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The Quantum-Classical Boundary: from Opto-Mechanics to Solid-State

Departamento de Física
Faculdade de Ciências da Universidade do Porto
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PhD Thesis supervised by Prof. João M. B. Lopes dos Santos

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To my adorable godfather
Joaquim Francisco Gonçalves Ferreira de Sousa
with love.
Acknowledgments

First I would like to thank my parents for being there for me throughout my studies, since primary school to university. I am also indebted to my godfather, who had been my inspiration since I was a little kid, not only for me but also to many people who had the chance to meet him. Unfortunately, he is not among us anymore, but he would have enjoyed sharing with me this enthusiastic journey through science. This thesis is dedicated to him.

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Resumo

Recentes avanços experimentais em vários campos da Física, desde a Óptica Quântica até ao Estado Sólido, trouxeram velhas questões da Mecânica Quântica para a linha da frente do debate científico. Até que ponto efeitos quânticos podem ser observados em sistemas grandes é ainda uma questão em aberto. Apesar disto, no laboratório, a fronteira quântica-clássica tem-se rapidamente movido em direcção ao mundo macroscópico: foi observada interferência em moléculas tão grandes quanto flurenos (1999, Viena), assim como sobreposição de currentes macroscópicas em dispositivos supercondutores de interferência quântica (2000, Nova Iorque).

Comum a todas estas experiências, é o fenómeno de perda de coerência; a irreversibilidade inevitável dos sistemas abertos, dita as escalas em que assinaturas quânticas podem ser observadas. A coerência quântica pode ser extremamente robusta, a saber, nos spins de electrões em defeitos de diamante devido ao grande hiato espectral destes materiais, mas pode ser muito frágil em sistemas massivos, dado os inúmeros canais de perda de coerência. Onde se encontra exactamente a fronteira quântica-clássica vai depender das peculiaridades do sistema físico em questão, em particular, da magnitude do acoplamento ao ambiente e a sua temperatura. Esta última grandeza, crê-se ser o principal obstáculo na obtenção de estados não-clássicos nas mais leves nano-estruturas mecânicas, onde nenhum efeito quântico foi ainda observado.

Motivados por estes desafios, e pela diferença fundamental entre correlações clássicas e entanglement, investigamos a fronteira quântico-clássica através das seguintes questões: podem correlações quânticas macroscópicas (e portanto, o comportamento quântico) persistir acima do limite de baixas temperaturas, e como podem estes efeitos ser usados, por exemplo, para correlacionar quanticamente outros sistemas?

A primeira parte é dedicada a um sistema paradigmático de opto-mecânica: mostra-se que as quadraturas de um estado coerente da luz e o movimento dum oscilador mecânico, acoplados através de pressão de radiação numa geometria de cavidade, podem ficar substancialmente correlacionados de forma genuinamente quântica. Inicialmente, consideramos um cenário ideal (isto é, sem perda de coerência) e, através dum procedimento de renormalização de subspaços do operador de estado, conjecturamos que o entanglement bipartido do sistema é robusto relativamente à temperatura. De seguida, num breve capítulo, discutimos um cenário realista onde uma fonte luminosa intensa é usada para popular uma cavidade com espelhos parcialmente reflectivos. É mostrado que um acoplamento efectivo, proporcional à amplitude interna da cavidade, surge no estado estacionário, o que confirma as conclusões tiradas acerca do sistema ideal: encontra-se entanglement macroscópico opto-mecânico persistente até temperatures muito acima da energia de ponto zero do oscilador mecânico.
Na segunda parte, focamo-nos num outro cenário promissor: a geração de entanglement robusto entre spins distantes, através de sistemas de Estado Sólido fortemente correlacionados. Com efeito, através de uma teoria de perturbações adequada, é estudado o problema de extracção de entanglement a partir destes sistemas. Inicialmente, consideram-se dois modelos de anti-ferromagnetismo a uma dimensão: a cadeia finita de Heisenberg e a cadeia infinita de Affleck-Kennedy-Lieb-Tasaki. Demonstramos que a geração de entanglement entre os dois spins, devido à interacção local com o sistema mediador, é extremamente eficiente: os spins adquirem entanglement quase completo mesmo a distâncias grandes. O cálculo do Hamiltoniano efectivo de interacção entre os spins, prova-se adequado para a investigação deste fenómeno em sistemas de muitos corpos de hiato finito e quando o acoplamento spin-sistema é fraco. No último capítulo, estes resultados são generalizados para possibilitar o cálculo das correlações spin-spin no regime não-perturbativo a temperatura finita. Comparando resultados analíticos com dados de Monte Carlo Quântico, é provada a existência de correlações quânticas nos spins a temperaturas muito mais elevadas do que anteriormente se julgava ser possível. Isto acontece no cenário bi-dimensional, devido ao surgimento de hiatos de energia consideráveis, mesmo em sistemas com um hiato intrínseco muito pequeno (desaparecendo no limite termodinâmico), devido apenas à presença dos spins externos.

A presente tese, mostra que as ferramentas de Informação Quântica podem ser usadas no sentido de melhor compreendermos a fronteira que separa o mundo quântico do mundo clássico em sistemas macroscópicos. As nossas descobertas sugerem uma forma de alargar esta fronteira em direcção ao mundo macroscópico, através do acoplamento dum espelho movível a um campo electromagnético confinado, e abrem novas possibilidades relativamente à computação e processamento de informação quântica em sistemas fortemente correlacionados a temperaturas realistas.
Summary

Recent experimental breakthroughs in miscellaneous fields of physics, from Quantum Optics to Solid State, have brought the old questions of Quantum Mechanics into the front line of scientific debate. To what extent bona fide quantum effects are observable in large systems is still an open question. Notwithstanding, in the laboratory, the quantum-classical boundary has been moving towards the macroscopic world very quickly: interference was observed in molecules as large as fullerenes (1999, Vienna) and superposition of macroscopic currents was achieved in superconducting quantum interference devices (2000, New York).

Common to all these experiments is the decoherence phenomenon; the unavoidable irreversibility of open systems, ultimately setting the scales where a quantum signature is hoped to be observed. The quantum coherence can be extremely robust, for instance, in single electron spins in diamond defects, due to its natural large gap to excited states, but can be extremely feeble in massive systems for many decoherence channels are available. Where the quantum-classical boundary exactly lies depends on the peculiarities of a given physical system and especially on the strength of coupling to the environment and on its temperature. In fact, it is believed that temperature is the main obstacle in achieving non-classical effects in light mechanical nanostructures where no quantum behaviour has been observed so far.

Motivated by these developments and the fundamental difference between classical correlations and entanglement, in this thesis we investigate the quantum-classical boundary by asking the following questions; can macroscopic quantum correlations, and thus quantum behavior, persist above the low-temperature threshold, and how such effects can be used, for instance, to entangle other systems?

In the first part, focusing on a paradigmatic opto-mechanical system, it is shown that the quadratures of a coherent state of light and the motion of a mechanical oscillator, coupled via radiation pressure in a cavity geometry, can be substantially quantum correlated. Initially, we consider an ideal scenario (i.e. no decoherence) and, by employing a renormalization procedure to finite dimensional subspaces of the complete density matrix, we conjecture that bipartite entanglement is very robust against temperature. The entropy of the subsystems discloses a macroscopic amount of quantum correlations and suggests that the mirror-light entanglement can be enhanced by adding more photons to the cavity. Afterwards, in a short chapter, we discuss a realistic scenario where a pumping bright source is used to populate a cavity with partially reflective mirrors. We show that an effective coupling emerges in the stationary regime that is proportional to the intra-cavity field amplitude, thus settling on solid grounds previous conclusions about the ideal system. We find opto-mechanical entanglement surviving at temperatures much above the mechanical oscillator’s ground state energy,
therefore overcoming the conventional criterion on temperature.

In the second part, we focus on yet another encouraging scenario, namely that of generating robust entanglement between distant spins by exploiting the highly correlated ground states of solid state systems. Indeed, by developing an adequate perturbation theory, we study the problem of entanglement extraction from non-critical many-body systems to probes endowed with a two-dimensional Hilbert space. Initially, we focus on two models of one-dimensional anti-ferromagnetism, namely the Heisenberg and the Affleck-Kennedy-Lieb-Tasaki spin chains, and show that entanglement generation between initially uncorrelated probes, weakly interacting with the many body bus, is extremely efficient, as they can share quasi-perfect entanglement even at large distances. The computation of the effective Hamiltonian of interaction of the probes defines a suitable framework to investigate the phenomenon in generic gapped quantum lattice systems. In the last chapter these results are generalized as to allow the computation of probe correlations in situations where adiabatic continuity between the eigenstates of the full many-body Hamiltonian and the unperturbed system holds. This encompasses the effect of temperature and the non-perturbative regime. By comparing analytic results against Quantum Monte Carlo data, we go far away perturbation theory limits and unveil probe-probe quantum correlations at temperatures much higher than previously thought possible. The latter happens in the two-dimensional scenario, where robust gaps are shown to emerge even in lattices with a very small gap (vanishing in the thermodynamic limit) solely due to the presence of the probes.

