec{n} = \frac{N(1 + 2\bar{k}) - 2k^2}{4} + \frac{n_z^2}{4}(6\bar{k}^2 - 2\bar{k}(N + 2\bar{k}) - N) \quad (5.21)
\]

From the orthogonality of the triplet \( \vec{n}_{1,2,3} \), it follows that \( n_{1z}^2 + n_{2z}^2 + n_{3z}^2 = 1 \); one can thus check that all inequalities but (5.17) are satisfied by \((\mathcal{A}_1, \mathcal{A}_2)\)-separable states. Concerning (5.17), its left hand side reads

\[
\delta = \frac{N}{2} \left( \Delta^2 k - \bar{k}(N - \bar{k}) \right) + \frac{n_{3z}^2}{2} \left( (N + 2)\bar{k}(N - \bar{k}) - 3N\Delta^2 k \right) \quad (5.22)
\]

where \( \Delta^2 k \equiv \bar{k}^2 - \bar{k}^2 \) is the variance of \( k \) with respect to \( \pi = \{p_k\}_{k=0}^N \). If \( \pi \) is chosen such that \( a \equiv \bar{k}(N - \bar{k}) > N\Delta^2 k \), then \( \delta \) becomes positive and thus (5.17) results violated by the corresponding \((\mathcal{A}_1, \mathcal{A}_2)\)-separable states (2.33) for all orthogonal triplets with
Consider the pure states $|l, N - l⟩$ in (2.28) with $l \neq 0, N$; in such a case, $p_k = \delta_{k,l}$, $⟨k⟩ = l$ and $\Delta^2 k = 0$, so that (5.17) is violated for $1 \geq n^2_{3c} > N/(N + 2)$.

The preceding discussion shows that the spin inequalities (5.12-5.14) are not an entanglement witness for states of identical Bosons. Indeed, inequalities witnessing mode-entanglement for multi-mode Bosons are found in [75, 76]. They are different from (5.12-5.14), hold also when the number of particles is not fixed and depend on the mode we exploit to describe the state, i.e. on the Bogolubov transformation we perform to change the modes. The simplest inequality derived for two-mode Bosons and related to the SU(2) Lie algebra (5.3) is

$$\Delta^2 J_x + \Delta^2 J_y \geq \frac{\langle a_1^* a_1 + a_2^* a_2⟩}{2} = \frac{N}{2} \Leftrightarrow \langle (ab)^* \rangle^2 \leq \langle a_1^* a_1 a_2^* a_2⟩.$$ (5.24)

Indeed, the latter inequality implies that (5.11) is violated for separable states, unless $\Delta^2 J_x = \Delta^2 J_y = N/4$ i.e. for the states $|0, N⟩$ and $|N, 0⟩$. The second form of this inequality can be generalized to inequalities involving arbitrary powers of the creation and annihilation operators:

$$\langle (a_1^* a_1^* b_2^* b_2^*) \rangle^2 \leq \langle (a_1^* a_1^* a_2^* a_2^*) \rangle^2.$$ (5.25)

Therefore, in order to witness mode-entanglement, one should apply these latter inequalities, as done in [81], instead of (5.12-5.14) or the spin squeezing criteria discussed in the following, that hold only for distinguishable particles, as wrongly suggested in [192, 194, 195].

### 5.2.2 Spin-squeezing

For any orthogonal triplet of space-directions $\vec{n}_{1,2,3}$, the Heisenberg uncertainty relations for the SU(2) operators $J_\vec{n}$ read

$$\Delta^2 J_{\vec{n}_1} \Delta^2 J_{\vec{n}_2} \geq \frac{1}{4} \langle J_{\vec{n}_1} \rangle^2.$$ (5.26)

One speaks of spin-squeezing when one of the variances can be made smaller than $\frac{1}{2} \langle J_{\vec{n}_1} \rangle$. The relevance of states satisfying this condition for achieving otherwise unavailable accuracies has been studied in relation to the measure of an angle $\theta$ by interferometric techniques. These are based on a rotation of an input state $\rho_0$ (5.1) around $\vec{n}_2$ and upon measuring on $\rho_0$ the collective spin $J_{\vec{n}_1}$, where $\vec{n}_2 \perp \vec{n}_1$. By choosing the remaining orthogonal
unit vector \( \vec{n}_3 \) such that \( \langle \vec{J}_{\vec{n}_3} \rangle = \text{Tr}(\rho_0 \vec{J}_{\vec{n}_3}) \neq 0 \), by error propagation, the uncertainty \( \delta \theta \) in the determination of \( \theta \) can be estimated by [185]

\[
\delta^2 \theta = \frac{\Delta^2 \vec{J}_{\vec{n}_1}}{\left( \partial_{\theta} \langle \vec{J}_{\vec{n}_2} \rangle \right)_{\theta=0}^2} = \frac{\Delta^2 \vec{J}_{\vec{n}_1}}{\langle \vec{J}_{\vec{n}_1} \rangle^2} = \frac{\xi^2_W}{N},
\]  

(5.27)
in terms of the spin-squeezing parameter

\[
\xi^2_W \equiv \frac{N \Delta^2 \vec{J}_{\vec{n}_1}}{\langle \vec{J}_{\vec{n}_1} \rangle^2}.
\]

(5.28)

The value \( \delta^2 \theta = 1/N \) is called shot-noise limit; in the case of distinguishable qubits, it gives the lower bound to the attainable accuracies when the input state \( \rho_0 \) is separable. Indeed, in such a case one finds \( \xi^2_W \leq 1 \). This result follows from the inequality \( \xi^2_S > \xi^2_W \)

where the new spin-squeezing parameter

\[
\xi^2_S \equiv \frac{N \Delta^2 \vec{J}_{\vec{n}_1}}{\langle \vec{J}_{\vec{n}_1} \rangle^2 + \langle \vec{J}_{\vec{n}_3} \rangle^2},
\]

(5.29)

has been introduced in [69, 70]; by means of the local structure of the collective spin operators \( J_{x,y,z} \), one can prove that \( \xi^2_S \) is always \( \geq 1 \) for separable states of distinguishable qubits. Therefore, using distinguishable qubits, the shot-noise limit can be beaten, namely accuracies better than \( 1/N \) can be achieved only if \( \xi^2_S < 1 \), that is only by means of entangled states. For sake of completeness, we mention the first spin-squeezing parameter

\[
\xi^2_{KU} = \frac{4 \Delta^2 \vec{J}_{\vec{n}_1}}{N},
\]

(5.30)

that was defined in [184]. The inequality \( \langle \vec{J}_x \rangle^2 \leq N/2 \) implies \( \xi_{KU} \leq \xi_W \). The equality holds if and only if \( \langle \vec{J}_{\vec{n}_1} \rangle^2 = N/2 \), whence \( \Delta^2_{\rho} \vec{J}_{\vec{n}_1} = N/4 \) and \( \xi^2_{KU} = \xi^2_W = 1 \). Furthermore,

\[
\frac{N}{2} \left( \frac{N}{2} + 1 \right) \geq \langle \vec{J}_{\vec{n}_1} \rangle^2 \rho + \langle \vec{J}_{\vec{n}_3} \rangle^2 \rho > \langle \vec{J}_{\vec{n}_1} \rangle^2 + \langle \vec{J}_{\vec{n}_3} \rangle^2 \Rightarrow \xi^2_{KU} < \frac{N + 2}{N} \xi^2_W.
\]

(5.31)
The first inequality saturates if and only if \( \langle \vec{J}_{\vec{n}_1} \rangle^2 = 0 \). The second inequality is never saturated. It is equivalent to \( \Delta^2_{\rho} \vec{J}_{\vec{n}_1} + \Delta^2_{\rho} \vec{J}_{\vec{n}_3} > 0 \). The equality would hold only if \( \Delta^2_{\rho} \vec{J}_{\vec{n}_1} = \Delta^2_{\rho} \vec{J}_{\vec{n}_3} = 0 \), which is impossible since it corresponds to a common eigenstate of \( \vec{J}_{\vec{n}_1} \) and \( \vec{J}_{\vec{n}_3} \). Some features of spin-squeezing are reviewed in [181]. Summarizing, the relations between the spin-squeezing parameters are as follows

\[
\xi^2_S \leq \xi^2_W, \quad \xi^2_{KU} \leq \xi^2_W, \quad \xi^2_{KU} < \frac{N + 2}{N} \xi^2_S.
\]

(5.32)
5.2 - Spin inequalities

Let us instead consider $N$ identical Bosonic qubits in the $(\mathcal{A}_1, \mathcal{A}_2)$-separable pure states $|k, N - k\rangle$ and any triplet of orthogonal spatial directions $\vec{n}_{1,2,3}$ with $\vec{n}_1 \neq \vec{z}$. Using (5.12-5.14) and $n_{1z}^2 + n_{2z}^2 + n_{3z}^2 = 1$, one computes

\[ \xi_S^2 = \frac{N \Delta^2 J_{\vec{n}_1}}{(J_{\vec{n}_1})^2 + (J_{\vec{n}_2})^2} = \frac{N}{n_{2z}^2 + n_{3z}^2} \frac{N + 2k(N - k)}{(2k - N)^2} = \frac{N(N + 2k(N - k))}{(2k - N)^2} \geq 1, \quad (5.33) \]

where $0 \leq k \leq N$. In the case of the $(\mathcal{A}_1, \mathcal{A}_2)$-separable density matrices (2.33), first observe that, thanks to the Cauchy-Schwartz inequality, one has $\sum_{k=0}^N p_k \langle J_k^2 \rangle_k \geq \langle J^2 \rangle$, where $\langle X \rangle_k$ denotes the mean-value of $X$ with respect to the number state $|k, N - k\rangle$. Then,

\[ \xi_S^2 \geq \frac{N \sum_{k=0}^N p_k \Delta^2 J_{\vec{n}_1}}{(J_{\vec{n}_1})^2 + (J_{\vec{n}_2})^2} = \frac{1 - n_{1z}^2}{n_{2z}^2 + n_{3z}^2} \frac{N \sum_{k=0}^N p_k (N + 2k(N - k))}{(\sum_{k=0}^N p_k (N - 2k))^2} \geq \frac{\sum_{k=0}^N p_k (k - \frac{N}{2})^2}{(\sum_{k=0}^N p_k (k - \frac{N}{2}))^2}, \quad (5.34) \]

where the last inequality follow from (5.33). A further application of the Cauchy-Schwartz inequality to the right hand side of the last inequality yields $\xi_S^2 \geq 1$ for all $(\mathcal{A}_1, \mathcal{A}_2)$-separable states when $n_1 \neq z$.

If one chooses $\vec{n}_1 = \vec{z}$, in the case of $(\mathcal{A}_1, \mathcal{A}_2)$-separable mixed states, one finds $\Delta^2 J_z \neq 0$ and $\langle J_{\vec{n}_2,\vec{n}_3} \rangle = 0$; therefore, $\xi_S^2$ and $\xi_W^2$ diverge. Instead, for $(\mathcal{A}_1, \mathcal{A}_2)$-separable pure states $|k, N - k\rangle$ also $\Delta_k J_z = 0$ whence $\xi_S^2$ and $\xi_W^2$ are not defined and must thus be computed by means of suitable limiting procedures.

Let us consider the $(\mathcal{A}_1, \mathcal{A}_2)$-entangled vector state

\[ |\Psi\rangle = \sum_{k=0}^N \sqrt{q_k} |k, N - k\rangle, \quad (5.35) \]

with real coefficients from a probability distribution $\pi = \{q_k\}_{k=0}^{N}$ over the stochastic variable $k$. Then, from (5.12-5.14) it follows that $\langle J_z \rangle = 0$ and $\Delta^2 J_z = \Delta^2 k$; therefore $\xi_S^2 = \xi_W^2$ and

\[ \xi_W^2 = \frac{N \Delta^2 J_z}{(J_z)^2} = \frac{N \Delta^2 k}{(\sum_{k=1}^{N} \sqrt{k(N - k + 1)} \sqrt{q_k q_{k-1}})^2}, \quad (5.36) \]
In the case of a Gaussian distribution peaked around \( k = \ell \neq 0, N \),

\[
q_k = \frac{1}{Z} \exp\left(-\frac{(k-\ell)^2}{\sigma^2}\right), \quad Z = \sum_{k=0}^{N} \exp\left(-\frac{(k-\ell)^2}{\sigma^2}\right),
\]

one finds

\[
\xi^2_{W} = \frac{2N}{\left(\sqrt{(\ell + 1)(N-\ell)} + \sqrt{\ell(N-\ell + 1)}\right)^2} + O\left(e^{-\frac{2}{N^2}}\right),
\]

\[
\xi^2_{KU} = \frac{8}{N} e^{-\frac{2}{N^2}} + O\left(e^{-\frac{2}{N^2}}\right).
\]

Thus, for sufficiently small \( \sigma \), \( \xi^2_S = \xi^2_W < 1 \) for all \( \ell \neq 0, N \). Chosing \( \ell = \frac{N}{2} \), one computes \( \xi^2_W = \xi^2_S = \frac{2}{N+2} + O\left(e^{-\frac{2}{N^2}}\right) \). As \( \sigma \to 0 \), the state \( |\Psi\rangle \) goes to a twin Fock state \( |N/2, N/2\rangle \) and the parameters \( \xi^2_W = \xi^2_S \) are much smaller than one for large \( N \). For \( \ell = 0, N \), we get

\[
\xi^2_W = 1 + O\left(e^{-\frac{2}{N^2}}\right), \quad \xi^2_{KU} = \frac{4}{N} e^{-\frac{2}{N^2}} + O\left(e^{-\frac{2}{N^2}}\right).
\]

On the other hand, by choosing

\[
|\Psi\rangle = \frac{p}{N} \sum_{k=0, k\neq N/2}^{N} |k, N-k\rangle + (1-p) \left| \frac{N}{2}, \frac{N}{2}\right\rangle, \quad 0 < p < 1,
\]

it turns out that \( \Delta^2k = p(N+2)(N+1)/12 \) so that (5.36) yields

\[
\xi^2_W = \frac{N(N+1)}{12\left(\sqrt{1-p + q}\right)^2},
\]

\[
\xi^2_{KU} = \frac{p(N+2)(N+1)}{3N}.
\]

where

\[
q = \sqrt{\frac{p}{N^2(N+2)}} \sum_{k\neq N/2, N/2+1} \sqrt{k(N-k+1)}.
\]
Letting $p \to 0$ one gets $|\Psi \rangle \to \left| \frac{N}{2}, \frac{N}{2} \right\rangle$ and, if $N > 3$,

$$\xi_w^2 \to \frac{N(N + 1)}{12} > 1.$$  \hfill (5.46)

The above two examples show that, when $\vec{n}_1 = \hat{z}$, the spin-squeezing parameters $\xi_{WS}$ are not well-defined: different values for $\xi_{WS}^2$ can be obtained by approaching a state $|k, N-k\rangle$ via different limit procedures. This fact is also of practical importance: indeed, in [192], approximations to Fock states $|k, N-k\rangle$ have been experimentally constructed that are characterized by spin-squeezing parameters shows $\xi_{W}^2 < 1$. This property arises from the fact that the approximations are $(\mathcal{A}_1, \mathcal{A}_2)$-entangled states. The previous discussion shows that some care has to be taken in constructing the perturbations of $|k, N-k\rangle$; indeed, not all $(\mathcal{A}_1, \mathcal{A}_2)$-entangled states arbitrarily close to it automatically $\xi_{WS}^2 > 1$. Therefore, the spin-squeezing parameters $\xi_{WS}^2$ are not always useful for metrological applications, a better quantity is the so-called quantum Fisher information [186, 188], which as we shall see below, is continuous and well defined for all Bosonic qubits.

Up to now we have perturbed the Fock states with superpositions of states. We notice that as soon as we superpose Fock states we get an $(\mathcal{A}_1, \mathcal{A}_2)$-entangled pure state. Thus, in order to regularize the limit of the spin squeezing we need entanglement which vanishes in the limit leaving some residual effects. In order to model a more realistic perturbation induced by some noise, we consider mixed states converging to pure Fock states. As a first preliminary example, we choose $(\mathcal{A}_1, \mathcal{A}_2)$-separable mixed states:

$$\rho = \sum_{k=0}^{N} p_k |k, N-k\rangle\langle k, N-k|.$$  \hfill (5.47)

Varying the weights $\{p_k\}_{k=0,\ldots,N}$, this states can reach any Fock state, when one of the weights goes to 1 and the others vanish. This states satisfy $\langle J_y \rangle_\rho = 0$, while $\Delta J_z^2 \neq 0$ for a proper mixture. Therefore, the spin-squeezing parameters with $\vec{n}_1 = \hat{z}$ are $\xi_S^2 = \xi_W^2$

$$\xi_w^2 \to \infty,$$  \hfill (5.48)

$$\xi_{KU}^2 = \frac{1}{N} \sum_{k=0}^{N} p_k (2k - N)^2 - \frac{1}{N} \left( \sum_{k=0}^{N} p_k (2k - N) \right)^2.$$  \hfill (5.49)

The parameter $\xi_{KU}^2$ goes continuously to zero as $p_k \to \delta_{k,k'}$, while the other parameters are still affected by a pathological behaviour.

In order to get a non pathological spin squeezeing we need $(\mathcal{A}_1, \mathcal{A}_2)$-entangled mixed states, such as
\[ \rho = (1 - p)|k, N - k\rangle\langle k, N - k| + p \rho', \]  
(5.50)

where \( \rho' \) is and \((\mathcal{A}_1, \mathcal{A}_2)\)-entangled state. The spin-squeezing parameters read (\( \hat{n}_1 = \hat{z}, \hat{n}_2 = \hat{x}, \hat{n}_3 = \hat{y} \))

\[
\xi_w^2 = \frac{N \left( k - \frac{N}{2}\right)^2 + \langle J_z \rangle_{\rho'} + 2 \left( k - \frac{N}{2}\right) \langle J_z \rangle_{\rho'} }{\langle J_z \rangle_{\rho'}^2} + O(1) \geq \frac{N \left( k - \frac{N}{2} + \langle J_z \rangle_{\rho'} \right)^2}{\langle J_z \rangle_{\rho'}^2} + O(1),
\]
(5.51)

\[
\xi_s^2 = \frac{N \left( k - \frac{N}{2}\right)^2 + \langle J_z \rangle_{\rho'} + 2 \left( k - \frac{N}{2}\right) \langle J_z \rangle_{\rho'} }{\langle J_z \rangle_{\rho'}^2 + \langle J_x \rangle_{\rho'}^2} + O(1) \geq \frac{N \left( k - \frac{N}{2} + \langle J_z \rangle_{\rho'} \right)^2}{\langle J_z \rangle_{\rho'}^2 + \langle J_x \rangle_{\rho'}^2} + O(1),
\]
(5.52)

\[
\xi_{KU}^2 = \frac{4p \langle J_z \rangle_{\rho'}^2}{N} + O(p^2) \geq \frac{4p \left( k - \frac{N}{2} + \langle J_z \rangle_{\rho'} \right)^2}{N} + O(p^2).
\]
(5.53)

The spin-squeezing of the state \( \rho \) depend on the spin-squeezing of \( \rho' \) even for small \( p \). For instance, if \( k = N/2 \), we get

\[
\xi_w^2 = \frac{N \langle J_z \rangle_{\rho'}^2}{p \langle J_z \rangle_{\rho'}^2} + O(1) \geq \frac{N \Delta_{\rho'}^2 J_z}{p \langle J_z \rangle_{\rho'}^2},
\]
(5.54)

\[
\xi_s^2 = \frac{N \langle J_z \rangle_{\rho'}^2}{p \langle J_z \rangle_{\rho'}^2 + \langle J_x \rangle_{\rho'}^2} + O(1) \geq \frac{N \Delta_{\rho'}^2 J_z}{p \langle J_z \rangle_{\rho'}^2 + \langle J_x \rangle_{\rho'}^2},
\]
(5.55)

\[
\xi_{KU}^2 = \frac{4p \langle J_z \rangle_{\rho'}^2}{N} + O(p^2) \geq \frac{4p \Delta_{\rho'}^2 J_z}{N},
\]
(5.56)

which are bounded by the the spin-squeezing parameters of \( \rho' \), apart a factor \( p \), and the equalities hold if \( \langle J_z \rangle_{\rho'} = 0 \). However, the parameter \( \xi_{KU}^2 \) continuously converges to zero while the parameters \( \xi_w^2 \) and \( \xi_s^2 \) diverge, as \( p \to 0 \).

The most general regularization we can consider is the following state
\[ \rho = (1 - p)|\psi_k(\chi)\rangle\langle\psi_k(\chi)| + p\rho', \]

where \(|\psi_k(\chi)\rangle \rightarrow |k, N - k\rangle\) as \(\chi \rightarrow 0\), and \(\chi\) may be a multivariate variable. If we first perform the limit \(\chi \rightarrow 0\), we get the same spin-squeezing parameters of the previous case. If we first perform the limit \(p \rightarrow 0\), we retrieve perturbations of Fock states given by pure states. Thus, any proper mixture does not provide a well defined regularization.

### 5.3 Quantum Fisher information

Quantum estimation theory allows a precise determination of the accuracy with which the phase change of an interferometer can be measured: the accuracy \(\delta \theta\) with which the phase \(\theta\) can be obtained in a rotation (5.1) involving the operator \(J_{\hat{n}}\) and the initial state \(\rho_0\) is limited by the following inequality [177, 178, 179, 188]:

\[ \delta^2 \theta \geq \frac{1}{F[\rho_0, J_{\hat{n}}]}, \]

where the quantity \(F[\rho_0, J_{\hat{n}}]\) is the so-called quantum Fisher information. A brief discussion on quantum estimation theory is presented in appendix E. One can show that the quantum Fisher information is a convex function of the quantum state \(\rho_0\), see appendix E, and in general [188]

\[ F[\rho_0, J_{\hat{n}}] \leq \frac{4}{N} \left( \Delta_{\rho_0} J_{\hat{n}} \right)^2, \]

where \(\Delta_{\rho_0} J_{\hat{n}} \equiv \langle J_{\hat{n}}^2 \rangle - \langle J_{\hat{n}} \rangle^2\) is the variance of the operator \(J_{\hat{n}}\) in the state \(\rho_0\), the equality holding only for pure initial states, \(\rho_0 = |\psi\rangle\langle\psi|\).

Given the interferometer, i.e. given the operator \(J_{\hat{n}}\) to be measured, one can optimize the precision with which \(\theta\) is determined by choosing an initial state that maximizes the corresponding quantum Fisher information.

In the case of distinguishable particles, it has been shown that for any separable state

\[ \rho_{\text{sep}} = \sum_k p_k \bigotimes_{j=1}^N \rho_k^{(j)}, \]

the quantum Fisher information is bounded by \(N\) [193]:

\[ F[\rho_{\text{sep}}, J_{\hat{n}}] \leq N. \]

The proof of the latter inequality directly follows from (5.11) and (5.59). Indeed, the inequality involving \(F[\rho_0, J_{\hat{n}}]\) given below (and similarly the set of inequalities discussed
in section 5.2.1 and [77, 78]) has been proved by using the decomposition of the collective operators \( J_\alpha, \alpha = x, y, z \), in terms of single-particle pseudo-spin: \( J_\alpha = \sum_i J_\alpha^{(i)} \), where \( J_\alpha^{(i)} \) refers to the \( i \)-th particle inside the trap. This is possible only if the particles are distinguishable. In the case of identical particles, single-particle operators like \( J_\alpha^{(i)} \) are not addressable, otherwise one would be able to distinguish the particles by mean of them: only observables that are symmetric with respect to all permutations of the \( N \) Bosons, like the \( J_\alpha \)'s, are in fact permitted. This means that by feeding the interferometer with separable initial states, the best achievable precision in the determination of the phase shift \( \theta \) is bounded by the so-called shot-noise-limit (also called the standard-quantum-limit):

\[
\delta^2 \theta \geq \frac{1}{N}.
\] (5.62)

On the other hand, quite in general, one finds

\[
F[\rho, J_\vec{n}] \leq N^2,
\] (5.63)

so that an accuracy in phase estimation better than the shot-noise-limit is in principle allowed, eventually reaching the so-called Heisenberg limit, \( \delta^2 \theta > 1/N^2 \), obtained when in (5.63) the equality holds. And indeed, many efforts have been devoted in order to find suitable input states \( \rho_0 \) and detection protocols that would allow such an ultimate sensitivity [181, 184, 185, 192, 193, 194, 195]. Notice that, because of (5.61), these states must be entangled. Actually, one can turn the argument around and use the quantum Fisher information for entanglement detection [193]; indeed, if for a state \( \rho \) one finds that \( F[\rho, J_\vec{n}] > N \), than the state is surely entangled.

In the previous section, it is showed that the spin-squeezing parameters are not well defined for \((\mathcal{A}_1, \mathcal{A}_2)\)-separable states of identical Bosons. In full generality, the relation between spin-squeezing and quantum Fisher information is

\[
F[\rho, J_{\vec{n}_1}] \Delta^2 J_{\vec{n}_2} \geq \langle J_{\vec{n}_1} \rangle^2,
\] (5.64)

where \( \vec{n}_{1,2,3} \) is a triplet of orthogonal spatial directions. In order to directly prove (5.64), we consider the measurement of the observable \( J_{\vec{n}_2} \). \( \lambda \) are the eigenvalues of \( J_{\vec{n}_2} \). \( p(\lambda, \theta) \) is the probability of measuring the value \( \lambda \) with the state \( \rho_\theta = e^{i\theta J_{\vec{n}_1}} \rho e^{-i\theta J_{\vec{n}_1}} \), and \( \langle J_{\vec{n}_2} \rangle_{\rho_\theta} = \text{Tr}(\rho_\theta J_{\vec{n}_2}) \) is the mean value of the operator \( J_{\vec{n}_2} \) with respect to the state \( \rho_\theta \). Deriving by \( \theta \) the relation \( \int d\lambda (\lambda - \langle J_{\vec{n}_2} \rangle_{\rho_\theta}) \rho(\lambda, \theta) = 0 \), we get

\[
\left( \partial_\theta \langle J_{\vec{n}_1} \rangle_{\rho_\theta} \right)^2 \leq \left( \int d\lambda (\lambda - \langle J_{\vec{n}_2} \rangle_{\rho_\theta}) \partial_\theta p(\lambda, \theta) \right)^2.
\]
\[
\leq \left( \int d\lambda (\lambda - \langle J_{\hat{n}_1} \rangle)^2 p(\lambda, \theta) \right) \left( \int d\lambda \frac{1}{p(\lambda, \theta)} (\partial_\theta p(\lambda, \theta))^2 \right), \tag{5.65}
\]

where we have used the Cauchy-Schwartz inequality. By the definition of quantum Fisher information (see appendix E.2),

\[
F[\rho, J_{\hat{n}_1}] \Delta_{\hat{n}_1}^2 J_{\hat{n}_2} \geq \Delta_{\hat{n}_2}^2 \langle J_{\hat{n}_3} \rangle^2 = \xi^2_W/N, \tag{5.66}
\]

which reduces to (5.64) for \( \theta = 0 \). The inequality (5.64) is termed generalized uncertainty relation: for pure state inequality (5.59) reduces to an equality and (5.64) is the standard Heisenberg principle. If \( \langle J_{\hat{n}_3} \rangle \neq 0 \), one gets the following relation between the quantum Fisher information and the squeezing parameter \( \xi^2_W \) in (5.28):

\[
\frac{1}{F[\rho, J_{\hat{n}_1}]} \leq \frac{\Delta^2 J_{\hat{n}_2}}{\langle J_{\hat{n}_2} \rangle^2} = \frac{\xi^2_W}{N}. \tag{5.67}
\]

The inequality (5.67) is easy to understand if we recall that \( 1/F[\rho, J_{\hat{n}_1}] \) is the best accuracy \( \delta^2 \theta \) and \( \xi^2_W/N \) is an attainable accuracy. In the case of distinguishable qubits, from (5.58) and (5.67) it follows that spin-squeezing, namely \( \xi^2_W < 1 \), opens the possibility of achieving \( \delta^2 \theta < 1/N \), thus of beating the shot-noise limit. There is no direct connection between the Sorensen’s spin-squeezing parameter \( \xi^2_W \) and the quantum Fisher information.

In the case of identical qubits and of \((A_1, A_2)\)-separable states, the right hand side of the above inequality diverges if \( \hat{n}_1 = \hat{z} \) as \( \langle J_{\hat{n}_3} \rangle = 0 \), while it does not make sense if \( \hat{n}_2 = \hat{z} \) for then also \( \Delta^2 J_{\hat{n}_2} = 0 \) whence, as already observed, \( \xi^2_W \) is not defined. However, the quantum Fisher information is always well-defined.

### 5.3.1 Sub-shot-noise

When dealing with identical particles, as in the case of the condensed Bosonic atoms confined in a double-well optical trap, these conclusions need to be re-qualified. When identical Bosons are enough far away from each other so that their wavefunctions do not spatially overlap, they effectively behave as distinguishable particles, and no symmetrization of the total wavefunction is needed [79]. However, this situation is hardly applicable to a gas of condensed ultracold atoms, where all particles share the same quantum state. As shown earlier, with respect to the bipartition \((A_1, A_2)\), a generic separable mixed state \( \rho \) is diagonal in the Fock basis (2.28), and can thus be written as in (2.33). For such a state, the quantum Fisher information can be explicitly computed, by means of equation
(E.28) in the appendix E:

$$F[\rho, J_n] = (1 - n_z^2) \left[ N + 2 \sum_{k=0}^{N} p_k (N - k) - 4 \sum_{k=0}^{N} \frac{p_k p_{k+1}}{p_k + p_{k+1}} (k + 1)(N - k) \right]. \quad (5.68)$$

In particular, in the case of a pure state, $\rho_k = |k, N - k\rangle\langle k, N - k|$, this expression results proportional to the variance of $J_n$ (see (5.59)),

$$F[\rho_k, J_n] = (1 - n_z^2) \left[ N + 2k(N - k) \right], \quad (5.69)$$

which is greater than $N$ for

$$0 \leq n_z^2 < \frac{2k(N - k)}{N + 2k(N - k)} < 1. \quad (5.70)$$

More specifically, when $\vec{n}$ lays in the plane orthogonal to the $z$ direction, so that $n_z^2 = 0$, one finds that $F[\rho_k, J_n] > N$ for $k \neq 0, N$. Recalling (5.58), this implies that in this case the phase uncertainty $\delta \theta$ is smaller than $1/\sqrt{N}$, thus beating the shot-noise-limit. Actually, when the two wells are filled by the same number of particles, so that the system is in the state $\rho_{N/2} = |N/2, N/2\rangle\langle N/2, N/2|$, one can even get close to the Heisenberg limit, since in this case:

$$F[\rho_{N/2}, J_n] = \frac{N^2}{2} + N. \quad (5.71)$$

Therefore, unlike in the case of distinguishable particles, the quantum Fisher information can attain a value greater than $N$ even with initial states that are separable with respect to the spatial bipartition. As a consequence, in general, the inequality (5.61) does not play any more the role of a separability condition when dealing with systems of identical particles.