The present thesis shows that Quantum Information tools can be used to better understand the quantum-to-classical boundary in mesoscopic and macroscopic systems. Our findings suggest a way to push this boundary towards the macroscopic world by coupling a moveable mirror to a confined quasi-classical electromagnetic field, and opens new possibilities towards quantum computation and information processing with strongly-correlated systems at realistic temperatures, i.e. much above their natural ground states.
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**List of Acronyms**

| Acronym | Description                             |
|---------|-----------------------------------------|
| 1D      | one-dimensional                         |
| 2D      | two-dimensional                         |
| 3D      | three-dimensional                       |
| AF      | Anti-Ferromagnetic                      |
| AKLT    | Affleck-Kennedy-Lieb-Tasaki             |
| CV      | Continuous Variable                    |
| DMRG    | Density Matrix Renormalization Group    |
| EM      | Electromagnetic                         |
| EPR     | Einstein-Podolsky-Rosen                |
| FM      | Ferromagnetic                           |
| GS      | Ground State                            |
| LASER   | Light Amplification by Stimulated Emission of Radiation |
| LDE     | Long-Distance Entanglement             |
| LOCC    | Local Operations and Classical Communication |
| PPT     | Positive Partial Transposition          |
| QI      | Quantum Information                    |
| QMC     | Quantum Monte Carlo                     |
| QND     | Quantum Non-Demolition                  |
| SQL     | Standard Quantum Limit                  |
| ZPF     | Zero-Point Fluctuations                 |
List of Acronyms
1. Introduction

This thesis is devoted to the study of the quantum-classical boundary at finite temperatures, in two distinct physical scenarios, and to its implications for fundamental physics.

This monograph consists of two large blocks as follows:

- in Chapter 2, we focus our attention on a very popular subject in current state-of-the-art optomechanics: the bona fide quantum behavior of a macroscopic mechanical oscillator driven by electromagnetic radiation pressure. We will argue that this system accomplishes the possibility of macroscopic entanglement. In Chapter 3, we will show that the same opto-mechanical setup, provided with an appropriate measurement apparatus, turns out to be an excellent candidate for an experiment aiming to test the quantum-to-classical transition at realistic temperatures;

- in Chapter 4, we show that spin-1/2 probes develop quantum correlations when they are locally coupled to gapped many-body systems; this is a different facet of the quantum-to-classical transition when the bulk system is perceived as a model for an environmental bath. The possibilities for quantum communication and computation entirely based on solid-state devices at finite temperatures will be analyzed in Chapter 5 where the emergence of gaps in various spin systems due to additional spin particles will be shown to accommodate bipartite spin-spin entanglement at temperatures much higher than previously considered possible.

The present chapter attempts to shed some light on the context and relevance of the topics covered in this thesis (Sec. 1.1) and also to make a comprehensive review of the basic results for the characterization of quantum correlations (Sec. 1.2 and 1.3): the theory of quantum entanglement. While experts may consider skipping the introduction, the reader new to Quantum Information concepts should find this section particularly helpful to learn the crucial difference between the classical correlations and their non-classical counterparts. To ensure the readability of the text, useful background related to major standard technical subjects will be given in special appendices at the proper time, and informal and easy to follow derivations will be favoured when possible over more rigorous (but often less illuminating!) mathematical approaches.

1.1. Context

Correlations between different systems have always been an active subject of study in various branches of theoretical physics. Ranging from criticality in classical statistical mechanics to many body
1. Introduction

effects in electronic systems, correlations appear as a fundamental property characterizing interacting systems. More recently, a new area of physics has emerged mainly from the Quantum Optics community: Quantum Information (QI) science. Originally motivated by a close examination of the foundations of Quantum Mechanics, the QI community envisaged quantum communication protocols and a new paradigm of computation based on the laws of Quantum Mechanics.

In the past few years, the interests of this community have broadened by extending the methods initially developed to characterize the quantum correlations in small Hilbert spaces (such as the polarization degree of freedom of two photons) to encompass the solid-state and condensed-matter systems from a new perspective: the so-called "entanglement" approach.

The entanglement theory provides a suitable framework to think about non-classical quantum information processing tasks (e.g. teleportation), and also paves the way for the resolution of the old question of the quantum-to-classical transition: when does a physical system loses every quantum signature and behaves classically?

Throughout this monograph, we will show that applying the entanglement approach to the study of interacting systems unveils how far we can hope to go on pushing the genuine quantum behavior of the microscopic world towards the macroscopic domain. The "boundary" is not the same in distinct physical scenarios, where many different kind of interactions may play a role, and it will show to be very sensitive to the initial conditions. Notwithstanding, the entanglement approach will prove to capture important subtleties of correlations in an unified picture.

1.2. Classical versus quantum correlations

1.2.1. Preliminaries

In general, an experimentalist has no way to prepare with perfect control a definite quantum state,

$$|\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle,$$

(1.1)

where \{ |n\rangle \} \in \mathcal{H} denotes a basis of the Hilbert space and \langle n|\psi\rangle are arbitrary complex amplitudes. Instead, he/she prepares a probabilistic ensemble of pure states \{ |\psi_n\rangle \} with associated probabilities \rho_n. For the moment, and without loss of generality, this ensemble will be taken to consist entirely of orthogonal (and normalized) individual states. At the end of the day, one is interested in averages of physical quantities, and thus it is instructive to see how physical averages look like when an ensemble of quantum states is assumed.

Bearing in mind these considerations, the prediction \langle A \rangle of a generic physical observable \hat{A} must be
the weighted average of the expectation values \( \langle \psi_n | \hat{A} | \psi_n \rangle \) for the pure states \( | \psi_n \rangle \),

\[
\langle A \rangle = \sum_n \rho_n \langle \psi_n | \hat{A} | \psi_n \rangle = \text{Tr} \left[ \hat{\rho} \hat{A} \right],
\]

(1.2)

where we have conveniently introduced the density matrix operator,

\[
\hat{\rho} := \rho = \sum_n \rho_n | \psi_n \rangle \langle \psi_n |.
\]

(1.3)

The spectrum of this operator may be thought as the quantum-mechanical analogue of the familiar Boltzmann weights in classical statistical-mechanics, \( \rho_n \sim e^{-\beta E_n} \), describing the probability of finding a canonical system in a configuration with definite energy \( E_n \) at temperature \( T = 1/k_B \beta \). The only difference being that in Quantum Mechanics there are not many different microscopic configurations contributing to the same macroscopic configuration \( n \), but rather an unique quantum state \( | \psi_n \rangle \) with energy given by the Schrödinger equation,

\[
\hat{H} | \psi_n \rangle = E_n | \psi_n \rangle,
\]

(1.4)

with \( \hat{H} \) denoting the system’s Hamiltonian. There will more to say about this analogy soon. Let us now look into the properties of the density matrix in more detail. From Eq. (1.3) we have,

\[
\text{Tr}[\rho] = \sum_n \rho_n \text{Tr}[| \psi_n \rangle \langle \psi_n |] = \sum_n \rho_n \langle \psi_n | \psi_n \rangle = 1,
\]

(1.5)

as both the \( \{ \rho_n \} \) and the individual states \( \{| \psi \rangle \} \) are assumed to be normalized, that is \( \sum_n \rho_n = 1 \) and \( \langle \psi_n | \psi_n \rangle = 1 \). The density matrix is Hermitian as can be seen by direct inspection (hence assuring that \( \rho_n \in \mathbb{R} \)). Moreover, since \( \rho_n \) must represent a probability, the density matrix \( \rho \) is semi-positive definite. The latter is a strong restriction in the class of matrices in \( \mathcal{H} \) allowed as acceptable density matrices:

\[
\langle \psi | \rho | \psi \rangle = \sum_n | \langle \psi | n \rangle |^2 \rho_n \geq 0.
\]

(1.6)

Eq. (1.6) is, for calculus purposes, an efficient way to check if a given matrix actually represents a physical state. Before moving forward, a comment is in order: the decomposition in Eq. (1.3) is not unique for mixed states of two or more quantum systems. This makes no difference at the time of evaluating a given physical quantity by means of Eq. (1.2), but will have important consequences for the discussion of entanglement in mixed states.

\[\text{Here it is assumed that the energy spectrum is non-degenerate. It can happen (and many times it does) that a given state is degenerate. This degeneracy is usually broken in realistic scenarios by the environment.}\]
1. Introduction

1.2.2. The randomness of quantum states

We have introduced the notation of density matrix defining ensembles of quantum states and its most elementary features. Now we prepare the grounds for the understanding of the difference between ordinary correlations of every-day life and quantum correlations, by reviewing the concept of entropy.

The notion of statistical ensembles appeared a long time ago in the description of systems surrounded by a (very large) heat bath, where the microscopic details of the system-bath interaction are discarded in favor of concrete answers for quantities of physical interest (such as the specific heat, etc.). The statistical description is also the appropriate framework to study classical communication problems where noise (as a source of uncertainty) cannot be neglected.

In general, only probabilities for the outcomes of physical observables can be predicted. This lack of knowledge about physical systems, lead us to the concept of entropy: let us imagine that we own $N$ copies of identical prepared systems (e.g. an atom in its ground state) and that $p_1,...,p_d$ are the a priori known probabilities of the different outcomes we may get ($d$ standing for the number of such outcomes; typically the dimension of the system’s Hilbert space). How much information do we gain about a single system by performing measurements on a large number of identically prepared systems? The answer is related to the number of possible ways to arrange the measurement’s results: assuming that $N$ is large, we expect that each outcome, labeled by $i$, materializes in average $\sim n_i = N p_i$ times, with $\sum n_i = N$. The number of arrangements is $k = N!/(n_1!...n_d!)$. In the limit $N \to \infty$, we get $\log k = \log(N!/(n_1!...n_d!)) \approx -N \sum_i p_i \log p_i$, naturally suggesting the quantity

$$H := - \sum_{i=1}^d p_i \log p_i,$$  \hspace{1cm} (1.7)

as a measure of the uncertainty. This is the famous Shannon entropy for the classical distribution $\{p_1,...,p_d\}$. It measures the ignorance we have about a physical system (prior to measurement) and achieves its maximal value if all the $p_i$ are equal.

The classical information theory was founded by Shannon [11] whose pioneering work is of paramount importance nowadays in technology and science. In a classical information problem (e.g. the transmission of a message from $A$ to $B$) $H$ quantifies the information that has been transmitted, which may seem a bit awkward for the physicist who usually thinks about entropy as ignorance rather than knowledge. This false impression, however, becomes clear by noting that $B$ cannot learn anything if the outcome is known to him/her prior to transmission, and does learn a good amount of information if he/she cannot predict any of the outcomes, i.e. if $p_i = 1/d, \forall i$.

In classical statistical mechanics, the entropy is the logarithm of the number of microstates ($\Omega$) of the system, $S = \ln \Omega$ (defined up to a constant due to the arbitrary dense volume of the phase

\[2\]Other functions of $k$ could be considered as measures of entropy, but this particular choice has suitable properties. For instance, it is additive: for two statistical independent systems it yields the sum of individual entropies.
space cells), where the Boltzmann’s constant was set to unit. In quantum statistical mechanics the Heisenberg principle imposes a limit on how small the phase space cells can be; there is no arbitrariness in counting the number of microstates. Let us consider the elementary example of a totally random mixture (also known as maximally mixed state in QI) of eigenstates occurring with the same probability, with \( \text{dim } \mathcal{H} = d \),

\[
\rho_d = \frac{1}{d} \sum_{n=1}^{d} |\psi_n\rangle \langle \psi_n| = \frac{1}{d}. \tag{1.8}
\]

The number of "microstates" is the number of pure states \( d \) and, therefore, the entropy reads \( S = \ln d \) according to Boltzmann’s formula. In quantum mechanics, however, we have to compute the entropy by the von Neumann formula,

\[
S(\rho) := -\text{Tr}[\rho \ln \rho]. \tag{1.9}
\]

This expression yields zero for every pure state, \( S(|\psi\rangle) = 0 \), and reaches its maximum value for a maximally mixed state, \( S(\rho_d) = \ln d \). Although there are many possible entropies (for a complete review on the subject see [2]), von Neumann’s formula has suitable physical properties (Appendix A.4) and plays a crucial role for the theory of entanglement as it will become apparent in the next section. For the moment, it is enough to realize that the familiar result for the Boltzmann entropy of a totally random mixture, \( S(\rho_d) = \ln d \), is straightforwardly obtained using Eq. (1.9), and that it is the quantum extension of the classical Shannon entropy. The latter can be seen by considering a density matrix in the general form given by Eq. (1.3) and computing its von Neumann entropy. This yields,

\[
S = -\sum_n \rho_n \ln \rho_n, \tag{1.10}
\]

which resembles the classical Shannon entropy [Eq. (1.7)] for a random variable.

The von Neumann entropy [Eq. (1.9)] is the best measure of how "mixed" a state is, although it has a major disadvantage compared to other types of entropy; excluding rather special situations it is very difficult to compute as it presupposes diagonalization of \( \rho \). For practical ends, one often adopts the so-called linear entropy instead. For a density matrix \( \rho \) living in a Hilbert space of dimension \( d \) it reads \( S_\mathcal{L}(\rho) := d/(d-1) \left(1 - \text{Tr}[\rho^2]\right) \). It has the nice virtue of being easy to compute in all situations and it is directly related to the purity of a state \( \mathcal{P}(\rho) := \text{Tr}[\rho^2] \),

\[
S_\mathcal{L}(\rho) = \frac{d}{d-1} (1 - \mathcal{P}(\rho)). \tag{1.11}
\]

The purity \( \mathcal{P} \in [0, 1] \) is one for pure states and decreases with the degree of mixture, i.e. as soon as more non-zero eigenvalues \( \rho_n \) appear in decomposition [Eq. (1.3)]. Depending on the context it may be more convenient to employ the purity rather than the linear entropy; indeed, both concepts will be employed in this monograph and, unless stated otherwise, the word entropy will be used to denote the von Neumann entropy [Eq. (1.9)].
1. Introduction

1.2.3. The EPR "super-correlations"

Very often, density matrices appear coupled to some sort of statistical description of a physical system; this could be due to the inability to control the states in a realistic experimental scenario (e.g. external noise or an intrinsic random process), or even as a mathematical tool to compute an average from an adequate statistical ensemble. This is not, however, the full story. For a system with several components (e.g. particles, degrees of freedom) the density matrix is an useful concept even when the full system is a pure one. In order to see this, let us consider the Bohm version of the famous Einstein-Podolsky-Rosen (EPR) paradox [3]. A spin-1 particle in the $S = 0$ state decays into two spin-1/2 particles ($A$ and $B$) in a singlet state:

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}} (|\uparrow_A, \downarrow_B\rangle - |\downarrow_A, \uparrow_B\rangle).$$ \hfill (1.12)

This is a very special state for reasons, which will become clear in the course of this chapter. On one hand, it is rotationally invariant: $\uparrow_A$ means that spin $A$ points in the positive direction of the $z$-axis or any other direction in three-dimensional (3D) space. This suggests an alternative, and perhaps more revealing, way of writing the state of the two particles:

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}} (|+A, -B\rangle - |-A, +B\rangle),$$ \hfill (1.13)

where now the meaning of $+_A$ is that the spin $A$ is pointing in the positive direction of a given (arbitrary) axis. From (1.13) we immediately see that whenever $A$ is detected in the positive direction, $B$ will be detected pointing out in the negative direction (provided the measurement is made along the same axis). This is already a curious feature of (1.13), but more is yet to come; if an observer decides to measure $B$ along a different direction, he/she will measure $+$ or $-$ with the same probability. The EPR paradox comes about when we imagine these particles to be separated over a large distance in such a way that a measurement performed in one of the particles cannot influence the result obtained for the other. If we measure $A$ along $x$, we can infer the corresponding outcome for $B$ [Eq. (1.13)]. If we now measure $B$ along $y$, we will have determined the spin of $B$ along two orthogonal directions! On the other hand, Quantum Mechanics does not allow for the simultaneous knowledge of the value of two non-commuting variables (such as the spin operators along $x$ and $y$). Hence, one can conclude that either Quantum Mechanics is incomplete or these two quantities cannot have simultaneous reality. This is the essence of the EPR paradox in a few lines. In order to see where the density

---

3Whatever direction $A$ is detected being spinning then $B$ will be found spinning in the opposite direction. This might suggest faster-than-light signaling, but this is of course not the case since two distant observers must agree on the measurement axis, which force them sending (perhaps by a phone call) a "classical" information which speed is bounded from above by the speed of light.
1.2. Classical versus quantum correlations

matrix shows up, we define the partial state of two systems $A$ and $B$,

$$
\rho_A := \text{Tr}_B \rho_{AB}
$$

$$
\rho_B := \text{Tr}_A \rho_{AB},
$$

(1.14)

where $\rho_{AB} = |\psi_{AB}\rangle\langle\psi_{AB}|$ for a generic state of two spin-1 particles $|\psi_{AB}\rangle$ and $\text{Tr}_A(B)$ denotes the partial trace with respect to $A(B)$. For the singlet [Eq. (1.13)], this yields,

$$
\rho_A = \rho_B = \frac{1}{2} (|+\rangle\langle+| + |−\rangle\langle−|) = \left( \begin{array}{cc} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{array} \right).
$$

(1.15)

The partial states are proportional to the identity matrix making the entropy maximal ($S(\rho_A) = S(\rho_B) = \ln 2$). These density operators do not correspond to any state vector, as can be concluded for lack of idempotence (note that for a pure state one has $\rho^2 = (|\psi\rangle\langle\psi|)^2 = \rho$, whereas in our example $\rho_A^2 = \rho_B^2 = \frac{1}{4} 1$). We see from (1.15) that there is more entropy in considering the subsystems $A$ and $B$, individually, than in considering the compound system 'A + B', $S(\rho_A) > S(\rho_{AB}) = 0$: that is, we have lost information about correlations while performing the trace! This is at odds with classical intuition; for two classical random variables ($A$ and $B$), the Shannon entropy obeys $H(A, B) \geq \max \{H(A), H(B)\}$, as $A$ (or $B$) cannot have more entropy than the overall system.