In spite of this, we have just seen that the accuracy with which the phase change can be determined in interferometers fed with such separable states can still beat the shot-noise-limit, provided that the rotation involved in the apparatus is not directed along the $z$ axis. When $\vec{n} = \hat{z}$, the quantum Fisher information (5.68) vanishes. From the physical point of view, this results follows from the fact that the Fock states in (2.28) are eigenstates of the operator $J_z$, so that separability is preserved by rotations generated by it: $e^{i\theta J_z} |k, N - k\rangle = e^{i\theta (2k - N)} |k, N - k\rangle$. In other words, in order to take advantage of the improvement in the accuracy of the phase determination, one has to use an experimental setup for which $\vec{n} \neq \hat{z}$. As observed before, such rotations are realized by operators that are non-local with respect to the spatial bipartition. In fact, only the exponential of $J_z$ happens to be a $(A_1, A_2)$-local operator, as shown in (5.5). Therefore, given the $(A_1, A_2)$ bipartition, it is not the entanglement of the states fed into the interferometer...
that help overcoming the shot-noise-limit in the phase estimation accuracy; rather, it is
the non-local character of the rotations operated by the apparatus on initially separable
states that allows \( \delta^2 \theta \) to be larger than \( 1/N \), with the possibility of closely approaching
the Heisenberg \( 1/N^2 \) limit.

This result can be physically interpreted in another, equivalent way, which will shed
further light on the notion of separability when dealing with identical particles. The idea is
to change description (and thus bipartition) through a suitable Bogolubov transformation,
following the discussion at the end of the previous Section.

Take the unit vector \( \vec{n} \) to lay in the plane orthogonal to the \( z \) axis, so that one can write
\( \vec{n} = (\cos \varphi, \sin \varphi, 0) \), \( \varphi \in [0, 2\pi] \). Then, the generator \( J_{\vec{n}} \) in (5.2) assumes the form:

\[
J_{\vec{n}} = \frac{1}{2} \left( e^{-i\varphi} a_1^* a_2 + e^{i\varphi} a_1 a_2^* \right),
\]

which clearly shows that its exponential is non-local in the \((A_1, A_2)\) bipartition. Never-
theless, it can become local in a different, suitably chosen bipartition. To this aim, let us
introduce a new set of mode operators \( b_1^\dagger, b_1, b_2^\dagger, b_2 \) through the following Bogolubov
transformation, that slightly generalizes the one in (5.6):

\[
b_1 = \frac{a_1 + e^{-i\varphi} a_2}{\sqrt{2}}, \quad b_2 = \frac{a_1 - e^{-i\varphi} a_2}{\sqrt{2}},
\]

(5.73)

together with their hermitian conjugates. In this new representation, one has:

\[
J_{\vec{n}} = \frac{1}{2} (b_1^\dagger b_1 - b_2^\dagger b_2),
\]

(5.74)
so that the unitary operator that implements the rotation around \( \vec{n} \),

\[
e^{i\theta J_{\vec{n}}} = e^{i\theta b_1^\dagger b_1^{\dagger}/2} e^{-i\theta b_2^\dagger b_2^{\dagger}/2}, \quad e^{i\theta b_1^\dagger b_1^{\dagger}/2} \in \mathcal{B}_1, \quad e^{-i\theta b_2^\dagger b_2^{\dagger}/2} \in \mathcal{B}_2,
\]

(5.75)
is indeed local with respect to the new bipartition \((\mathcal{B}_1, \mathcal{B}_2)\), where \( \mathcal{B}_1 \) is the subalgebra of
polynomials in \( b_1^\dagger, b_1 \), while \( \mathcal{B}_2 \) is the one of polynomials in \( b_2^\dagger, b_2 \). In this new language,
the state \(|N/2, N/2\rangle\) representing the situation of equal filling of the two wells, is no longer
separable with respect to this new bipartition; in fact, one finds (see (5.9)):

\[
\left| \begin{array}{c}
N - N/2 \\
N/2 - N/2
\end{array} \right| = \frac{e^{iN\varphi/2}}{2^{N/2}(N/2)!} \sum_{k,l=0}^{N/2} \binom{N/2}{k} \binom{N/2}{l} (-1)^{N/2-l} (b_1^\dagger)_k (b_2^\dagger)_l (b_1)_k (b_2)_l \left| 0 \right>,
\]

(5.76)
while, as seen in the previous Section, any pure \((\mathcal{B}_1, \mathcal{B}_2)\)-separable state must be a Fock
state of the form \( b_1^{m_1} b_2^{l_1} |0\rangle\).
Despite these changes, the value of the quantum Fisher information for the initial state $|N/2, N/2\rangle$ and the observable $J_n$ is unchanged and still given by (5.71), since it does not depend on the representation used to compute it. This means that if one is able to build an experimental setup, together with a suitable measure procedure, which can be modelled in terms of the energy modes $b_i, b_i^\dagger$ instead of the original spatial modes $a_i, a_i^\dagger$, then the accuracy $\delta \theta$ with which the phase $\theta$ may be determined can still approach the Heisenberg limit. In such a case, the improvement in sensitivity with respect to the standard shot-noise-limit is due to the $(B_1, B_2)$-entanglement of the initial state $|N/2, N/2\rangle$ and not to the non-locality of the transformation that takes place inside the apparatus.

Notice that even approximating a number state $|\ell, N-\ell\rangle$ by an experimentally more realistic superposition $|\Psi\rangle = \sum_{k=0}^{N} \sqrt{q_k} |k, N-k\rangle$ of states $|k, N-k\rangle$ with coefficients as in (5.38), may beat the shot noise limit. Indeed, one computes

$$F[|\Psi\rangle \langle \Psi|, J_y] = 4 \Delta^2 J_y = N + 2\ell(N-\ell) + O \left( e^{-\frac{1}{\sigma^2}} \right),$$

which can be kept $> N$ by suitably small $\sigma$. As a side remark, we notice that the quantum Fisher information and the Wineland’s spin-squeezing parameter give the same accuracy, for the Gaussian superposition $|\Psi\rangle$ with $\ell = N/2$ at the lowest order of $\sigma$. Indeed, the equality holds in (5.67) at the lowest order of $\sigma$, with $\vec{n}_1 = \hat{y}, \vec{n}_2 = \hat{\zeta}$ and $\vec{n}_3 = \hat{x}$. Thus, the spin-squeezing give the best accuracy for such states, that may model the state the authors of [192] prepared tempting to generate a twin Fock state $|N/2, N/2\rangle$.

Instead, making the quantum Fisher information larger than $N$ is impossible without $(A_1, A_2)$-non-locality; indeed, $F[\rho_\ell, J_z] = 4 \Delta^2 J_z = 0$. Even considering the $(A_1, A_2)$-entangled perturbation $|\Psi\rangle$ does not help; indeed,

$$F[|\Psi\rangle \langle \Psi|, J_z] = 4 \Delta^2 J_z = 8e^{-\frac{1}{\sigma^2}} + O \left( e^{-\frac{1}{2\sigma^2}} \right).$$

Therefore, the lower bound to the error in (5.58) becomes arbitrarily large when $\sigma \to 0$.

When dealing with $(A_1, A_2)$-separable mixed states $\rho_{A-sep}$ (2.33), the quantum Fisher information is (5.68). Thus, if $F[\rho_\ell, J_\alpha] > N$ holds for a certain $\ell$, then, by continuity, $F[\rho_{A-sep}, J_\alpha] > N$ for a probability distribution $\pi = \{p_k\}_{k=0,...,N}$ suitably peaked around $k = \ell$, hence able to overcome the shot-noise limit. On the other hand, from the previous section we know that for all such mixed states $\xi^2_W > \xi^2_S > 1$; therefore, based on this lower bound to the squeezing parameter, we would wrongly discard such states as not useful for metrological applications.
5.4 Heisenberg limit

In this section, we address the problem to achieve exactly the Heisenberg limit, that is \( \delta^2 \theta = 1/N^2 \). From (5.58), in order to get the Heisenberg limit the quantum Fisher information has to be maximum \( F[\rho, J_\hat{\theta}] = N^2 \) (see equation (5.63)). Since the quantum Fisher information is a convex function of \( \rho \), as proved in the appendix E, its maximum is reached for pure states. Moreover, the quantum Fisher information is invariant under Bogolubov transformations. For pure states the quantum Fisher information is proportional to the variance of \( J_\hat{\theta} \): \( F[\rho, J_\hat{\theta}] = 4\Delta_\rho^2 J_\hat{\theta} \). In order to maximize the variance of \( J_\hat{\theta} \), we chose an equal weighted superposition of an eigenvector of \( J_\hat{\theta} \) attaining the minimum eigenvalues and of an eigenvector of \( J_\hat{\theta} \) attaining the maximum eigenvalues. For convenience, we can fix this freedom such that the operator \( J_\hat{\theta} \) generates a local interferometer \( \hat{n} = \hat{z} \). Thus, the most general states that achieves the Heisenberg limit are the so-called \( N_00N_\phi \) states

\[
|N00\phi\rangle \equiv \frac{1}{\sqrt{2}} \left[ (a_1^\dagger)^N + e^{i\phi} (a_2^\dagger)^N \right] |0\rangle = \frac{|N,0\rangle + e^{i\phi}|0,N\rangle}{\sqrt{2}}, \quad (5.79)
\]

\[
F[|N00\phi\rangle \langle N00\phi|, J_\hat{\theta}] = N^2. \quad (5.80)
\]

5.5 Fluctuating particle number

Until now, we focused on a system with a fixed number of identical Boson. These systems are described by states without coherent superposition among states with different numbers of particles. In this section we will focus on some interesting results, that arise when we allow superposition of states with different numbers of particles.

Before starting the discussion, it is useful to shed light into the definition of shot-noise for a system of \( N \) fixed identical Bosons in order to generalize it. The shot-noise is the best accuracy we can get with “classical” states. Since the best accuracy is equivalent to maximize the quantum Fisher information that is convex (E.25), we can refer only to pure states. The classical states of one-dimensional particles, or single modes with an unconstrained number of particles, e.g. in quantum optics, are the standard coherent states (D.1). The classical states of the \( SU(2) \) Lie algebra, defined by (5.3), are the so-called coherent-like states:

\[
|\xi, \varphi; N\rangle = \frac{1}{\sqrt{N!}} \left( \sqrt{\xi} e^{i\varphi} a_1^\dagger + \sqrt{1-\xi} e^{-i\varphi} a_2^\dagger \right)^N |0\rangle. \quad (5.81)
\]

Some of their properties are stated in the appendix D, see also [10, 3, 26]. Therefore, the
shot-noise of a system with $N$ fixed identical Bosons, is defined by the minimal accuracy, i.e. the maximal quantum Fisher information, achievable with a coherent-like state.

The quantum Fisher information of any coherent-like state is actually bounded by $N$. It is enough to show that the quantum Fisher information is bounded by $N$ for $J_{\vec{z}} = J_z$ and any coherent-like state. Indeed, the rotation that transforms the operator $J_z$ into a general operator $J_{\vec{n}}$ is a Bogolubov transformation

$$b_1 = \sqrt{\epsilon} e^{\frac{\epsilon}{2}} a_1 + \sqrt{1 - \epsilon} e^{-\frac{\epsilon}{2}} a_2, \quad b_1 = -\sqrt{1 - \epsilon} e^{\frac{\epsilon}{2}} a_1 + \sqrt{\epsilon} e^{-\frac{\epsilon}{2}} a_2. \quad (5.82)$$

Any Bogolubov transformation moves coherent-like states into coherent-like states, changing the parameters $\xi$ and $\phi$. The quantum Fisher information is

$$F[|\xi,\phi;N⟩⟨\xi,\phi;N|, J_z] = 4N\xi(1 - \xi) \leq N, \quad (5.83)$$

where the inequality holds because $0 \leq \xi \leq 1$. The coherent-like states are also the most stable against noises [158]. It means that any other state affected by a dissipative dynamics deviates from itself much more than the coherent-like states. Therefore, the states that are harder to be destroyed in the experiments can not beat the shot-noise.

Now, consider coherent superpositions of states with different numbers of two-mode Bosons:

$$\sum_{n,m} c_{n,m} (a_1^\dagger)^m (a_2^\dagger)^n |0⟩, \quad \sum_{n,m} |c_{n,m}|^2 = 1. \quad (5.84)$$

These coherent superpositions can be forbidden by imposing the superselection rule that the total number of particles be conserved, so that any quantum state is a statistical mixture of eigenstates of the operator $N_{12} = a_1^\dagger a_1 + a_2^\dagger a_2$ and all meaningful observables must commute with it. Indeed, the operator $N_{12}$ is effectively a c-number that is conserved in each eigenspace, and at most incoherent fluctuation are allowed. Allowing the states (5.84) is equivalent to breaking the superselection rule. This fact has two physical consequences: the first one is to allow quantum fluctuations of the total number of particles, the second one is the existence of a second phase reference frame corresponding to a second party. Let us consider two observers relative to two different reference frames for the phase conjugated to the total number of particles, where $\phi$ is the angle relating them. If the first observer prepares the state $|\psi⟩$, the second observer describes the same state as $e^{i\phi N_{12}}|\psi⟩$ in his reference frame, where $e^{i\phi N_{12}}$ is the phase-shift needed to change the reference frame. The existence of reference frames is implied by the addressability of any phase-shift $e^{i\phi N_{12}}$. The phase $\phi$ can be completely controlled and measured by means of operators which do not commute with $N_{12}$. On the other hand, if the second observer does
not have any information about the phase relating the two reference frames, he describes the state as an incoherent unbiased average

$$\rho = \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{i\phi N_{12}} |\psi\rangle \langle \psi| e^{-i\phi N_{12}} = \frac{1}{2\pi} \sum_{N,N'} e^{i\phi N} P_N |\psi\rangle \langle \psi| P_{N'} e^{-i\phi N'} = \sum_N P_N |\psi\rangle \langle \psi| P_N,$$

(5.85)

where $P_N$ is the projector onto the eigenspace of $N_{12}$ with eigenvalue $N$. Biased averages are allowed for partial knowledge of $\phi$. Therefore, the lack of a reference frame is equivalent to forbidding coherent superpositions of states belonging to different eigenspaces of $N_{12}$. Moreover, being restricted to states (5.85) means that all meaningful observables commute with $N_{12}$. Such observables are $O = \sum_N O_N P_N$, and can not distinguish between the state $|\psi\rangle \langle \psi|$ and $\rho$:

$$\langle \psi| O |\psi\rangle = \sum_N \langle \psi| P_N O_N P_N |\psi\rangle = \text{Tr}(\rho O).$$