The special form of (1.15) implies that the average of any observable defined in the Hilbert space of spin-1/2 will not change when a change of basis is performed — this is just what the rotational invariance of the singlet means — and hence the spins will be perfectly anti-correlated in every direction, yielding subsystems totally mixed. Let us compare the singlet state with the following ”classical mixture” of two spins:

$$
\sigma_{AB} = \frac{1}{2} (|↑_A, ↓_B\rangle\langle↑_A, ↓_B| + |↓_A, ↑_B\rangle\langle↓_A, ↑_B|).
$$

(1.16)

The mixed state $\sigma_{AB}$ yields the same partial states of the singlet [Eq. (1.15)] and also displays a perfect anti-correlation along the $z$ axis. However, the situation for $\sigma_{AB}$ is distinct in two ways: when measured along a different direction, say $x$, the particles appear uncorrelated, and, this time, the partial entropies do not surpass the total entropy. While one could attribute the violation of a classical bound on entropies to the particular case of the EPR pair in a singlet state, this is a general feature of non-classical bipartite states.

1.2.4. Beyond classical correlations

On general grounds, the averages of operators defined in the Hilbert space of one subsystem is completely determined by its partial state. Hence, for every operator $O_A$ defined in the Hilbert space
1. Introduction

of $A$, one has

$$
\langle O_A \rangle = \langle \psi_{AB} | O_A \otimes 1_B | \psi_{AB} \rangle = \text{Tr}_A \left[ O_A \rho_A \right].
$$

(1.17)

The last equality can be checked by inserting the definition of partial state [Eq. (1.14)]. The analogous holds true for operators defined in the Hilbert space of $B$. This confirms the idea expressed in the previous section: the knowledge of partial states is sufficient, as long as we just care about the local properties of $A$ and $B$, but as soon as we ask about non-local properties, we need the information of the full density matrix $\rho_{AB}$ (the state vector $|\psi_{AB}\rangle$, in the EPR example).

The Anti-Ferromagnetic (AF) correlations in the singlet state [Eq. (1.13)] are much stronger than what they could ever be classically, being maximal in every spatial direction. Two particles in such states are said to display the so-called entanglement (i.e. genuine quantum correlations). This is a unique feature of compound systems in quantum mechanics, and will be addressed in detail in Sec. 1.3 Here we make a glimpse of entanglement in two-level systems (also known as qubits).

In a classical framework, we would say that correlations among spins-1/2 do exist both for AF and Ferromagnetic (FM) states, since the connected correlation,

$$
\langle O_A O_B \rangle_c := \langle O_A O_B \rangle - \langle O_A \rangle \langle O_B \rangle
$$

(1.18)

can be non-zero in both cases. In order to see this, we take the primary matrices of the Clifford algebra (the famous Pauli matrices) — which, together with the identity matrix, form an orthogonal basis of the complex Hilbert space of all $2 \times 2$ matrices, and therefore can be employed to write any physical state of the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$ of two spin-1/2 particles,

$$
\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
$$

(1.19)

and consider the special set of $SU(2)$ rotational invariant states:

$$
\rho_{AB}(f) = \frac{1}{4} \left( 1_A \otimes 1_B + f \sum_{\alpha=x,y,z} \sigma^\alpha_A \otimes \sigma^\alpha_B \right).
$$

(1.20)

The partial states are maximally mixed, $\rho_A(f) = \rho_B(f) = \frac{1}{2} 1_2$, from our symmetry requirement, and the correlations can be readily obtained using the properties of the Pauli algebra:

$$
\text{Tr} \left[ \sigma^i \right] = 0
$$

(1.21)

$$
\sigma^i \sigma^j = \epsilon^{ij}_k \sigma^k + \delta^{ij} 1_2,
$$

(1.22)

where $\epsilon^{ij}_k$ is the Levi-Cevitta symbol and the summation over repeated indexes is implicit. Since $\langle \sigma^\alpha_{A,B} \rangle = 0$, we get,

$$
\langle \sigma^\alpha_A \sigma^\beta_B \rangle_c = \text{Tr} \left[ \sigma^\alpha_A \sigma^\beta_B \rho_{AB}(f) \right] = f.
$$

(1.23)
1.3. Entanglement theory

There is a constraint on $f$ resulting from the density matrix being semi-positive definite, $\rho_{AB}(f) \geq 0$. The eigenvalues of Eq. (1.20) read:

$$\rho_1 = \frac{1-3f}{4},$$

$$\rho_2 = \rho_3 = \rho_4 = \frac{1+f}{4},$$

from which we readily obtain,

$$f \in [-1, \frac{1}{3}].$$

This constraint is physically natural since the correlations are bounded from definition (1.18). When $f = -1$ the singlet state (1.13) is recovered and, in this case, we say that the spins are fully anti-correlated. The reverse case happens when $f = 1/3$ and the correlations are as much FM as a rotational invariant state can afford; to achieve higher FM correlations (max $\rho \langle \sigma_A^z \sigma_B^z \rangle = 1$) we need to consider different states (and thus break rotational invariance).

It is no coincidence that AF correlations can be "stronger" than FM correlations for rotational invariant states: quantum correlations not only are maximal for the singlet state $f = -1$, but also cease to exist when $f \geq -1/3$ (Sec. 1.3.3)! Indeed, whereas for classical spins AF and FM correlations are on equal footing, for quantum spins there are non-classical correlations which only emerge for sufficiently robust AF interactions. Hence, for rotational invariant states, besides the usual distinction between ferromagnetic correlations ($f \in [0, 1/3]$) and antiferromagnetic correlations ($f \in [-1, 0]$), we have a more symmetrical classification of correlations:

$$f \in [-1, -1/3] \rightarrow \text{quantum correlations};$$

$$f \in [-1/3, 1/3] \rightarrow \text{classical correlations}.$$ 

What is so special about states with AF correlations in the range $[-1, -1/3]$ besides the 'spooky action at distance' as conceived by EPR? The answer is that the states with $f < -1/3$ are necessarily written as an entangled superposition of different branches: they are entangled in any local basis! In the next section, we will see that this forces the correlations to be highly non-classical in a very precise sense. Fig. 1.3 displays, in a density plot, the amount of quantum correlations for two spins-1/2 interacting via an AF Heisenberg Hamiltonian as function of (isotropic) magnetic field and temperature.

1.3. Entanglement theory

Bipartite physical states displaying EPR correlations cannot be prepared by two observers by separate local operations (unitary transformations, measurements, etc.) and classical communication (exchange of information by classical means). As a matter of fact, the correlation in the singlet
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state [Eq. (1.13)] is so peculiar that leads to interesting QI possibilities with no correspondence in the classical information theory. Perhaps, the most genuine QI task is quantum teleportation [4]. It has been experimentally implemented with photons [5, 6, 7, 8] and also with atoms [9, 10]. In it, quantum states of fields are "teleported" through the space among observers sharing an invaluable kind of correlation: entanglement.

1.3.1. Local operations, separable states and the fundamental law of QI

Let us start by making precise the meaning of Local Operations and Classical Communication (LOCC) before defining entanglement in a rigorous way. There are several ways one can formalize the concept of LOCC but here we will adopt the formalism of separable actions — the reader is referred to [11], and references therein for a complete survey on the subject. Before introducing the set of separable actions, it is useful to recall the set of elementary quantum operations one can perform in a given system which are allowable operations in the context of QI:

1. unitary transformations (time evolution) — a system evolves under some Hamiltonian and its density matrix changes according to

\[ \rho \mapsto \rho(t) = U\rho U^\dagger, \]

with \( U = U(t) \) being the corresponding (unitary) evolution operator;

2. measurements — a physical state can change via the process of measurement. One can label the possible measurement outcomes by an index \( i = 1, \ldots, K \), where \( K \) stands for the number of such possible outcomes. Associated with each of these outcomes is a projector \( P_i \) that obeys

\[ P_i P_j = \delta_{ij} P_i, \quad \sum_{i=1}^{K} P_i = 1_K. \]

A given outcome \( i \) will happen with probability \( p_i = \text{Tr}[P_i \rho P_i] \) and the state will change according to

\[ \rho \mapsto \frac{P_i \rho P_i}{\text{Tr}[P_i \rho P_i]}. \]

The latter is called a selective projective measurement and it is said complete if all projectors \( P_i \) are one-dimensional. A non-selective projective measurement will not discriminate between the different subspaces spanned by \( P_i \) entailing the following map:

\[ \rho \mapsto \sum_{i=1}^{K} P_i \rho P_i. \]

3. enlargement of the Hilbert space — one can attach to a quantum system, described by the Hilbert space \( \mathcal{H} \), an ancilla with support in an auxiliary Hilbert space \( \mathcal{Y} \). Let \( \rho \) and \( \sigma \) denote
the state of the system and ancilla, respectively. The appending of the ancilla to the original system is described by

\[ \rho \mapsto \rho \otimes \sigma. \quad (1.31) \]

The map above is a natural quantum operation, since any system can be thought as being part of a larger system.

4. partial trace — finally one may be interested in discarding the ancilla (with support in \( \mathcal{V} \)) and perform a quantum operation in the final system \( S \):

\[ \rho \mapsto \rho_S = \text{Tr}_V \rho. \quad (1.32) \]

The classes 1—4 of allowable quantum operations can be combined together. The resulting action will be described by a positive linear map from the whole state space onto itself. LOCC is the class of quantum operations in a bipartite scenario where two parties, \( A \) and \( B \), perform any combination of 1—4 in their own Hilbert space, \( \mathcal{H}_A \) and \( \mathcal{H}_B \), respectively, and also in additional ancillas they might have at their disposal. In the LOCC setup, \( A \) and \( B \) are even allowed to exchange "classical information" containing results of local measurements they get; if \( A \) communicates the result of his/her measurement to the distant party \( B \), then \( B \) may apply a specific quantum operation which can depend on the result obtained by \( A \). Recall, for instance, the teleportation protocol: \( A \) performs a joint measurement of two particles (one in an unknown state and another particle belonging to an entangled pair that \( A \) shares with \( B \)). The result of the measurement is transmitted to \( B \), who, depending on the outcome \( A \) obtained, performs an unitary transformation in his/her particle [4].

On quite general grounds, we can describe any combination of allowable quantum operations by superoperators acting in the compound system. The superoperators are trace-preserving completely positive maps and, at the operator level, can always be written as [12, 13]:

\[ \rho \mapsto \rho' = \mathcal{S}(\rho) = \sum_i S_i \rho S_i^\dagger, \quad (1.33) \]

where \( \rho \) and \( \rho' \) are any two density matrices in the state space. The \( \{S_i\} \) are known as Kraus operators in [Q1] and describe the action of superoperators. These states may have different dimensions (if for instance, the quantum operation above is meant to denote an enlargement of the Hilbert space by an ancilla) and thus the Kraus operators are not operators in the usual sense in Quantum Mechanics [14].

In a simple unitary evolution, this map would just contain one such operator, \( \mathcal{S}(\rho) = U \rho U^\dagger \), but more involved situations can be considered. The trace-preserving character of the superoperator manifests as \( \sum_i S_i^\dagger S_i = 1 \) for it implies \( \text{Tr} \mathcal{S}(\rho) = 1 \). Curiously, any trace-preserving quantum operation can be mapped to a situation where an ancilla \( a \) (with density matrix \( \sigma \)) is added to the

\[ A \text{ map } \mathcal{S} \text{ is said completely positive if } \mathcal{S} \otimes 1_N \text{ is also positive with } N \in \mathbb{N}. \]

This property is essential since many actions will leave unchanged the state of auxiliary particles that might exist; in their Hilbert space, the map acts as the identity operator. Interestingly, this condition is more general than simple positivity of \( \mathcal{S} \): there are positive maps that are not completely positive (in Sec. 1.3.3 we will see their implication to entanglement theory).
1. Introduction

system (initially in the state $\rho$, uncorrelated with $a$), which is left to evolve unitarily and then traced out \[15\]; for every quantum operation $\mathcal{S}$ there exists a density matrix $\sigma$ and an unitary operator $U$ such that,

$$\mathcal{S}(\rho) = \text{Tr}_a [U (\rho \otimes \sigma) U^\dagger].$$  \hspace{1cm} (1.34)

The map (1.33) being trace-preserving, it does not encompass the class of measurements "reducing" the wave-function, but can be easily generalized as to do so by relaxing its trace-preserving character, that is allowing quantum operations $\mathcal{S}_m$ which, although completely positive, are not trace-preserving: $\text{Tr} \mathcal{S}_m(\rho) \leq 1$. To this end we let $\mathcal{S}$ to be decomposable in a sum, $\sum_m \mathcal{S}_m$, in which, each $\mathcal{S}_m$ is not trace-preserving. The map now acquires the following form:

$$\rho \mapsto \mathcal{S}_m(\rho) = \sum_i \mathcal{S}_{m,i} \rho \mathcal{S}_{m,i}^\dagger,$$  \hspace{1cm} (1.35)

and $\sum_m \sum_i \mathcal{S}_{m,i}^\dagger \mathcal{S}_{m,i} = 1$, such that for each $m$ we can have $\sum_i \mathcal{S}_{m,i}^\dagger \mathcal{S}_{m,i} \leq 1$. This decomposition of unity is called a Positive Operator Valued Measure (POVM); the $\mathcal{S}_{m,i}^\dagger \mathcal{S}_{m,i}$ are the elements of the POVM which is being measured and $\mathcal{S}_{m,i}$ are Kraus operators. The "classical information" associated with the outcome $m$ (e.g. a spin projection $-1$ or 1) indicates which superoperator $\mathcal{S}_m$ acted on the state space, and thus it is said that this kind of operation is partially classical. This generalizes the concept of projective measurements introduced above, and it is known as a generalized measurement.

Now we are in position to define LOCC more formally following references \[12, 16\]. For pedagogical purposes, we first introduce the concept of Local Operations. Let $\mathcal{H}_A \otimes \mathcal{H}_B$ denote the Hilbert space as usual and $\rho_{AB}$ be the density matrix of the compound system. Associated to the parties $A$ and $B$ we have Kraus operators $A_i$ and $B_j$, respectively. With these definitions, Local Operations is the class of operations for which the corresponding superoperator is "nonmeasuring" (i.e. trace-preserving), and it is a direct product of superoperators acting alone in $A$ and $B$, that is $\mathcal{S} = \mathcal{S}_A \otimes \mathcal{S}_B$. At the operator level this map reads,

$$\rho_{AB} \xrightarrow{\text{LO}} \mathcal{S}(\rho_{AB}) = \sum_{i,j} (A_i \otimes B_j) \rho_{AB} (A_i^\dagger \otimes B_j^\dagger).$$  \hspace{1cm} (1.36)

Finally, we introduce the concept of separable actions; this is the class in which each $\mathcal{S}_m$ (non trace-preserving in general) is separable, in the sense that its Kraus operators are separable, $S_{m,i} = A_i \otimes B_i$, resulting in the following map:

$$\rho_{AB} \xrightarrow{\text{LOCC}} \mathcal{S}_m(\rho_{AB}) = \sum_i (A_i \otimes B_i) \rho (A_i^\dagger \otimes B_i^\dagger).$$  \hspace{1cm} (1.37)

Note that in the map above the individual actions of $A$ and $B$ may be correlated in a way not necessarily decomposable into direct products each acting in the respective subsystem, and therefore it accomplishes the possibility for classical communications. The separable map of Eq. (1.37) can be implemented using local operations and classical communication only \[17\]. Although every LOCC...
1.3. Entanglement theory

Figure 1.1.: The amount of non-separability of a state $\rho \equiv \rho_{AB}$ can be thought as the distance of $\rho$ to the closest separable state $\sigma \equiv \sigma_A \otimes \sigma_B$ [21]. The set of all bipartite density matrices is represented by $\mathcal{T}$ and the set of separable states by $\mathcal{D}$. At the center of the inner circle lies the most separable state for a given $d$-dimensional Hilbert space: the identity matrix.

Having reviewed the concept of quantum operations on states and the LOCC scenario, we are now able to introduce formally the concept of entanglement. Let us denote the set of all density matrices by $\mathcal{T}$ and the set of the separable density matrices by $\mathcal{D}$. The latter being the subset of bipartite states which can be prepared by LOCC alone.