(5.86)

However, there is a widespread belief that the number of particles should be conserved forbidding fluctuations, at least in a non-relativistic regime. Indeed, we can restore the superselection rule of the total number of particles adding additional modes, which play the role of a reference frame [61]. Let us consider a third mode $(a_3, a_3^\dagger)$ and the following eigenstate of the total number of particles $N_T = a_1^\dagger a_1 + a_2^\dagger a_2 + a_3^\dagger a_3$

$$\sum_{n,m \in \mathbb{Z}} c_{n,m} (a_1^\dagger)^n (a_2^\dagger)^m (a_3^\dagger)^{N-n-m} |0\rangle = \sum_{n,m \in \mathbb{Z}} c_{n,m} |n, m, N - n - m\rangle_{123}. \quad (5.87)$$

We used the eigenvalues of the operators $a_1^\dagger a_1, a_2^\dagger a_2$ and $a_3^\dagger a_3$ as quantum numbers in order to write the states (5.87). We can choose the eigenvalues of the operators $a_1^\dagger a_1, a_2^\dagger a_2$ and $N_T$ as quantum numbers, writing the same state as

$$\sum_{n,m \in \mathbb{Z}} c_{n,m} |n, m, \rangle_{12} |N\rangle_T. \quad (5.88)$$

As discussed in sections 2.3.1, 2.3.4 and [31, 60], this change of quantum numbers corresponds to a change of the tensor product structure from $P_N \mathbb{F}^{123} P_N$ to the new one $(\bigoplus_{M=0}^N P_M \mathbb{F}^{12} P_M) \otimes \mathbb{C}$, where $P_N$ is the projector onto the subspace of $N$ fixed particles, $\mathbb{F}^{123}$ is the Fock space of a three-mode system, $\mathbb{F}^{12}$ is the Fock space of a two-mode system, and $\mathbb{C}$ is the unidimensional Hilbert space spanned by the vector $|N\rangle_T$. In this section,
we consider a tensor product structure which identifies the mode degrees of freedom in the formalism of the second quantization. It should not be confused with the more usual tensor product structure which identifies the particles in the formalism of the first quantization. Since the third quantum number is the total number of particles, it has the same value for every state. Therefore, tracing out the third quantum number gives the state (5.84). For a review on superselection rules, see [61] and reference therein.

In the light of these remarks, there are several possible choices states of two-mode Bosons without superselection rules which are closest to classical states. The first one are the standard two-mode coherent states

\[
|\alpha_1\rangle|\alpha_2\rangle = e^{\alpha_1 a_1^\dagger}a_1|0\rangle = e^{\alpha_2 a_2^\dagger}a_2|0\rangle, \quad j = 1, 2. \tag{5.89}
\]

The second one is the embedding of the standard two-mode coherent states into a three-mode state with a fixed number of particles:

\[
|\alpha_1, \alpha_2; N\rangle = e^{-|\alpha_1|^2 - |\alpha_2|^2} \sum_{0\leq n, m \leq N} \frac{\alpha_1^n \alpha_2^m}{\sqrt{n! m!}}|n, m\rangle|N - n - m\rangle. \tag{5.90}
\]

The third choice is a generalization of coherent-like states (5.81) for three-mode Bosons:

\[
|\xi_{1,2}, \varphi_{1,2}; N\rangle = \frac{1}{\sqrt{N!}} \left( \sqrt{\xi_1} e^{i\varphi_1} a_1^\dagger + \sqrt{\xi_2} e^{i\varphi_2} a_2^\dagger + \sqrt{1 - \xi_1 - \xi_2} a_3^\dagger \right)^N |0\rangle. \tag{5.91}
\]

We now look for the sharp upper bound of quantum Fisher information evaluated for these classical states and an operator \(J_n\), which defines the shot-noise. The quantum Fisher information for the states (5.89) and (5.90) is

\[
F[|\alpha_1\rangle|\alpha_2\rangle|\alpha_1, \alpha_2; N, J_n] = \langle \alpha_1|\alpha_2|N_{12}|\alpha_1, \alpha_2; N, J_n \rangle \tag{5.92}
\]

\[
F[|\alpha_1, \alpha_2; N\rangle|\alpha_1, \alpha_2; N, J_n] = \langle \alpha_1, \alpha_2; N|N_{12}|\alpha_1, \alpha_2; N \rangle. \tag{5.93}
\]

On the other hand, it is enough to compare the quantum Fisher information for states as in (5.91) and the operator \(J_z = J_z\). The rotation that transforms the operator \(J_z\) into a general operator \(J_n\) is a Bogolubov transformation (5.82), which transforms coherent-like states into coherent-like states, changing the parameters \(\xi_{1,2}\) and \(\varphi_{1,2}\). The quantum Fisher information is
\[ F_1(5.95) \]

\[ = \frac{4}{N} \langle \xi_{1,2}, \varphi_{1,2}; N | J_z \xi_{1,2}, \varphi_{1,2}; N \rangle^2 \leq \langle \xi_{1,2}, \varphi_{1,2}; N | N_{12}^2 \xi_{1,2}, \varphi_{1,2}; N \rangle. \]

Therefore, a quantum state \( \rho \) beats the shot-noise if \( F[\rho, J_n] > \text{Tr}(\rho N_{12}) \), i.e. \( \delta^2 \theta < 1/\text{Tr}(\rho N_{12}) \).

The main result of this section is to show that a \( (\mathcal{A}_1, \mathcal{A}_2) \)-separable state can reach the sub-shot-noise even with the \( (\mathcal{A}_1, \mathcal{A}_2) \)-local interferometer generated by \( J_z \), when we extend our analysis to superpositions of states with different numbers of particles. As an example, we consider the state

\[ |\psi \rangle = \frac{1}{2} \left( \frac{a_1^\dagger}{\sqrt{n!}} + \frac{a_2^\dagger}{\sqrt{m!}} \right) \left( \frac{a_2^\dagger}{\sqrt{n!}} + \frac{a_3^\dagger}{\sqrt{m!}} \right) |0 \rangle = \frac{1}{2} (|n \rangle + |m \rangle) (|n \rangle + |m \rangle), \quad (5.95) \]

whose mean total number of particles is \( \langle \psi | N_{12} \psi \rangle = n + m \). The quantum Fisher information evaluated with the operators \( J_{x,y,z} \) reads

\[ F_1[|\psi \rangle \langle \psi |, J_x] = F_1[|\psi \rangle \langle \psi |, J_y] = n + m + \frac{(n + m)^2}{2} = \langle N_{12} \rangle + \frac{\langle N_{12} \rangle^2}{2}, \quad (5.96) \]

\[ F_1[|\psi \rangle \langle \psi |, J_z] = \frac{(n - m)^2}{2} = \frac{\langle N_{12} \rangle - 2m)^2}{2} = \frac{\langle N_{12} \rangle - 2m)^2}{2}. \quad (5.97) \]

The \( (\mathcal{A}_1, \mathcal{A}_2) \)-nonlocal interferometers generated by \( J_{x,y} \) give a quantum Fisher information which scales as \( O\left(\langle N_{12} \rangle^2 \right) \). The \( (\mathcal{A}_1, \mathcal{A}_2) \)-local interferometer generated by \( J_z \) as well does, if \( 2n \ll \langle N_{12} \rangle \) or \( 2m \ll \langle N_{12} \rangle \). Even if an \( (\mathcal{A}_1, \mathcal{A}_2) \)-local interferometer beats the shot-noise once fed with \( (\mathcal{A}_1, \mathcal{A}_2) \)-separable states, there is still a kind of non locality in the game. Indeed, once we add a third mode to restore the superselection rule, the state (5.95) becomes

\[ |\tilde{\psi} \rangle = \frac{1}{2} \left( (a_1^\dagger)^n(a_2^\dagger)^m(a_3^\dagger)^{N-2n} + (a_1^\dagger)^m(a_2^\dagger)^n(a_3^\dagger)^{N-2m} + \right. \]

\[ + \left. \left( (a_1^\dagger)^n(a_3^\dagger)^m + (a_2^\dagger)^m(a_3^\dagger)^n \right) (a_3^\dagger)^{N-n-n} \right) |0 \rangle = \]

\[ = \frac{1}{2} \left( |n, n \rangle |N - 2n \rangle + |m, m \rangle |N - 2m \rangle + (|n, m \rangle + |m, n \rangle) |N - n - m \rangle \right). \quad (5.98) \]

Therefore, the nonlocal resource is the entanglement between the two modes describing the double well and the third mode representing the reference frame.
5.6 Localization and identification of particles

In the previous sections, we stressed the difference between distinguishable qubits and identical two-mode Bosons. In this section, we want to discuss how to switch between the two cases. This issue is interesting since interferometric experiments with BEC are discussed according to the theory of spin squeezing and quantum metrology applied to distinguishable particles [192, 194, 195]. Results that hold for distinguishable qubits are then naively extended to identical two-mode Bosons. Therefore, it makes sense to discuss how identical particles turn into distinguishable, in order to see which relations remain valid and which do not in the transition. Identical particles are not addressable: their formal label is a dummy index and every state and operator must be symmetric under any permutation of that index. In order to make them distinguishable, we need an additional degree of freedom. After performing some operations, the new degree of freedom may play the role of a label. A similar analysis is discussed in [79].

Let us start with a general state of \( N \) identical Bosons. In the formalism of the first quantization, it reads

\[
|\psi\rangle = \sum_{\{x_j,\sigma_j\}} c_{\{x_j,\sigma_j\}} \left( \bigotimes_{j=1}^{N} |x_j\rangle \otimes |\sigma_j\rangle \right), \quad \sum_{\{x_j,\sigma_j\}} |c_{\{x_j,\sigma_j\}}|^2 = 1, \tag{5.99}
\]

where \( x_j \) and \( \sigma_j \) label two degrees of freedom of the \( j \)-th particle, for instance the position and the hyperfine level, for instance in a system of ultracold atoms trapped by a two-well potential. The coefficients \( c_{\{x_j,\sigma_j\}} \) are completely symmetric under any simultaneous permutation of \( \{x_j\} \) and \( \{\sigma_j\} \) (i.e. of the dummy index \( j \) labelling but not addressing the particles). In the second quantization, the previous state reads

\[
|\Psi\rangle = \sum_{\sum_{n_{x,\sigma}} n_{x,\sigma} = N} C_{\{n_{x,\sigma}\}} \prod_{x,\sigma} (a_{x,\sigma}^\dagger)^{n_{x,\sigma}} |0\rangle, \quad \sum_{\sum_{n_{x,\sigma}} n_{x,\sigma} = N} |C_{\{n_{x,\sigma}\}}|^2 = 1, \quad [a_{x,\sigma}, a_{x',\sigma'}^\dagger] = \delta_{x,x'} \delta_{\sigma,\sigma'}, \tag{5.100}
\]

where \( x \) and \( \sigma \) label the degrees of freedom of the single particle, and \( n_{x,\sigma} \) counts the number of particles in the mode \( (x,\sigma) \). In some experiments with BEC [194, 195], the useful information for quantum metrology is encoded in the hyperfine degree of freedom \( \sigma \). Thus, the position \( x \) may be used to localize and distinguish the particles. When all the modes in the state \( |\Psi\rangle \) share the same spatial mode, we get a state with a single effective degree of freedom:
\[ |\Psi \rangle = \sum_{n_{\sigma}} \hat{C}_{(n_{\sigma})} \prod_{\sigma} \left( a_{\sigma}^{\dagger} \right)^{n_{\sigma}} |0\rangle, \quad a_{\sigma} = \sum_{x} f_{x} a_{x,\sigma}, \quad (5.101) \]

where \( f_{x} \) is any function such that \( \sum_{x} |f_{x}|^2 = 1 \). The latter state can not distinguish the particles. The states exploited in the experiments with BEC \([194, 195]\) belong to this class.

On the other hand, if there are some correlations between the two degrees of freedom \( x = x(\sigma) \), e.g. \( x(\sigma) \neq x(\sigma') \) if \( \sigma \neq \sigma' \), then the particles are effectively localized and then spatially distinguishable.

Since we are going to discuss the transition between identical and distinguishable particles, it is more convenient to adopt the formalism of the first quantization. In order to distinguish the particles we have to correlate the two degrees of freedom, such that one, let say the spatial one \( x \), may serve as a label. Thus, we have to confine the particles in not overlapping regions \( V_{j} \). This localization is performed by spatial measurement described by the symmetrized projector

\[ P_{V}^{\text{sym}} = \sum_{\mathcal{P}} \left( \prod_{j=1}^{N} \left( P_{V_{\mathcal{P}(j)}} \otimes \Lambda_{\mathcal{P}(j)} \right) \right) |\psi \rangle \otimes |\sigma_{j} \rangle, \quad (5.102) \]

where we summed over all permutations \( \mathcal{P} \) of the index \( j \) and \( g_{x} \) is any function such that \( \sum_{x \in V_{j}} |g_{x}|^2 = 1 \ \forall j \). The latter operator need to be symmetric, i.e. invariant under any permutation of particles, since it acts on a state of identical particles. The result of the localization is the state

\[ P_{V}^{\text{sym}}|\psi \rangle = \sum_{\mathcal{P}} \left( \sum_{(\sigma_{j})} \left( \sum_{(x_{j} \in V_{\mathcal{P}(j)})} \hat{g}_{x_{j}} \right) \prod_{j=1}^{N} |V_{\mathcal{P}(j)} \rangle \otimes |\sigma_{j} \rangle \right). \quad (5.103) \]

If we want to use the spatial localization as a way to address each single particle, as far as the hyperfine levels are concerned, we have to consider only the following operators

\[ \text{span} \left\{ \sum_{\mathcal{P}} \left( \prod_{j=1}^{N} \left( P_{V_{\mathcal{P}(j)}} \otimes \Lambda_{\mathcal{P}(j)} \right) \right) \right\}_{|\Lambda_{j} \rangle}, \quad (5.104) \]

where \( \Lambda_{j} \) is an operator acting on the hyperfine states. If all the operators \( \Lambda_{j} \)'s are the identity, we recover the operator of localization \( P_{V}^{\text{sym}} \) (5.102). The operator (5.104) is
still symmetric, as it must be since it acts on states of identical particles. Moreover, the product of two operators of the form (5.104) still belongs to the same class

\[ \sum_{\mathcal{P}} \bigotimes_{j=1}^{N} \left( P_{V_{\mathcal{P}(j)}} \otimes \Lambda_{\mathcal{P}(j)} \right) = \sum_{\mathcal{P}} \bigotimes_{j=1}^{N} \left( P_{V_{\mathcal{P}(j)}} \otimes \Lambda_{\mathcal{P}(j)} \Lambda_{\mathcal{P}'(j)} \right), \]  

(5.105)

because the regions \{V_j\} do not overlap, \( P_{V_j} P_{V_{j'}} = \delta_{j,j'} P_{V_j} \). Now, we notice that we have introduced correlations between the two degrees of freedom: any operation on the hyperfine levels of the \( j \)-th unaddressable particle is locally performed in the spatial region \( V_j \). The outcomes of a localization experiment are the expectation values of operators of the form (5.104) with respect to the state \( |\psi\rangle \). Since the operators (5.104) and the states \( |\psi\rangle \) are both symmetric, we get the same result if we compute the expectations of

\[ \sum_{\mathcal{P}} \bigotimes_{j=1}^{N} \left( P_{V_{\mathcal{P}(j)}} \otimes \Lambda_{\mathcal{P}(j)} \right) \]  

with respect to the state \( |\psi\rangle \) for any fixed permutation \( \mathcal{P} \). Alternatively, exploiting the property (5.105) and the symmetry of both the operators and the state \( |\psi\rangle \), we get

\[ \Lambda \in \text{span} \left\{ \sum_{\mathcal{P}} \bigotimes_{j=1}^{N} \left( P_{V_{\mathcal{P}(j)}} \otimes \Lambda_{\mathcal{P}(j)} \right) \right\} \Rightarrow \]

\[ \Rightarrow \langle \psi | \Lambda | \psi \rangle = \langle \psi | P_{V}^{\text{sym}} \Lambda P_{V}^{\text{sym}} | \psi \rangle = \langle \psi | \bigotimes_{j=1}^{N} P_{V_{\mathcal{P}(j)}} \Lambda \bigotimes_{j=1}^{N} P_{V_{\mathcal{P}'(j)}} | \psi \rangle, \]  

(5.106)

for any fixed permutation \( \mathcal{P} \). Thus, we can effectively consider a not symmetrized localized state

\[ \bigotimes_{j=1}^{N} P_{V_{\mathcal{P}(j)}} | \psi \rangle = \sum_{\{\sigma_j\}} \left( \sum_{\{x_j\} \in V_{\mathcal{P}(j)}} c_{\{x_j,\sigma_j\}} \prod_{j=1}^{N} g_{x_j} \right) \bigotimes_{j=1}^{N} | V_{\mathcal{P}(j)} \rangle \otimes | \sigma_j \rangle. \]  

(5.107)

In other words, we can localize the particles and act locally on their hyperfine levels. This is equivalent to use the states \( |V_j\rangle \) to label and identify the particles. In the formalism of the second quantization, This procedure corresponds to consider only the subalgebra generated by the operators \( \{a_{V_{j,\sigma}}, a_{V_{j,\sigma}}^{\dagger}\} \), where \( a_{V_{j,\sigma}} = \sum_{x \in V_j} g_x a_{x,\sigma} \). Since \( [a_{V_{j,\sigma}}, a_{V_{j',\sigma'}}^{\dagger}] = \delta_{j,j'} \delta_{\sigma,\sigma'} \), we are considering sectors of the Fock space, corresponding to not overlapping regions \( V_j \), as if they were generated by different vacua.

In conclusion, once we allow only operations (5.104), the actual state of the system is either (5.103) or (5.107), which are equivalent as soon as we identify the spatial degrees
of freedom \( \{V_j\} \) with particle labels. In the physical situation of localized particles we can apply the standard notion and criteria of entanglement for distinguishable particles to the states (5.103) or (5.107), getting the same properties. Following the definition 2.3.1, the commuting subalgebras which identify non-locality among particles are

\[
A_j = \left\{ \sum_{p} 1^{(1)} \otimes \cdots \otimes 1^{(j-1)} \otimes \left( P_{V_{p(j)}} \otimes \Lambda_{p(j)} \right) \otimes 1^{(j+1)} \otimes \cdots \otimes 1^{(N)} \right\},
\]

where \( 1^{(l)} \) is the identity matrix on either the spatial and the hyperfine degrees of freedom of the \( l \)-th particle.
Part III

Conclusions
The focus of this thesis is upon coherent and decoherent effects in quantum many-body systems. A many-body system can play the role of an environment, whose effects on the coherence and entanglement of a smaller system deserve to be investigated. On the other hand, one can look at how the coherent and non-local features of the many-body system are affected by reversible transformations. In the part I, we outlined the motivations of the thesis, introduced some basic notion relative to the dissipative dynamics induced by the interaction with an environment, and then briefly reviewed the phenomenon of quantum entanglement.

In chapter 3, we have seen that two atoms, initially prepared in a separate state, can get entangled as a result of their independent interaction with a common bath made of thermal quantum fields even when their internal frequencies are unequal. This result is based on a novel Markovian approximation of the reduced atom dynamics, that allows to exhibit an explicit dependence on the time scale $\Delta t$, measuring the interval over which the atoms feel the presence of the environment. This conclusion contrasts with the one obtained through the usual weak coupling limit approach to the atom reduced dynamics; in that case, the entanglement power of the external environment is reduced to zero for atoms with unequal frequencies as a consequence of the procedure of taking the ergodic average. In the light of the discussed results, this conclusion appears however a mathematical artifact, originating in letting $\lambda$ go to zero and $\Delta t$ to infinity, conditions hardly met in actual physical situations. Because of the Riemann-Lebesgue lemma, the ergodic average, on which the so-called “rotating wave approximation” is based, is strictly justified only in the limit $\lambda \to 0$ and $\Delta t \to \infty$. Instead, for weakly coupled baths with finite $\Delta t$, environment assisted entanglement generation is always allowed, and can be controlled through the external parameters, the bath inverse temperature $\beta$ and the atom spatial separation $\ell$. All the above considerations are based on the condition (2.11) for entanglement enhancement; when satisfied, it assures that quantum correlations among the two atoms are generated as soon as $t > 0$. It is however unable to determine the fate of this quantum correlations as time increases and in particular in the asymptotically long time regime. On general grounds, one expects that the effects of decoherence and dissipation that counteract entanglement production be dominant at large times, so that no entanglement is left in the end. There are however instances in which the entanglement generated at the beginning of the evolution persists also for asymptotically long times [98, 148, 149]. In order to fully clarify this situation, a complete study and classification of the set of the steady states of the refined master equation (3.11-3.14) is necessary. Only partial results on the classification the steady states of completely positive quantum dynamical semigroups have been so far obtained [92, 108].

In chapter 4, we have proposed an approach to the study of open quantum systems based on quantum symplectic tomography. In many contexts the reduced dynamics of a
system coupled with its environment is modeled by phenomenological master equations with some general features, but with unknown parameters. Hence, it would be highly appealing to find a way to assign some values to these parameters. We have tackled this problem for a wide class of Markovian and non-Markovian Gaussian-shape-preserving master equations. The key point of our approach lies in using Gaussian states as probes, as information on the dissipative dynamics can be inferred via a limited number of tomograms. For the non-Markovian master equations, we have proposed two alternative procedures, integral and differential, to reconstruct the unknown quantities. In order to provide an explicit example of how these different approaches work, we have applied them to a benchmark model made up of a harmonic oscillator coupled to a Bosonic bath, whose unknown parameters are the coupling constant, the temperature and the bath frequency cut-off.

Besides measuring unknown parameters, our procedure proves useful also in case those are already known. Indeed, it could be employed as a preliminary consistency test for the adopted master equation, when the reconstruction procedure assumes that the time-dependent master equation coefficients are previously known functions of a set of time-independent quantities. This is for example the case of a microscopical derivation (and related approximations) of the master equation. In this perspective, the agreement between the measured and theoretically expected time-independent parameters provides a necessary validity condition for the adopted approximation scheme. Along the same line of thought, we also extended this approach to the reconstruction of the whole set of time-dependent master equation coefficients. This provides a sound, reliable and complete experimental check of the goodness of the approximation scheme underlying a master equation.

This result leads to some interesting applications. Once retrieved the unknown master equation coefficients, it is possible to compute the dynamical evolution of any physical quantity whose analytical expression is known. The indirect-measurement scheme we propose could be then employed to make predictions on system loss of coherence due to the external environment. In order to perform this kind of analysis one can consider some quantities such as the spread and the coherence length in both position and momentum [133], provided their analytical expressions are available for an arbitrary time \( t \) (e.g. see [154]). Working in the coherent state representation, the evolution of the system of interest from an arbitrary initial state can be in principle predicted. Therefore, it is possible to perform the proposed indirect analysis of the decoherence processes. For example, if we consider an initial Schrödinger-cat state, highly interesting due to its potentially long-range coherence properties and its extreme sensitivity to environmental decoherence [127], we can re-write it as a combination of four Gaussian functions. Therefore, due to the linearity of the master equation, it can be possible to derive analytically the state
evolution and to analyze its loss of coherence by means of the procedure we propose. Furthermore, our procedure might also prove useful to test the theoretical predictions associated to a given model, such as the crossing of the Lindblad-non Lindblad border investigated in [143]. Our proposal opens up several interesting questions which are going to be the subject of further future investigation. In facts how our approach can be recast within an estimation theory perspective represents a relevant open scenario. Another relevant point to investigate is whether the proposed protocol can be enhanced by employing entangled Gaussian states as a probe. Finally, whether or not the proposed procedure can be generalized and employed in presence of memory kernels is a challenging question. Indeed, reconstructing the unknown parameters of Gaussian noisy evolutions with memory represents both a highly involved and interesting task.

In chapter 5, the standard notion of separability, holding for a many-body system made of \( N \) distinguishable particles, is replaced by a generalized one for a system of identical particles, that makes use of a “dual” language, focusing on the algebra \( \mathcal{A} \) of operators of the system instead of the set of its quantum states. One fixes a partition of \( \mathcal{A} \) in terms of a set of commuting subalgebras and defines as separable those states for which the associated expectation values of any factorized element of this partition can be written as a convex combination of products of expectation values. The notion of separability is thus linked to a specific partition of \( \mathcal{A} \), so that a given many-body state can be separable with respect to one partition, but result entangled with respect to a different one. Nevertheless, this generalized definition of separability reduces to the familiar one expressed in terms of the single-particle tensor product structure in the case of a system of distinguishable particles.

We have applied these considerations to the specific case of a system of \( N \) ultracold atoms trapped in an optical double-well potential, whose dynamics is very well captured by a two-mode Bose-Hubbard Hamiltonian. As we have seen, the second quantized language makes the application to this case of the new, generalized notion of separability very transparent and further allows the discussion of various related issues in quantum metrology. In fact, through state preparation and trapping potential control, this system has been shown to realize a highly sensitive Mach-Zhender interferometer, able to measure phase differences with a very high accuracy. Quite in general, the square error \( \delta^2 \theta \) in the determination of the phase difference \( \theta \) accumulated inside the interferometer is bounded by the inverse of the quantum Fisher information \( F \), whose value can not exceed \( N^2 \). This gives the smallest possible error in the estimation of the phase, \( \delta \theta \geq 1/N \), the Heisenberg limit, which, for large \( N \), is a huge improvement with respect to the standard shot-noise-limit, \( \delta \theta \geq 1/\sqrt{N} \).

In the case of a system of distinguishable particles, it has been proven that in order to beat the shot-noise-limit in the accuracy of the phase determination one needs to feed
the interferometer with suitably \( N \)-body entangled states. Indeed, one can show that for all separable states one has: \( F \leq N \); as a consequence, the condition \( F > N \) signals the presence of entanglement and at the same time allows \( \delta \theta \) to be smaller than \( 1 / \sqrt{N} \). When the interferometer is filled with identical particles, the condition \( F > N \) is no longer a univocal signal of state entanglement. Indeed, we have explicitly seen that in this case a quantum Fisher information larger than \( N \) may be obtained either via a non-local operation on separable states or via local operations on entangled states. Notice, however, that the notion of locality vs. non-locality and that of separability vs. entanglement need always to be referred to given algebraic bipartitions of the full algebra of observables.

Many-body entanglement has also been related to spin squeezing [181, 184, 185, 69, 70, 192, 193, 194, 195]. For instance, in the case of distinguishable particles, a state for which the inequality \( N (\Delta J_z)^2 \geq \langle J_z \rangle^2 + \langle J_x \rangle^2 \) is violated is surely entangled and spin squeezed. Actually, a complete set of inequalities obeyed by all separable states have been discussed in [77, 78]: violation of just one of them is enough to signal entanglement. Let us remark that in the case of a system of identical particles, some of these inequalities are violated even for separable states, thus losing their role as entanglement witness. In this respect, when dealing with systems of identical particles, spin squeezing does not seem an unambiguous, useful resource for quantum metrology.

More specifically, in relation to the actual realization of a BEC-based interferometric experiment with a double-well optical trap, beam-splitting is usually implemented through lowering and raising of the inter-well potential barrier, while the subsequent phase estimation is obtained through number counting of particles inside the two wells. The algebraic bipartition that is relevant in this case is thus the spatial bipartition \((A_1, A_2)\), where local observables are those that can be expressed as the product of operators pertaining to the first and second well, respectively. A sub-shot-noise accuracy in the determination of the phase difference \( \theta \) can then be obtained by acting with a non-local operation, \( i.e. \) a transformation generated by \( J_x \) or \( J_y \), on mode-separable states, \( e.g. \) the balanced Fock state \(|N/2, N/2\rangle\). Nevertheless, as shown in section 5.3.1, a different point of view can be equivalently adopted: it is based on an alternate measurement protocol, in which the energy bipartition \((B_1, B_2)\) becomes relevant. In this case, a local operation suffices to get a sub-shot-noise phase estimation accuracy, provided it acts on an entangled initial state. The practical realization of such a new type of BEC-based interferometer is surely an interesting experimental challenge.
Appendix

Some integrals

We indicate here how to compute the integrals that appear in the expressions of the Kossakowski matrix $C_{ij}^{(a)}$, (3.55) and (3.56), and in that of the effective Hamiltonian interaction term $H_{\text{eff}}^{(12)}$, (3.66) and (3.67). In the high temperature case, the explicit evaluation of (3.55) involves the computation of integrals of the following two types:

$$I_1 = \int_{-\infty}^{+\infty} dx \, \sin(c \, x) \, \text{sinc}(x - a) \, \text{sinc}(x - b) ,$$

$$I_2 = \int_{-\infty}^{+\infty} dx \, \sin(c \, x) \, \text{sinc}(x - a) \, \text{sinc}(x - b) ,$$

(A.1)

(A.2)

with $a, b, c$ positive constants. By decomposing the products of trigonometric functions in terms of linear combinations of sines and cosines, one can split e.g. $I_1$ into the sum of three simpler integrals:

$$I_1 = I_0 + I(c) - I(-c) ,$$

(A.3)

with

$$I_0 = \frac{\cos(a - b)}{2} \int_{-\infty}^{+\infty} dx \, \frac{\sin(c \, x)}{(x - a)(x - b)} ,$$

$$I(c) = \frac{1}{4} \int_{-\infty}^{+\infty} dx \, \frac{\sin((2 - c)x - a - b)}{(x - a)(x - b)} .$$

(A.4)

(A.5)

By first changing the integration variable to $y = (2 - c)x - a - b$ in $I(c)$, with $c \ll 2$, and then reducing the denominators in partial fractions in both integrands, one can express $I_0$ and $I(c)$ as combinations of the following integral (e.g. see [1]):

$$\int_{-\infty}^{+\infty} dx \, \frac{\sin(\alpha \, x)}{x + z} = \pi \cos(\alpha z) , \quad \alpha > 0 .$$

(A.6)
Explicitly, one finds:

\[ I_0 = -\pi \frac{\cos(a - b)}{a - b} \sin \left[ \frac{(a + b)c}{2} \right] \sin \left[ \frac{(a - b)c}{2} \right], \quad (A.7) \]

\[ I(c) = \frac{\pi}{4(a - b)} \left( \cos \left[ a(c - 1) + b \right] - \cos \left[ a + b(c - 1) \right] \right), \quad (A.8) \]

so that, recalling (A.3), one finally obtains:

\[ I_1 = \pi \sin \left[ \frac{(a + b)c}{2} \right] \sin \left[ \frac{(a - b)(1 - c/2)}{a - b} \right]. \quad (A.9) \]

This result holds for \( c \leq 2 \); when \( c > 2 \), one is forced to use a different integration variable in the expression of \( I(c) \) in (A.4)-(A.5), \( y' = (c - 2)x + a + b \), and as a result ends up with a vanishing value for \( I_1 \). As a function of the parameter \( c \), the integral \( I_1 \) is however continuous, since the expression in (A.9) also vanishes at the boundary point \( c = 2 \).