**Definition.** A bipartite state $\sigma_{AB}$ is said to be separable if it can be written as a convex mixture of product states $\rho_A \otimes \rho_B$,

$$\sigma_{AB} := \sum_i p_i \rho_A^i \otimes \rho_B^i,$$

(1.38)

with $p_i$ representing probabilities. Any state $\rho_{AB}$, which cannot be written in this form, is said to be entangled or to display entanglement.

Werner [19] showed that, contrary to EPR-like states such as the spin singlet [Eq. (1.13)], separable states [Eq. (1.38)] trivially satisfy a local hidden variable model [20], hence not violating Bell inequalities. The set (1.38) is clearly convex since if $\sigma_1 \in \mathcal{D}$ and $\sigma_2 \in \mathcal{D}$, then $\sigma = p\sigma_1 + (1-p)\sigma_2$ with $p \in [0,1]$ is also a separable state. Recalling that the definition of density matrix implies that the convex mixture of any two density matrices is also a valid state, and following [21], we introduce a convenient picture where the set of bipartite states is divided into two regions: the separable set $\mathcal{D}$ and the entangled set $\mathcal{T} \setminus \mathcal{D}$ — see Fig. 1.1.

The way to prepare a separable state (1.38) is straightforward: $A$ samples from the distribution $p_i$ and communicates the result of the outcome to $B$, which in turn creates $\rho_B^i$. We remark that the
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correlations in these states are said to be classical not because the states $\rho_{A(B)}$ are classical at all (they are arbitrary quantum states), but rather because they do not permit non-classical tasks as teleportation or dense-coding (by which two classical bits of information are sent at the expense of just one quantum-bit) [22, 23]. Moreover, these states do not violate classical upper bounds in entropic inequalities (see Appendix A.4).

The most important [QI] contention is the postulate stating that two parties, by means of LOCC, cannot increase the amount of quantum correlations they share. This obviously implies that one has some well-defined entanglement measure, for instance, capable of giving the distance of a given (potential) entangled state $\rho$ to the closest separable state $\sigma$ in the sense of Fig. 1.1. We have not introduced this measure yet, but we shall not be concerned with it for the moment. Let us rather think of the particular case where two parties share no entanglement at all. In this case, all they can do by local operations and classical communication is to prepare states which are a mixture of product states of the form

$$|\Psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle.$$  \hfill (1.39)

This can be seen by taking a generic separable state [Eq. (1.38)] and check that it remains separable under the action of a LOCC map [Eq. (1.37)]. The strong assertion that one cannot create entanglement by means of LOCC in cases where the initial state is not of the form given above, is not yet demonstrated for generic states $\rho_{AB}$ (partially because the difficulty of computing known entanglement measures for mixed states) and constitutes what is known as the fundamental law of QI. It can be formulated in two different ways [22]:

1. [restricted form] The parties $A$ and $B$ cannot, with no matter how small probability, by LOCC transform a separable state into an entangled state;

2. [general form] The parties $A$ and $B$ cannot increase the amount of entanglement they share solely by LOCC.

Clearly the singlet state [Eq. (1.13)] cannot be recast in the form (1.39) by means of local unitary transformations $U_A \otimes U_B$ \footnote{If this were the case the entropy of the partial states would be zero and not maximal, since $\text{Tr}_A \left[ U_A \otimes U_B |\Psi_{AB}\rangle \langle \Psi_{AB}| U_A^\dagger \otimes U_B^\dagger \right] = |\psi_B\rangle \langle \psi_B|$ which again is a pure state yielding zero entropy.} but according to the restricted form of the postulate, this will be the case even if parties $A$ and $B$ communicate and make generalized measurements in their particles. In what follows, we make further insight into the fundamental postulate and its consequences for QI by introducing the entanglement measure for pure states.
1.3. Entanglement theory

1.3.2. The entanglement measure for pure states

The problem of computing the entanglement for arbitrary bipartite states (i.e., general mixed states) is an extremely hard one, and has only been solved satisfactorily for Hilbert spaces of the form $\mathbb{C}^2 \otimes \mathbb{C}^2$ [24] and for Gaussian states [25] (for a survey of the subject see [16, 21, 26, 27, 28]). Remarkably, however, there exists an unique entanglement measure for bipartite pure states of arbitrary dimension resulting from a link between entanglement and thermodynamics. In this section, we outline the main ingredients leading to this conclusion.

**Theorem.** <Schmidt, [29]> Every pure state $|\psi_{AB}\rangle$ of a composite system of two parties in $\mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$, with $d_A = \dim \mathcal{H}_A$ and $d_B = \dim \mathcal{H}_B$, can be written in the Schmidt form:

$$
\sum_{i=1}^{d_A} \sum_{j=1}^{d_B} c_{ij} |\phi_i\rangle_A \otimes |\phi_j\rangle_B \rightarrow \sum_{i=1}^{r} \sqrt{p_i} |u_i\rangle_A \otimes |v_i\rangle_B, \quad (1.40)
$$

where $c_{ij} \in \mathbb{C}$, $\{|u_i\rangle_A\}$ and $\{|v_i\rangle_B\}$ are orthogonal complete bases (the Schmidt bases) of the Hilbert spaces of subsystem A and B, respectively, $r \leq \min\{d_A, d_B\}$, and $p_i$ are positive real numbers called Schmidt coefficients (phase factors can always be absorbed in the Schmidt basis).

The decomposition (1.40) is unique when the coefficients $\sqrt{p_i}$ are all different from one another and has some attractive properties. The partial states are diagonal in the Schmidt basis and have a common eigenvalue spectrum:

$$
\rho_A = \sum_{i=1}^{r} p_i |u_i\rangle \langle u_i| \quad \text{(1.41)}
$$

$$
\rho_B = \sum_{i=1}^{r} p_i |v_i\rangle \langle v_i|. \quad \text{(1.42)}
$$

The latter, provides an useful shortcut to the Schmidt weights $p_i$ by simply computing the partial states and picking up its eigenvalues. The number of non-zero eigenvalues ($r$) is the Schmidt rank of the decomposition (1.40). Entangled states of bipartite pure states are those with Schmidt rank higher than one, and the respective degree of entanglement $E_{AB}$ can be measured by the Shannon entropy [Eq. (1.7)] of the Schmidt weights (or equivalently by the entropy of partial states):

$$
E_{AB} = -\sum_{i=1}^{r} p_i \ln p_i. \quad \text{(1.43)}
$$

In particular, for any $2 \otimes 2$ system, the maximal entanglement occurs for $r = 2$ and $p_1 = p_2 = 1/2$, whereas for $r = 1$ the state is separable. The entropy associated with the Schmidt coefficients $\{p_i\}$ will not change under local unitary transformations. Moreover, according to the fundamental law of QI, the entropy $E_{AB}$ can never increase under LOCC.
1. Introduction

Definition. The maximally entangled state of a bipartite $\mathbb{C}^d \otimes \mathbb{C}^d$ system reads

$$|\Psi_{AB}^{\text{max}}\rangle := \frac{1}{\sqrt{d}} (|u_1, v_1\rangle + ... + |u_d, v_d\rangle);$$

(1.44)

where $|u_i(v_i)\rangle$ are Schmidt basis (or any other locally equivalent basis).

Definition. The entropy of entanglement of a bipartite pure state $|\psi_{AB}\rangle$ reads

$$E(|\psi_{AB}\rangle\langle\psi_{AB}|) := -\text{Tr}[\rho_A \ln \rho_A] = -\text{Tr}[\rho_B \ln \rho_B].$$

(1.45)

For generic $d \otimes d$ systems, the maximal entropy of entanglement occurs for maximum Schmidt rank when all weights are equal, $\max_{\rho} E = \ln d$ [see Eq. (1.43)]. These are the states that are locally unitarily equivalent to $|\Psi_{AB}^{\text{max}}\rangle$. Maximally entangled states allow to prepare any bipartite state $\rho_{AB}$ solely by LOCC [30, 31, 32, 33, 34], as well as enhancing many of the non-classical tasks (hence their name "maximally entangled states").

For QI purposes (e.g. perfect teleportation), we might be interested in distilling a number of maximally entangled pairs of particles out from a certain number of partially entangled particles just by LOCC (imagine the situation where no maximally entangled pair is available but one has access to two or more partially entangled pairs). This procedure is known as entanglement concentration, and its study in the early nineties turned out to yield seminal conclusions for entanglement theory, as we will briefly see. The initial partially entangled state shared by $A$ and $B$ is denoted by $\Psi_i$,

$$\Psi_i = |\Psi_{A_1B_1}\rangle \otimes |\Psi_{A_2B_2}\rangle \otimes ... |\Psi_{A_nB_n}\rangle$$

(1.46)

whereas $\Psi_f$ denotes the state of the final product of the entanglement concentration procedure, i.e. maximally entangled pairs (the state of the remaining, non entangled, particles is not represented). With this notation, the first particle of each pair, namely $A_1...$ and $A_{k(n)}$, belongs to $A$ and the remaining particles, namely $B_1...$ and $B_{k(n)}$, are in possession of $B$; each of the $\Psi_{A_iB_i}$ represents the same partial entangled state and thus, from now on, it will be simply denoted by $|\Psi_{AB}\rangle$. How many maximally entangled pairs ($k$) can $A$ and $B$ extract by means of standard quantum operations?