From the result (A.9), one further obtains:

\[ \lim_{c \to 0} \left( \frac{I_1}{c} \right) = \int_{-\infty}^{+\infty} dx \, x \, \text{sinc}(x - a) \, \text{sinc}(x - b) = \pi \left( \frac{a + b}{2} \right) \text{sinc}(a - b). \quad (A.10) \]

The integral \( I_2 \) in (A.2) can be evaluated using similar manipulations. When \( c \leq 2 \), one explicitly finds

\[ I_2 = \frac{\pi}{a - b} \left( \frac{\sin(ac/2)}{a} \sin \left[ a(1 - c/2) - b \right] + \frac{\sin(bc/2)}{b} \sin \left[ a - b(1 - c/2) \right] \right), \quad (A.11) \]

while for \( c > 2 \), a simpler expression holds:

\[ I_2 = \pi \, \text{sinc} \, a \, \text{sinc} \, b. \quad (A.12) \]

Here again one sees that \( I_2 \) is a continuous function of \( c \), since the expression in (A.11) reduces to the one in (A.12) at the boundary value \( c = 2 \). Further, from the expression in (A.11), one easily obtains the following limiting results:

\[ \lim_{c \to 0} \left( \frac{I_2}{c} \right) = \int_{-\infty}^{+\infty} dx \, \text{sinc}(x - a) \, \text{sinc}(x - b) = \pi \, \text{sinc}(a - b). \quad (A.13) \]

and similarly,

\[ \lim_{a,b \to 0} I_2 = c \int_{-\infty}^{+\infty} dx \, \text{sinc}(c \, x) \, (\text{sinc} \, x)^2 = \pi \, c \left( 1 - \frac{c}{4} \right). \quad (A.14) \]
The integrals appearing in the evaluation of the Hamiltonian contribution $H_{\text{eff}}^{(12)}$ can instead be all reduced to expressions of the form:

$$J = \int_{-\infty}^{+\infty} dx \cos(c x) \text{sinc}(x - a) \text{sinc}(x - b).$$  \hspace{1cm} (A.15)

With the help of manipulations similar to the one used above, $J$ can be reduced to combinations of the following integral [1]:

$$\int_{-\infty}^{+\infty} dx \frac{\cos(\alpha x)}{x + z} = \pi \sin(\alpha z), \quad \alpha > 0.$$  \hspace{1cm} (A.16)

When $c \leq 2$, the integral in (A.15) can be cast in the following form:

$$J = \pi \cos \left[ \frac{(a + b)c}{2} \right] \frac{\sin \left[ (a - b)(1 - c/2) \right]}{(a - b)},$$

while it vanishes for $c > 2$. In the limit of vanishing $a$ and $b$, it reduces to $J = \pi(1 - c/2)$. 
In this appendix the basic definitions of the representation of quantum states in the phase-space are sketched. For a review on the Weyl-Wigner-Moyal representation and its properties see [16]. In 1927, Weyl proposed a correspondence between functions on the phase-space and quantum mechanical operators [20]. Given a function $A(q, p)$ in its Fourier expansion

$$A(q, p) = \int dx \, dk \, e^{i(xq + kp)} \alpha(x, k),$$

(B.1)

we associate the quantum mechanical operator by exchanging the exponential function with the Weyl operator $e^{i(x\hat{q} + k\hat{p})}$. The operator reads

$$\hat{A}(q, p) = \int dx \, dk \, e^{i(x\hat{q} + k\hat{p})} \alpha(x, k).$$

(B.2)

In 1932, Wigner derived a representation of quantum states on the phase-space which has given rise of a lot of works and applications [21]. Even if Wigner stated a phase-space analogous only for density matrices, it can be defined for every operators as follows

$$W_A(q, p) = \frac{1}{\pi\hbar} \int_{-\infty}^{+\infty} dy \exp \left( \frac{i2py}{\hbar} \right) \langle q - y|\hat{A}|q + y \rangle,$$  

(B.3)

being the Wigner original formula if $A$ is a density operator.

In 1949, Moyal proved that the Weyl and the Wigner correspondences are equivalent [25]: $\mathcal{A}(q, p) = W_A(q, p)$. Therefore Wigner solved the inverse of the Weyl’s problem. Indeed, the Wigner function can be recast in terms of the so called characteristic function $\text{Tr}(\hat{A} \, e^{i(x\hat{q} + k\hat{p})})$.
\[ W_A(q, p) = \frac{1}{(2\pi\hbar)^2} \int dx \, dk \, e^{-\frac{i}{\hbar}(xq + kp)} \text{Tr}(\hat{A} e^{\frac{i}{\hbar}(x\hat{q} + k\hat{p})}), \quad (B.4) \]

\[ \text{Tr}(\hat{A} e^{\frac{i}{\hbar}(x\hat{q} + k\hat{p})}) = \int dq \, dp \, e^{\frac{i}{\hbar}(xq + kp)} W_A(q, p). \quad (B.5) \]

An explicit inverse formula of (B.3) is

\[ \hat{A}(q, p) = \int dx \, dk \, dq \, dp \, (2\pi\hbar)^2 e^{\frac{i}{\hbar}(x\hat{q} + k\hat{p})} e^{-\frac{i}{\hbar}(xq + kp)} W_A(q, p). \quad (B.6) \]

## B.1 Symplectic tomography

Given a time-evolving quantum state \( \rho(t) \) its Wigner function defines a generalization on phase-space of a classical probability distribution [21, 25] and is defined as

\[ W(q, p, t) = \frac{1}{\pi \hbar} \int_{-\infty}^{+\infty} dy \, \exp \left( \frac{i2py}{\hbar} \right) \rho(q - y, q + y, t). \quad (B.7) \]

If the system dynamics is described by a GSP master equation, and the initial state is Gaussian, the Wigner function preserves the Gaussian form of the state. Indeed, it can be expressed as a function of its first and second order momenta:

\[ W(q, p, t) = \frac{1}{2\pi \sqrt{\Delta q_t \Delta p_t - \sigma(q, p)_t^2}} \cdot \exp \left[ -\frac{\Delta q_t^2 (p - \langle p \rangle)_t^2 + \Delta p_t^2 (q - \langle q \rangle)_t^2 + 2\sigma(q, p)_t (q - \langle q \rangle)_t (p - \langle p \rangle)_t}{2[\Delta q_t^2 \Delta p_t^2 - \sigma(q, p)_t^2]} \right]. \quad (B.8) \]

Given the Wigner distribution of a quantum system, the Radon transform [19] represents the key ingredient to perform a tomographic analysis. This invertible integral transformation allows to retrieve the marginal probability densities of the system, i.e. the probability density along straight lines in phase space:

\[ X - \mu q - \nu p = 0. \quad (B.9) \]

The formal expression of the Radon transform, for a generic quantum state, is then given by

\[ \varpi(X, \mu, \nu) = \langle \delta(X - \mu q - \nu p) \rangle = \int_{\mathbb{R}^2} W(q, p, t)\delta(X - \mu q - \nu p) \, dq \, dp. \]
From equation (B.8) it follows that for a Gaussian wave packet the Radon transform can be explicitly written as:

\[ \varpi(X, \mu, \nu) = \frac{1}{\sqrt{2\pi}\sqrt{\Delta q^2\mu^2 + \Delta p^2\nu^2 + 2\sigma(q, p)\mu\nu}} \cdot \exp \left[ -\frac{(X - \mu \langle q \rangle - \nu \langle p \rangle)^2}{2[\Delta q^2\mu^2 + \Delta p^2\nu^2 + 2\sigma(q, p)\mu\nu]} \right], \] (B.11)

with the following constraint on the second cumulants:

\[ \Delta q^2\mu^2 + \Delta p^2\nu^2 + 2\sigma(q, p)\mu\nu > 0. \] (B.12)

This constraint is obeyed for each value of the parameters \( \mu \) and \( \nu \) if and only if \( \Delta q^2\Delta p^2 - \sigma(q, p)^2 > 0 \). This inequality is the Robertson-Schrödinger relation [22], that is a generalization of the Heisenberg principle.

Equation (B.10) also implies a homogeneity condition on the tomographic map, i.e. \( |c| \varpi(cX, c\mu, c\nu) = \varpi(X, \mu, \nu) \). This condition can be used in the choice of parameters \( \mu, \nu \). In fact, if one uses polar coordinates \((r, \theta)\), i.e. \( \mu = r \cos \theta, \nu = r \sin \theta \), the homogeneity condition can be used to eliminate the parameter \( r \). From equation (B.9) it emerges that the coordinates of the phase space need to be properly rescaled in order to have the same dimensions. For instance, we can set \( q \rightarrow \sqrt{\frac{\hbar}{\pi}} q \) and \( p \rightarrow \sqrt{\frac{1}{\hbar m}} p \). In particular if \( \omega = 0 \), i.e. for a free particle interacting with the environment, we can choose the same rescaling with a fictitious frequency defined by \( \hbar \tilde{\omega} = \Delta p^2_0/2m \), imposing \( q \rightarrow \frac{\Delta p_0}{\sqrt{2}\hbar} q \) and \( p \rightarrow \frac{1}{\sqrt{2\Delta p_0}} p \). In general, every rescaling assigning the same dimensions to \( q \) and \( p \) is suitable for our purpose.
Sampling theorems

Here we provide some details about the Nyquist-Shannon and the additive random sampling theorems, for a full review on this topic see [4, 5]. The simpler sampling theorem, known as Nyquist-Shannon theorem, deals with functions whose Fourier transform has a compact support. The theorem allows these functions to be reconstructed starting from a discrete and infinite set of values. The theorem is stated as follows:

**Theorem C.0.1** (Nyquist-Shannon theorem). *If a function \( F(t) \) has no frequency higher than \( W \), that is the support of its Fourier transform is contained in \([-2\pi W, 2\pi W]\), then it is completely determined by giving its ordinates at a series of points spaced \( \frac{1}{2W} \) apart. The reconstruction formula is*

\[
F(t) = \sum_{n=-\infty}^{\infty} F\left(\frac{n}{2W}\right) \frac{\sin(2\pi W t - n)}{\pi(2\pi W t - n)}.
\]  

(C.1)

The most frequent sources of error are the truncation error, the aliasing error, the round-off error and the jittering error. The truncation error arises from considering a finite sampling instead of an infinite one, as in practice it is unfeasible to sample and store an infinite number of values (unless some regular behavior of the function to reconstruct can be postulated). The aliasing error occurs whenever a function which is not band-limited is reconstructed by means of procedures suitable for band-limited functions which is often the case since band-limited functions are very peculiar. Whenever a truncation or an aliasing error occurs, it means that there are different functions matching the exploited sampling, anyway there exist conditions to bind this kind of errors [4, 5]. Whereas the two previous errors are sampling-related, whereas the round-off and the jittering error are linked to the precision of the experimental apparatus. In particular, the round-off error
is caused by errors affecting the sampling values and, finally, the jittering error is due to errors affecting the sampling times.

A remarkable generalization of the sampling theorem is developed in [6, 8] and requires an additive random sampling. The function is sampled at additively randomly chosen points \( t_n = t_{n-1} + \gamma_n \), where \( \{\gamma_n\} \) is a family of independent identically distributed random variables, whose probability distribution \( p(t) \) obeys the following constraints

\[
p(t) \in L^2(\mathbb{R}), \quad p(t) = 0 \quad \text{for} \quad t < 0, \quad \mathbb{E}[\gamma_n] = h < \infty, \quad (C.2)
\]

where \( \mathbb{E}[\cdot] \) is the expected value and \( h \) is the average spacing of the sampling. Additive random samplings may be alias-free, namely they may provide reconstructions without any aliasing error. As a consequence, non band-limited functions may as well be reconstructed. Examples of alias-free samplings are discussed in [6, 8]. The following theorem provides the condition for an additive sampling to be alias-free:

**Theorem C.0.2 (Additive random sampling).** An additive random sampling is alias-free if the characteristic function \( \phi(\omega) = \mathbb{E}[e^{j\omega t}] \) takes no values more than once on the real axis.

Conversely, if the characteristic function \( \phi(\omega) \) takes the same value at two different points of the open upper half-plane, then aliasing occurs with an additive random sampling.

The probability distribution \( p_n(t) \) of \( t_n \) is defined by the relations:

\[
p_n(t) = \int_{-\infty}^{\infty} dp_{n-1}(t-u)p(u) = \int_{0}^{\infty} dp_{n-1}(t-u)p(u),
\]

\[
p_1(t) = p(t). \quad (C.3)
\]

Since the functions \( p_n(t) \) are linearly independent [6], we can apply the orthogonalization procedure to them thus obtaining the orthonormal set \( \{q_n(t)\}_n \):

\[
\int_{0}^{\infty} d\tau q_n(t)q_m(t) = \delta_{n,m}. \quad (C.4)
\]

The function \( q_n(t) \) can be expressed as a linear combination of \( p_n(t) \):

\[
q_n(t) = \sum_{m=1}^{n} b_{n,m} p_n(t). \quad (C.5)
\]
To reconstruct the function $F(t)$, we define the averages

$$f_n = \int_{-\infty}^{\infty} d\tau p_n(t) F(t) = \int_{0}^{\infty} d\tau p_n(t) F(t), \quad \text{(C.6)}$$

where we have used $p_n(t) = 0$ (equation (C.2)). From equation (C.5), we get

$$\beta_n = \int_{0}^{\infty} d\tau q_n(t) F(t) = \sum_{m=1}^{n} b_{n,m} f_n, \quad \text{(C.7)}$$

The reconstruction formula can then be written as

$$F(t) = \sum_{n=1}^{\infty} \beta_n q_n(t), \quad \text{(C.8)}$$

where the sum converges in the $L^2$-norm. We emphasize that in this case the input sampling is not a countable set of values but rather a countable set of averages (C.6) as the sample spacing is a random variable itself and we make an average over all possible spacings. If the spacing distribution is highly picked on $h$, i.e. $p(t) = \delta(t - h)$, the spacing variance vanishes $\mathbb{E}[\gamma^2_n] = \mathbb{E}[\gamma_n]$, and the reconstruction procedure recovers the usual one with equally spaced samplings. If the spacing variance is comparable with its mean value $\mathbb{E}[\gamma^2_n] - \mathbb{E}[\gamma_n] \sim h^2$, then all spacings are highly probable and we get an effective continuous sampling. An unavoidable source of error in the implementation of this sampling theorem is that it involves functions defined on arbitrarily small times [6, 8] whereas any experimental apparatus exhibits a dead working time interval to record and process data. Finally we note that we want to reconstruct functions defined only for $t > 0$ hence we do not encounter any lower truncation error. The upper truncation error can be also avoided by reconstructing slightly different functions: $F(t)(1 - \theta(t - \bar{t}))$ instead of $F(t)$. The differences arise from the integral transforms involved in the reconstruction formula, but if we are interested in reconstructing functions in the experimentally accessible timescales, values greater than the threshold $\bar{t}$ of experimentally reachable times can be neglected. The same trick can be exploited to avoid errors due to a finite input size for an additive random sampling. Indeed if the sampling probability is well localized, each $p_n(t)$ is localized as well. The probabilities $p_n(t)$ localized at times larger than the threshold $\bar{t}$ do not contribute and the corresponding $f_n$ vanish.
Coherent states

In this appendix the definition and some properties of coherent states of the Heisenberg and the \(SU(2)\) or \(U(2)\) Lie algebras are stated. For a general review on coherent states of Lie groups and Lie algebras, see [10]. In the next section, we will show that, when the number of particles is large, the richer \(U(2)\) Lie algebra contracts in the Heisenberg Lie algebra and the corresponding coherent states identify with each other.

Standard coherent states for one mode are defined by one of the following equations

\[
a|\alpha\rangle = \frac{\alpha}{\sqrt{\hbar}} |\alpha\rangle, \quad |\alpha\rangle = e^{\frac{i\hbar}{2\sqrt{\hbar}} \alpha} |0\rangle = e^{\frac{i|\alpha|^2}{2\hbar}} \sum_{n=0}^{\infty} \frac{\alpha^n (e^\dagger)^n}{n! |\hbar|^n} |0\rangle, \quad (D.1)\]

where \(a^\dagger\) and \(a\) are respectively the creation and the annihilation operator of a single particle. Coherent states are not orthogonal: indeed

\[
\langle \beta | \alpha \rangle = e^{-\frac{|\alpha|^2}{\hbar}} e^{\frac{|\alpha|^2}{\hbar}} = e^{-\frac{1}{\hbar} |\alpha|^2}, \quad |\langle \beta | \alpha \rangle|^2 = e^{-\frac{1}{\hbar} |\alpha|^2}. \quad (D.2)\]

In order to get a completeness relation we need to normalize their integral by a factor \(\pi\):

\[
\frac{1}{\pi} \int d^2 \alpha |\alpha\rangle \langle \alpha| = 1, \quad (D.3)\]

where we put \(d^2 \alpha = d \text{Re} \alpha \, d \text{Im} \alpha\).

We shall develop some similarities between coherent states and coherent-like states of \(N\) identical Bosons, defined as

\[
|\xi, \varphi; N\rangle = \frac{1}{\sqrt{N!}} \left( \sqrt{\xi} e^{l_\varphi} a_1^\dagger + \sqrt{1-\xi} e^{-l_\varphi} a_2^\dagger \right)^N |0\rangle. \quad (D.4)\]
The first similarity we shall show concerns the action of annihilation operators on the coherent-like states. One can straightforwardly compute

\[ a_1 |\xi, \varphi; N \rangle = \sqrt{N} \xi |\xi, \varphi; N - 1 \rangle, \]  
(D.5)

\[ a_2 |\xi, \varphi; N \rangle = \sqrt{N(1 - \xi)} e^{-i\xi} |\xi, \varphi; N - 1 \rangle. \]  
(D.6)

Coherent-like states pertaining to subspaces with a different number of particles are actually orthogonal: \( \langle \xi, \varphi; N - 1 |\xi, \varphi; N \rangle = 0 \), whenever \( N \) is finite. However, if \( N \) goes to infinity, the subspaces with \( N \) and \( N - 1 \) particles become isomorphic. Physically speaking, adding the \( N \)-th particle to \( N - 1 \) Bosons in the same superposition state do not abruptly change the global features of the state. Therefore, coherent-like states behave as if they were eigenstates of the annihilation operators. This feature exactly holds for standard coherent states.

Coherent-like states are not orthogonal:

\[ \langle \eta, \vartheta; N |\xi, \varphi; N \rangle = \left( \xi \eta + (1 - \xi)(1 - \eta) + 2 \sqrt{\xi \eta (1 - \xi)(1 - \eta)} \cos(\vartheta - \varphi) \right)^{\frac{N}{2}} \cdot \]  
\[ \cdot e^{i N \tan(\frac{\vartheta - \varphi}{2}) \frac{\sqrt{1 - \xi(1 - \eta)}}{\sqrt{1 - \xi(1 - \eta)}}}. \]  
(D.7)

Coherent-like states as well form an overcomplete basis. In order to get a completeness relation, we need to normalize their integral by a suitable factor:

\[ \frac{N + 1}{2\pi} \int d\xi d\varphi |\xi, \varphi; N \rangle \langle \xi, \varphi; N| = 1. \]  
(D.8)

Furthermore, the ground state of a quadratic Hamiltonian in \( a_{1,2} \) and \( a_{1,2}^\dagger \) is a coherent-like state. Such a Hamiltonian makes coherent-like states evolve into coherent-like states. The Bose-Hubbard model provides a generic quadratic Hamiltonian, in the superfluid phase \( (U_{1,2}/T \ll 1) \), neglecting the interaction term \( U \). These features are satisfied by standard coherent states with respect to quadratic Hamiltonian in their creation and annihilation operators (alternatively in position and momentum).

For all these reasons, coherent-like states are good candidates to play the same role as standard coherent states, in the limit of large \( N \).
D.1 Contraction of the Lie algebra $U(2)$ to the Heisenberg Lie algebra $h(4)$

The similarities between standard coherent states and coherent-like states are consequences of a deeper algebraic connection, discussed in [3, 26]. The coherent-like states, termed coherent atomic states in [26], belong to the Fock space of $N$ identical Bosons, spanned by the Fock states (2.28). The subalgebra of quadratic polynomials in the creation and annihilation operators $a_{1,2}, a_{1,2}^\dagger$ which preserve the number of particles is the envelop of

$$J_x = \frac{1}{2}(a_1^\dagger a_2 + a_1 a_2^\dagger), \quad J_y = \frac{1}{2i}(a_1^\dagger a_2 - a_1 a_2^\dagger), \quad J_z = \frac{1}{2}(a_1^\dagger a_1 - a_2^\dagger a_2).$$

$1$ is the identity operator. The number operator $(a_1^\dagger a_1 + a_2^\dagger a_2)$ might as well be considered. However, it acts on the Fock space of $N$ (fixed) identical Bosons as the identity does.

Furthermore, we define the ladder operators

$$J_\pm = J_x \pm iJ_y.$$  \hspace{1cm} (D.10)

The sets $\{J_x, J_y, J_z\}$ and $\{J_+, J_-, J_z\}$ are representations of the Lie algebra $SU(2)$, while the sets $\{J_x, J_y, J_z, 1\}$ and $\{J_+, J_-, J_z, 1\}$ are representations of the Lie algebra $U(2)$, with respect to the following Lie brackets

$$[J_x, J_z] = iJ_z, \quad [J_y, J_z] = iJ_x, \quad [J_z, J_x] = iJ_y, \quad [J_x, J_y, J_z, 1] = 0, \quad [J_+, J_-, J_z, 1] = 0.$$  \hspace{1cm} (D.11)

Consider the following transformation

$$\begin{pmatrix} h_+ \\ h_- \\ h_3 \\ 1 \end{pmatrix} = A \begin{pmatrix} J_+ \\ J_- \\ J_z \\ 1 \end{pmatrix}, \quad A = \begin{pmatrix} c & 0 & 0 & 0 \\ 0 & c & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2c} \\ 0 & 0 & -\frac{1}{2c} & 1 \end{pmatrix}.$$  \hspace{1cm} (D.13)

As soon as $c \in (0, \infty)$, the transformation $A$ is not singular and we can define its inverse

$$A^{-1} = \begin{pmatrix} \frac{1}{c} & 0 & 0 & 0 \\ 0 & \frac{1}{c} & 0 & 0 \\ 0 & 0 & 1 & -\frac{1}{2c^2} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$  \hspace{1cm} (D.14)
The operators \( \{ h_+, h_-, h_3, 1 \} \) are a Lie algebra, satisfying the relations

\[
[h_+, h_-] = 2c^2 h_3 - 1 , \quad [h_3, h_\pm] = \pm h_\pm , \quad [h_\pm, 1] = 0 .
\]  
(D.15)

When \( c \) is finite, the transformation is invertible and the transformed Lie algebra is isomorphic to the original one. When \( c \to 0 \), the transformation \( A \) becomes singular and its inverse fails to exist. Nevertheless, the commutation relations (D.15) are well defined and identical to the commutation relations of the Heisenberg Lie algebra \( h(4) \). Such a transformation is called contraction of a Lie algebra. Thus, the original Lie algebra \( U(2) \), \( \{ J_+, J_-, J_z, 1 \} \), is contracted into the Heisenberg Lie algebra \( h(4) \), \( \{ h_+, h_-, h_3, 1 \} \), with respect to the usual Lie brackets (i.e. commutators). We can now identify

\[
h_+ \leftrightarrow a^\dagger , \quad h_- \leftrightarrow a , \quad h_3 \leftrightarrow a^\dagger a , \quad 1 \leftrightarrow 1 .
\]  
(D.16)

In a slightly different and more general approach to contractions of Lie algebra (see[3]), we can define new Lie brackets as

\[
[X, Y]_c = A^{-1} [AX, AY] .
\]  
(D.17)

The new Lie brackets of the \( U(2) \) Lie algebra reads

\[
[J_+, J_-] = 2c^2 J_z - 1 , \quad [J_z, J_\pm] = \pm J_\pm , \quad [J_\pm, 1] = 0 .
\]  
(D.18)

We have moved the effects of the transformation \( A \) from the operators to the Lie brackets. As \( c \to 0 \), the new Lie brackets are identical to the usual Lie brackets (commutators) of the Lie algebra \( h(4) \). Thus, we can state that the original \( U(2) \) Lie algebra, \( \{ J_+, J_-, J_z, 1 \} \), endowed with the usual Lie brackets (commutators) is contracted into the Heisenberg Lie algebra \( h(4) \), \( \{ J_+, J_-, J_z, 1 \} \), with respect to the new Lie brackets \( [X, Y]_c' = \lim_{c \to 0} [X, Y]_c \).

By consistency with the physical interpretation of the Heisenberg Lie algebra \( h(4) \), i.e. a quantum harmonic oscillator, we require that the lowest eigenvalues of \( h_3 \) vanishes. The latter condition corresponds to \( c = 1/\sqrt{N} \) [26]. After the singular transformation \( A \), as \( c \to 0 \), the coherent-like states become the usual coherent states of the contracted Heisenberg Lie algebra \( h(4) \) [26]. This limit corresponds to an infinite number \( N \) of Bosons.

Several properties of the standard coherent states holds for coherent-like states [3, 26], satisfying more involved relations due to the greater complexity of the Lie algebra \( U(2) \).

In conclusion, the standard coherent states and the coherent-like states are equivalent under the discussed Lie algebra contraction.
Appendix E

Estimation theory

In this appendix, we shall briefly review quantum estimation theory. Some seminal works and useful reviews on this topics are [176, 177, 178, 57, 179, 180, 182, 186, 188].

The goal of quantum estimation theory is to estimate parameters and physical quantities, even those not corresponding to Hermitian operators. Examples are time, phases, position both in quantum mechanics and quantum field theory, coupling constants, temperature, entanglement monotones, parameter governing unitary and dissipative dynamics. We can distinguish two kinds of theories. The global estimation theory looks for a POVM (Positive Operator Valued Measurement, i.e. a generalized not necessarily projective measurement [55]) minimizing a suitable cost function, averaged over all possible values of the parameters to be estimated. The resulting estimation is independent on the parameters one try to estimate. On the other hand, the local estimation theory minimizes the accuracy (e.g. the variance) of the estimation, once the parameters are fixed. Local estimation theory provides hopefully better performance, since the parameters are fixed, but the best estimation and its (minimal) accuracy depend on them. Quantum estimation theory provides generalized uncertainty relation, exploiting many generalized measurement (POVM), as it happens in data analysis and classical statistics (e.g. maximun likehood and minimum squares methods). In the following, we shall focus on local estimation theory with a single parameter.

E.1 Classical estimation theory

Here, we state the classical estimation theory, which gives the basis for the quantum generalization. The parameter to be estimated is $\lambda$. We call $\lambda_{\text{est}}$ its estimation. The estimation depends on a set $\{x_j\}_{1..M}$ of results of $M$ measurements. The conditioned probability
to measure $x_j$ given the value $\lambda$ is $p(x_j | \lambda)$. We define the average over all measurement as

$$\langle \cdot \rangle_\lambda = \int \left( \cdot \right) \prod_{j=1}^{M} dx_j p(x_j | \lambda).$$

(E.1)

We can define four different quantities giving the accuracy $\delta^2 \lambda$ of the estimation $\lambda_{\text{est}}$:

$$\langle (\lambda_{\text{est}} - \langle \lambda_{\text{est}} \rangle_{\lambda})^2 \rangle_{\lambda},$$

(E.2)

$$\langle (\lambda_{\text{est}} - \lambda)^2 \rangle_{\lambda},$$

(E.3)

$$\left\langle \left( \frac{\lambda_{\text{est}}}{d(\lambda_{\text{est}})} - \langle \lambda_{\text{est}} \rangle_{\lambda} \right)^2 \right\rangle_{\lambda},$$

(E.4)

$$\left\langle \left( \frac{\lambda_{\text{est}}}{d(\lambda_{\text{est}})} - \lambda \right)^2 \right\rangle_{\lambda}.$$  

(E.5)

The quantity (E.2) has two drawbacks. First it does not give a good accuracy for biased estimations, i.e. if $\langle \lambda_{\text{est}} \rangle_{\lambda} \neq \lambda$. Then it gives a wrongly scaled accuracy for an estimation $\lambda_{\text{est}}$ that has a different unit of measurement compared with the parameter $\lambda$. To correct the first drawback we can compare $\lambda_{\text{est}}$ directly with $\lambda$, instead of $\langle \lambda_{\text{est}} \rangle_{\lambda}$. This is done in the quantity (E.3). To correct the second drawback we can re-scale the estimation, as done in (E.4). The quantity (E.5) corrects both the drawbacks. For unbiased estimations, i.e. $\langle \lambda_{\text{est}} \rangle_{\lambda} = \lambda$, the previous quantities are all equivalent. For sake of simplicity, we shall deal with unbiased estimation. Thus, the accuracy of the estimation is $\delta^2 \lambda = \langle (\lambda_{\text{est}} - \langle \lambda_{\text{est}} \rangle_{\lambda})^2 \rangle_{\lambda}$.