C. H. Bennett and co-authors showed that the entropy of entanglement of the initial state $\Psi_i$ equals the number of maximally entangled pairs (i.e. the number of pairs in $\Psi_i$) one can extract asymptotically (i.e. $n,k \to \infty$ with $n/k$ kept constant) by means of LOCC [13] — see Fig. 1.2

$$n \text{ partially entangled pairs in the state } \Psi_i \xrightarrow{\text{LOCC}} k = E(\Psi_i)/E(\Psi_{AB}^{\text{max}}) \text{ maximally entangled pairs}.$$  

In other words, the initially amount of entanglement in $n$ pairs of particles [which, according to Eq. (1.45), equals $E = nE(\Psi_{AB})$; see also Appendix A.4 for the additivity property of the von
Neumann entropy] will determine how many maximally entangled pairs we might get by standard quantum operations. Let us outline some of the consequences of this conclusion; suppose that two observers share some amount of entanglement in the form of \( n \) pairs of qubits, each one in a partial entangled state,

\[
|\Psi_{AB}\rangle = \cos \theta \, |\uparrow_A \downarrow_B\rangle + \sin \theta \, |\downarrow_A \uparrow_B\rangle.
\]

(1.48)

By LOCC they can concentrate their amount of entanglement into \( k \leq n \) pairs of particles, but never increase the amount of entanglement (i.e. the number of singlets) they share. That nature does not allow to create new entangled states from a previous entangled state solely by local operations can be understood with a simple example. Let us imagine that two parties share an entangled state of \( k \) pairs plus one extra pair in a separable state \( |\Psi_i\rangle = |\Psi_{AB}\rangle^{\otimes k} \otimes |\Phi_A \otimes \Phi_B\rangle \), and they wish to get a final entangled state of \( k+1 \) pairs, such as \( |\Psi_f\rangle = |\Psi_{AB}\rangle^{\otimes k+1} \). The final state has an higher Schmidt rank\(^6\) and hence making this transformation impossible (in agreement with the the fundamental law of QI).

On the other hand, this can never happen with local operations and classical communication\(^3\)[30, 31, 32, 33], and hence making this transformation impossible (in agreement with the the fundamental law of QI).

The entanglement concentration procedure is reversible in the sense that the two parties can start with \( k \) maximally entangled pairs and distribute their entanglement among \( n \) pairs:

\[
|\Psi_{AB}^{\text{max}}\rangle^{\otimes k} \otimes (|\Phi_A \otimes \Phi_B\rangle)^{n-k} \xrightarrow{\text{LOCC}} |\Psi_{AB}\rangle^{\otimes n}.
\]

(1.49)

Moreover, by local operations, the entanglement can be shifted from one pair to another pair,

\[
|\Psi_{AB}^{\text{max}}\rangle \otimes (|\Phi_A \otimes \Phi_B\rangle) \xrightarrow{\text{LOCC}} (|\Phi_A \otimes \Phi_B\rangle) \otimes |\Psi_{AB}^{\text{max}}\rangle.
\]

(1.50)

None of these transformations violates the fundamental law, which by using Eq. (1.45) can now be expressed as,

\[
E(\rho_{AB}) \geq E(\Phi(\rho_{AB})),
\]

(1.51)

where \( \Phi(X) = \sum A_i \otimes B_i \sum_{i=1}^{r} \phi_i \otimes \phi_i \) is a LOCC map [Eq. (1.37)] and \( A_i(B_i) \) the Kraus operators of \( A \) and \( B \), respectively. The considerations made so far and specially the above equation suggest an analogy with the second law of thermodynamics, which goes much beyond the common definitions we have encountered (namely, the entanglement entropy and the von Neumann entropy).

---

\(^6\)In the multipartite scenario of the present example (\( 2k + 2 \) qubits in the state \( |\Psi_{AB}\rangle^{\otimes k} \otimes (|\Phi_A \otimes \Phi_B\rangle) \)) the Schmidt rank is the minimal number of product terms in a decomposition of \( |\Psi_i\rangle \) in the form \( \sum_{i=1}^{r} \sqrt{p_i} |u_i\rangle_A \otimes |u_i\rangle_B \) with \( p_i \geq 0 \) and \( |u_i\rangle \in \mathbb{C}^2 \) — compare with Eq. (1.40); see also reference [35].

\(^7\)The impossibility of increasing the Schmidt rank under LOCC can be easily shown in the bipartite scenario [32]: consider a state \( |\phi_{AB}\rangle \) with Schmidt decomposition given by \( \sum_{i=1}^{r} \sqrt{p_i} |u_i\rangle_A \otimes |u_i\rangle_B \) with \( |u_i\rangle_{AB} \in \mathbb{C}^{d_A(d_B)} \). Unitary local transformations will just re-define the vectors \( |u_i\rangle_{AB} \) changing neither the number of terms, \( r \), nor the probabilities \( p_i \). This, however, will no longer be the case if one of the parties, say \( A \), decides to make a projective measurement on his/her particle; if the outcome \( m \) is obtained then the state will be \( |\phi_{AB}(m)\rangle = \sum_{i=1}^{r} \sqrt{p_i} |P_i(m)| |u_i\rangle_A \otimes |u_i\rangle_B \), where \( P_i(m) \) is the projector corresponding to the outcome \( m \). The new state has at most \( r \) non-vanishing terms in accordance with the general statement that the Schmidt rank never increases under LOCC.
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Figure 1.2.: The entanglement concentration procedure (see [13]) takes \( n \) partial entangled states (represented in the left by particles connected with dashed lines) and transform them into \( k \leq n \) perfect singlets (blue particles connected by lines) plus some separable pairs (in the right). In the asymptotic limit, the conversion rate \( k/n \) reads
\[
E(\Psi_{AB})/E(\Psi_{AB}^{\text{max}}),
\]
where \( \Psi_{AB} \) denotes the compound state of a pair in the left.

The existence of a \textit{reversible} transformation gathering the entanglement of \( n \) systems into a smaller number of pairs \( k \) [Eq. (1.49)] when approaching the thermodynamic limit (with \( n/k \) finite) is the crucial result that lead S. Popescu and D. Rohrlich to the unique measure of entanglement [36]. It is instructive to review their argument; the key observation is that the good entanglement measure should be the one yielding the same value for any of two reversibly convertible entangled states [Eq. (1.49)]. Indeed, the problem of finding the unique entanglement measure \( \mathcal{E} \) for pure states is reduced to a much simpler one: finding the proper measure for \( k \) maximally entangled pairs. This measure must be proportional to \( k \) [36], which comes about since the reversibility of the entanglement concentration procedure is just strictly true in the asymptotic limit (\( n \to \infty \), see [13]) forcing to consider intensive quantities like the ratio of the total entanglement to the entanglement of a pair, instead of the total entanglement. The entanglement measure for a single pair in the initial state \( \mathcal{E}(|\Psi_{AB}\rangle) \) is related to the entanglement of a maximally pair \( \mathcal{E}(|\Psi_{AB}^{\text{max}}\rangle) \) by:

\[
\mathcal{E}(|\Psi_{AB}\rangle) = \lim_{n,k \to \infty} \left( \frac{k}{n} \mathcal{E}(|\Psi_{AB}^{\text{max}}\rangle) \right). \tag{1.52}
\]

On the other hand, for the entanglement concentration problem [Eq. (1.49)], we have seen that this limit was computed to be the entropy of entanglement. Thus, \( \mathcal{E}(|\Psi_{AB}\rangle) = E(|\Psi_{AB}\rangle) \) for every pure state \( |\Psi_{AB}\rangle \): thermodynamic arguments and the results from entanglement concentration uniquely determine the measure of entanglement for pure states obeying the fundamental law (1.51): the entropy of entanglement [Eq. (1.44)].
1.3. Entanglement theory

1.3.3. The entanglement of mixed states

In the QI literature we find a considerable number of proposals for entanglement measures. Some of these quantities have a well defined operational meaning, as the entanglement entropy in the previous section. Other measures, like the relative entropy of entanglement [21, 22], lack direct physical significance, but still may be very useful in multiple contexts (providing a simple interpretation of the amount of entanglement in a given state, classifying correlations in quantum many-body systems, etc.). Before introducing the entanglement for mixed states, we outline the main mathematical properties that a "good" measure of entanglement should satisfy:

1. The entanglement in a bipartite state $\rho_{AB}$ in the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ is a mapping $E(.)$ from density matrices into positive real numbers:

$$\rho_{AB} \in \mathcal{T} \rightarrow E(\rho_{AB}) \in \mathbb{R}^+,$$

and it is maximum for states locally equivalent to the maximally entangled state:$U_A \otimes U_B |\Psi_{AB}^{\text{max}}\rangle$;

2. $E(\rho_{AB}) = 0$ if and only if $\rho_{AB} \in \mathcal{D}$;

3. $E(\rho_{AB})$ does not increase under LOCC [Eq. (1.37)];

4. For pure states it reduces to the entropy of entanglement, $E(|\psi_{AB}\rangle\langle \psi_{AB}|) = S(\rho_A) = S(\rho_B)$.