Defining $\Delta \lambda = \lambda_{\text{est}} - \langle \lambda_{\text{est}} \rangle_{\lambda}$, the following identity is trivial

$$0 = \int \Delta \lambda \prod_{j=1}^{M} dx_j p(x_j | \lambda).$$

(E.6)

Differentiating by $\lambda$, we get

$$\int \left( \prod_{j=1}^{M} dx_j p(x_j | \lambda) \right) \left( \sum_{l=1}^{M} \frac{\partial}{\partial \lambda} \ln p(x_j | \lambda) \right) \Delta \lambda = \frac{d}{d \lambda} \langle \lambda_{\text{est}} \rangle_{\lambda} = 1.$$  

(E.7)

Applying the Cauchy-Schwartz inequality, we get

$$\left( \int \left( \prod_{j=1}^{M} dx_j p(x_j | \lambda) \right) \left( \sum_{l=1}^{M} \frac{\partial}{\partial \lambda} \ln p(x_j | \lambda) \right) \Delta \lambda \right)^2 \leq \left( \int \left( \prod_{j=1}^{M} dx_j p(x_j | \lambda) \right)^2 \right) \left( \int \left( \sum_{l=1}^{M} \frac{\partial}{\partial \lambda} \ln p(x_j | \lambda) \right)^2 \right).$$
\begin{align}
\delta^2 \lambda M F_{\text{cl}}[p(x|\lambda)] &\geq 1, \quad (E.10)
\end{align}

where the classical Fisher information \( F_{\text{cl}}[p(x|\lambda)] \) is defined as

\begin{align}
F_{\text{cl}}[p(x|\lambda)] &= \int dx p(x|\lambda) \left( \frac{\partial}{\partial \lambda} \ln p(x|\lambda) \right)^2 = \int dx \frac{1}{p(x|\lambda)} \left( \frac{\partial}{\partial \lambda} p(x|\lambda) \right)^2. \quad (E.11)
\end{align}

This bound is sharp and is saturated for \( M \to \infty \) by the maximum likelihood estimation. For finite \( M \), the bound is saturated only for some special distributions \( p(x|\lambda) \). The Fisher information is a convex function of the conditioned distribution \( p(x|\lambda) \) [7], that is

\begin{align}
F_{\text{cl}}[p(x|\lambda)] \leq \sum_k q_k F_{\text{cl}}[p_k(x|\lambda)], \quad (E.12)
\end{align}

if

\begin{align}
p(x|\lambda) = \sum_k q_k p_k(x|\lambda), \quad p_k(x|\lambda) \geq 0, \quad \int dx p_k(x|\lambda) = 1, \quad q_k \geq 0, \quad \sum_k q_k = 1. \quad (E.13)
\end{align}
E.2 Quantum estimation theory

In quantum mechanics a measurement is implemented by a POVM. A POVM is defined by a set of positive operators \( \{ E_x \} \), such that \( E_x \geq 0 \) and \( \int dxE_x = 1 \). Given a quantum density operator \( \rho \), to measure the outcome \( x \) corresponds to the operation \( \rho \rightarrow \sqrt{E_x} \rho \sqrt{E_x} \) and the probability to get the outcome \( x \) is \( p(x) = \text{Tr}(E_x \rho) \). If we want to estimate a parameter \( \lambda \) in a quantum context, we perform measurements on a family of states depending on \( \lambda \), \( \rho_\lambda \). Thus, the conditioned probability of the outcome \( x \) given the value \( \lambda \) is \( p(x | \lambda) = \text{Tr}(E_x \rho_\lambda) \). We define the symmetric symmetric logarithmic derivative as a Hermitian operator \( L_\lambda \) such that

\[
\frac{\partial}{\partial \lambda} \rho_\lambda = \frac{1}{2} \{ L_\lambda, \rho_\lambda \}.
\]

(E.14)

With these definitions we get

\[
\frac{\partial}{\partial \lambda} p(x | \lambda) = \text{Tr} \left( E_x \frac{\partial}{\partial \lambda} \rho_\lambda \right) = \text{Re} \left( \text{Tr} \left( \rho_\lambda E_x L_\lambda \right) \right),
\]

(E.15)

and the following expression for the Fisher information

\[
F_{cl} [p(x | \lambda)] = \int dx \frac{(\text{Re} (\text{Tr} (\rho_\lambda E_x L_\lambda)))^2}{\text{Tr}(\rho_\lambda E_x)}.
\]

(E.16)

The Fisher information depends on the parameter \( \lambda \), via the state \( \rho_\lambda \), and on the probability distribution of our outcomes, i.e. the POVM.

We now maximize the Fisher information over all possible POVMs. Instead of performing the maximization, we straightforwardly compute a sharp upper bound.

\[
F_{cl} [p(x | \lambda)] \leq \int dx \left| \frac{\text{Tr}(\rho_\lambda E_x L_\lambda)}{\sqrt{\text{Tr}(\rho_\lambda E_x)}} \right|^2 = \int dx \left| \text{Tr} \left( \sqrt{\rho_\lambda} \sqrt{E_x} \sqrt{E_x} \sqrt{\rho_\lambda} \right) \right|^2 \leq \int dx \text{Tr} \left( E_x L_\lambda \rho_\lambda L_\lambda \right) = \text{Tr} \left( L_\lambda \rho_\lambda L_\lambda \right) = \text{Tr} \left( \rho_\lambda L_\lambda^2 \right) = \text{Tr} \left( L_\lambda \frac{\partial}{\partial \lambda} \rho_\lambda \right) \equiv F_Q[\rho_\lambda].
\]

(E.17)

The first inequality of the previous formula is saturated if and only if \( \text{Tr}(\rho_\lambda E_x L_\lambda) \in \mathbb{R} \). The second inequality comes from the Cauchy-Schwartz inequality

\[
|\text{Tr}(A^\dagger B)|^2 \leq \text{Tr}(A^\dagger A) \text{Tr}(B^\dagger B), \quad \text{where} \quad A = \sqrt{E_x} \sqrt{\rho_\lambda} \quad \text{and} \quad B = \sqrt{E_x} L_\lambda \sqrt{\rho_\lambda}.
\]

(E.18)
and is saturated if and only if $A = B$. Both the inequalities are saturated if $\{E_x\}$ is the set of eigenprojectors of $L_\lambda$. It is a sufficient not necessary condition, as shown in [189]. The quantity $F_0[\rho_1]$ is called quantum Fisher information and together with the Cramér-Rao inequality gives a sharp, attainable, bound for the accuracy of our quantum estimation known as quantum Cramér-Rao bound or generalized uncertainty relation:

$$\delta^2\lambda M F_0[\rho_1] \geq 1.$$  \hfill (E.19)

The symmetric logarithmic derivative and the quantum Fisher information define the best accuracy of the estimation. They also define the measurement that minimize the accuracy and a possible unbiased estimator $O_\lambda = \lambda \mathbf{1} + \frac{L_\lambda}{F_0[\rho_1]}$. Indeed, since $\text{Tr}(\rho_\lambda L_\lambda) = \frac{d}{d\lambda} \text{Tr}(\rho_\lambda) = 0$, we get $\text{Tr}(\rho_\lambda O_\lambda) = \lambda$ and $\text{Tr}(\rho_\lambda O_\lambda^2) = \lambda^2 + \frac{1}{F_0[\rho_1]}$. Therefore, the average of the operator $O_\lambda$ with respect to the state $\rho_\lambda$ is an optimal unbiased estimation of the parameter $\lambda$, whose variance is $\text{Tr}(\rho_\lambda O_\lambda^2) - (\text{Tr}(\rho_\lambda O_\lambda))^2 = \frac{1}{F_0[\rho_1]}$.

Explicit basis-independent formulas for the symmetric logarithmic derivative and the quantum Fisher information are

$$L_\lambda = 2 \int_0^\infty dt e^{-\rho_\lambda t} \left( \frac{\partial}{\partial \lambda} \rho_\lambda \right) e^{-\rho_\lambda t}, \quad F_0[\rho_1] = 2 \int_0^\infty dt \text{Tr} \left( e^{-\rho_\lambda t} \left( \frac{\partial}{\partial \lambda} \rho_\lambda \right)^2 \right).$$  \hfill (E.20)

writing the spectral decomposition of the desity matrix $\rho_\lambda = \sum_n p_n(\lambda) |\psi_n(\lambda)\rangle \langle \psi_n(\lambda)|$, we get

$$L_\lambda = 2 \sum_{n,m} \frac{\langle \psi_m(\lambda)| \frac{\partial}{\partial \lambda} \rho_\lambda |\psi_n(\lambda)\rangle}{p_n(\lambda) + p_m(\lambda)} |\psi_m(\lambda)\rangle \langle \psi_n(\lambda)|,$$  \hfill (E.21)

$$F_0[\rho_1] = 2 \sum_{n,m} \frac{|\langle \psi_m(\lambda)| \frac{\partial}{\partial \lambda} \rho_\lambda |\psi_n(\lambda)\rangle|^2}{p_n(\lambda) + p_m(\lambda)},$$  \hfill (E.22)

where the sums are defined only for indices corresponding to $p_n + p_m \neq 0$.

The quantum Fisher information is convex, as a consequence of the convexity of the classical Fisher information. Let’s call $\bar{E}_x$ the POVM that maximaxes the classical Fisher information: $F_{cl}[\rho(x|\lambda)] \leq F_0[\rho_1] = F_{cl}[\bar{p}(x|\lambda)]$, where $\bar{p}(x|\lambda) = \text{Tr}(\rho_\lambda \bar{E}_x)$. Since the classical Fisher information is convex, we compute

$$F_{cl} \left[ \text{Tr}(\rho_\lambda \bar{E}_x) \right] \leq \sum_k q_k F_{cl} \left[ \text{Tr}(\rho_{k,\lambda} \bar{E}_x) \right].$$  \hfill (E.23)
if
\[ \rho_\lambda = \sum_k q_k \rho_{k,\lambda}, \quad \rho_{k,\lambda} \geq 0, \quad \operatorname{Tr} \rho_{k,\lambda} = 1, \quad q_k \geq 0, \quad \sum_k q_k = 1. \] (E.24)

The POVM that maximizes the classical Fisher information pertaining the state \( \rho_{k,\lambda} \) is \( \bar{E}^{(k)}_x \):
\[ F_{\text{cl}} \left[ \operatorname{Tr} \left( \rho_{k,\lambda} \bar{E}^{(k)}_x \right) \right] \leq F_{\text{cl}} \left[ \operatorname{Tr} \left( \rho_{k,\lambda} \tilde{E}^{(k)}_x \right) \right] = F_Q [\rho_{k,\lambda}]. \]
The POVM \( \tilde{E}^{(k)}_x \) is in general different from \( \bar{E}^{(k)}_x \), but by definition of quantum Fisher information
\[ F_{\text{cl}} \left[ \operatorname{Tr} \left( \rho_{k,\lambda} \bar{E}^{(k)}_x \right) \right] = F_{\text{cl}} \left[ \operatorname{Tr} \left( \rho_{k,\lambda} \tilde{E}^{(k)}_x \right) \right]. \]

Thus, from (E.23) we get
\[ F_Q [\rho_\lambda] = F_{\text{cl}} \left[ \operatorname{Tr} (\rho_\lambda \bar{E}_x) \right] \leq \sum_k q_k F_{\text{cl}} \left[ \operatorname{Tr} \left( \rho_{k,\lambda} \tilde{E}^{(k)}_x \right) \right] = \sum_k q_k F_Q [\rho_{k,\lambda}]. \] (E.25)

### E.2.1 Unitary paths of states

In this section, we focus on unitary paths of states
\[ \rho_\lambda = e^{-i(h-\chi)\lambda} \rho_0 e^{i(h-\chi)\lambda}, \quad \frac{\partial}{\partial \lambda} \rho_\lambda = -i[h, \rho_\lambda], \] (E.26)
where \( h = h^\dagger \) is a Hermitian operator, \( \chi \) is a c-number and no choice of \( \chi \) affects the path. This path changes the eigenvectors \( |\psi(\lambda)\rangle = e^{-i(h-\chi)\lambda} |\psi(0)\rangle \) of the states, but not its eigenvalues and its rank: \( \rho_\lambda = \sum_n p_n |\psi_n(\lambda)\rangle \langle \psi_n(\lambda)| \). The explicit formulas for the symmetric logarithmic derivative and the quantum Fisher information read
\[ L_\lambda = 2 \sum_{n,m} (\psi_m(0)|h-\chi|\psi_n(0)) \frac{p_n - p_m}{p_n + p_m} |\psi_m(\lambda)\rangle \langle \psi_n(\lambda)|, \] (E.27)
\[ F_Q [\rho_\lambda] = 2 \sum_{n,m} \frac{(p_n - p_m)^2}{p_n + p_m} (\psi_m(0)|h-\chi|\psi_n(0))^2. \] (E.28)

For pure states \( \rho_\lambda = |\psi(\lambda)\rangle \langle \psi(\lambda)| \), these formulas are very simplified. Exploiting \( \rho_\lambda = \rho_\lambda^2 \), we get
\[ \frac{\partial}{\partial \lambda} \rho_\lambda = \frac{\partial}{\partial \lambda} \rho_\lambda^2 = \left\{ \rho_\lambda, \frac{\partial}{\partial \lambda} \rho_\lambda \right\}, \] (E.29)
thus \( L_\lambda = 2 \frac{\partial}{\partial \lambda} \rho_\lambda \) and
\[ F_Q [\rho_\lambda] = \operatorname{Tr} \left( L_\lambda \frac{\partial}{\partial \lambda} \rho_\lambda \right) = -2 \operatorname{Tr} \left( [h, \rho_\lambda]^2 \right) = 4 \langle \psi(\lambda)|h^2|\psi(\lambda)\rangle - 4 \langle \psi(\lambda)|h|\psi(\lambda)\rangle^2 = \]
\[
4\Delta^2 \lambda h = 4\langle \psi(0)|h^2|\psi(0)\rangle - 4\langle \psi(0)|h|\psi(0)\rangle^2 = 4\Delta^2_0 h.
\] (E.30)

The quantum Fisher information of pure states is the variance of the generator \( h \), independent on \( \lambda \). The quantum Fisher information of mixed states is bounded by the variance of \( h \). Choosing \( \chi = \text{Tr}(\rho_\lambda h) \) in (E.28), we get

\[
F_Q[\rho_\lambda] \leq 2 \sum_{n,m} (p_n + p_m) (\psi_m(0)|h - \text{Tr}(\rho_\lambda h)|\psi_n(0))^2 = 4\text{Tr}(\rho_\lambda h^2) - 4(\text{Tr}(\rho_\lambda h))^2 = 4\Delta^2 h =
\]

\[
= 4\text{Tr}(\rho_\lambda h^2) - 4(\text{Tr}(\rho_\lambda h))^2 = 4\Delta^2_0 h.
\] (E.31)

The Cramér-Rao bound (E.10) now reads as an uncertainty relation

\[
\delta^2 \lambda \Delta^2 h \geq \frac{1}{4M},
\] (E.32)

being the bound sharp for pure states.

### E.2.2 Generalizations

There are some interesting generalizations of the above discussed quantum Fisher information. For instance, there are different definitions of Fisher informations, connected different distances in the Hilbert space [57, 180, 190]. The definition discussed above is connected to the Bures distance [186]. Moreover, different equivalent formulas of classical Fisher information give inequivalent quantum analogues [191]. There is also a generalization of the quantum Fisher information for multiple parameters. In this case, the quantum Fisher information becomes a matrix. However, the definition based on the symmetric logarithmic derivatives is no longer in general a sharp, attainable, bound for the covariance matrix of the estimation [179, 191].
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