When the mapping $E(.)$ satisfies the first three conditions, we call it an entanglement monotone, and if besides that it satisfies the last condition we call it an entanglement measure. Presently, no entanglement measure $E(.)$ for mixed states is known, for the constraints (3-4) are hard to realize together within the general space state $\mathcal{T}$, and there is no guaranteed reversibility in entanglement manipulations [Eq. (1.49)], as in the pure state case, just to name a few reasons. However, for the special case of two qubits ($\mathcal{H}_A = \mathcal{H}_B = \mathbb{C}^2$), two important and widely-used entanglement monotones do exist: the concurrence [24] and the negativity [37]. The former is an explicit formula for $\rho_{AB} \in 2 \otimes 2$ that equals the minimum over all the possible decompositions of $\rho_{AB}$ into pure states [Eq. (1.3)],

$$E(\rho_{AB}) = \min \sum_i p_i E(|\psi_i\rangle\langle \psi_i|),$$

with $\rho_{AB} = \sum_i p_i |\psi_i\rangle\langle \psi_i|$. The latter is based on the so-called Positive Partial Transposition (PPT) criterion [38]. It is instructive to review the main argument leading to the concept of PPT. We consider a generic bipartite separable state, $\sigma_{AB} = \sum_i p_i \rho_A^i \otimes \rho_B^i$, and note that partial transposition $\Lambda(.)$ with respect to one of the subsystems, say $A$, still yields a valid density matrix,

$$(\Lambda_A \otimes 1_B) \sigma_{AB} = \sum_i p_i \Lambda(\rho_A^i) \otimes \rho_B^i \in \mathcal{T},$$

with $\lambda_{AB} \in 2 \otimes 2$ that equals the minimum over all the possible decompositions of $\rho_{AB}$ into pure states [Eq. (1.3)].
1. Introduction

Hence, like any density matrix, the state after partial transposition must remain positive-semidefinite. This is the PPT criterion,

\[(\Lambda_A \otimes 1_B)\sigma_{AB} \geq 0.\]  

(1.55)

The transposition map \(\Lambda_A\) is positive but not completely positive [Eq. (1.33)]; there will be states \(\rho_{AB}\) for which \((\Lambda_A \otimes 1_B)\rho_{AB} \nless 0\) thus violating PPT; these states are entangled. This extraordinary simple separability condition by Asher Peres was of breakthrough importance in the entanglement theory of mixed states, and alone is already a stronger marker of non-separability than the usual violation of Bell inequalities [38]. In order to see how it works, we apply partial transposition to a rotational invariant state of two qubits [Eq. (1.20)] and compute the eigenvalues of the outcome,

\[(\Lambda_A \otimes 1_B)\rho_{AB}(f) = \frac{1}{4} (\mathbb{1}_A \otimes \mathbb{1}_B + f \Lambda_A (\vec{\sigma}_A) \cdot \vec{\sigma}_B).\]  

(1.56)

The transposition only affects the \(y\)-component of the Pauli matrices [Eq. (1.19)], \(\Lambda(\sigma^y) = -\sigma^y\), yielding the following set of eigenvalues [compare with Eqs. (1.24)-(1.25)]: \(\rho_1 = \rho_2 = \rho_3 = (1 - f)/4\) and \(\rho_4 = (1 + 3f)/4\). From direct inspection, we conclude that the rotational invariant state is entangled for \(f \in [-1, -1/3]\), whereas for \(f \in [-1/3, 1/3]\) is separable (as mentioned without proof in Sec. 1.2).

Remarkably, it has been shown that PPT is sufficient and necessary for separability of \(2 \otimes 2\) and \(2 \otimes 3\) cases [39]. In larger Hilbert spaces, however, there are states which are not separable, but still remain positive after partial transposition. The kind of entanglement present in those states is referred to as bound entanglement in opposition to the ordinary entanglement (as the one shared among two qubits), also known as free entanglement. The reason for this distinction stems from the non-distillability of the bound entangled states: the procedure of entanglement concentration under LOCC [Eq. (1.49)] is only possible when the parties share free entanglement. The amount of negativity of the state after partial transposition (i.e. the sum of the negative eigenvalues) is related to the actual free entanglement existing in the state, and it was shown to be a full entanglement monotone [37],

\[N(\rho_{AB}) := \frac{1}{2} ||(\Lambda \otimes 1)\rho_{AB}|| - 1,\]  

(1.57)

where \(||A|| := Tr[\sqrt{A^\dagger A}]\) is the trace norm. For the two qubits rotational invariant state [Eq. (1.20)] the negativity is a linear function of the correlation \(\langle \sigma_A^z \sigma_B^z \rangle\) and it has a discontinuity in the first derivative for \(f = -1/3\),

\[N(\rho_{AB}(f)) = -\theta \left(-f - \frac{1}{3}\right) \frac{1 + 3f}{4}.\]  

(1.58)

The maximal entanglement occurs for \(f = -1\) (the singlet state) in agreement with what we expect from an entanglement monotone. When dealing with more than two particles, the negativity defined as (1.57) has a drawback however; it suffers from non-additivity, i.e. \(N(\rho_{AB} \otimes \rho_{CD}) \neq N(\rho_{AB}) + N(\rho_{CD})\).
Figure 1.3.: The density plot shows the degree of entanglement of the AF Heisenberg magnet $\Xi$ [Eq. (1.60)] as measured by the concurrence. The dashed lines separate regions where the entanglement differs by more than 20%. The first dashed line (on the left hand-side) is a transition line ($\beta \simeq 0.14$) separating separable states (left) from entangled ones (right). For small $\beta$ the entanglement completely vanishes, i.e. the temperature is so high that no quantum correlations survive. At the top, $E(\Xi)$ disappears exponentially fast since large magnetic fields tend to align the spins in the opposite direction of $\vec{B}$ producing a separable state. At bottom-right the system is practically in its ground-state (a singlet state) and thus entanglement is nearly maximal.

$N(\rho_{CD})$, and, occasionally, it may be more convenient to use the logarithmic negativity instead,

$$E_N(\rho_{AB}) := \log_2 \| (\Lambda \otimes 1) \rho_{AB} \|.$$  \hfill (1.59)

The logarithmic negativity is an additive entanglement monotone with two desirable properties: it has a clear operational meaning and is an upper bound to the distillable entanglement [40, 41].

Before ending this section, let us apply the concepts we have learned to a simple physical model: two quantum spins in an isotropic magnetic field $\vec{B} = h(1,1,1)/\sqrt{3}$ interacting via an AF Heisenberg model. Adopting the standard summation convention for repeated indices and dropping the subscripts identifying the particles and denoting the partition function by $Z$, the canonical thermal state $\Xi$ of the system becomes,

$$\Xi = 2^r e^{-\beta (\sigma^x \otimes \sigma^x + B^y \sigma^y \otimes 1 + B^z \sigma^z \otimes 1)}$$

$$= \frac{1}{4} \left( 1 \otimes 1 + C(\beta, h) \sigma^y \otimes \sigma^y + m(\beta, h) \sum_{\mu} (\sigma^\mu \otimes 1 + 1 \otimes \sigma^\mu) \right),$$

with $\sigma^\mu := \sigma^\mu$ and $\mu = x, y, z$. The last line follows from the and the properties of Pauli matrices [Eqs. (1.21) and (1.22)]. The two-body correlation $C(\beta, h)$ and the local magnetization $m(\beta, h)$ then

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univocally determine the entanglement. When applying partial transposition,

\[(\Lambda \otimes 1)\Xi: \sigma^y \rightarrow -\sigma^y, \quad (1.62)\]

according to PPT the eigenvalues will remain positive (and thus defining a physical density matrix) only if \(\Xi\) is separable (i.e. if it can be written as a convex sum of product states) — see Fig. 1.3 for a detailed discussion about entanglement in this model.

We have seen that entanglement in bipartite pure states is a well understood problem and that a single measure singles out from adequate QI definitions and thermodynamics considerations. On the other hand, other types of entanglement (e.g. tripartite entanglement), or bipartite entanglement of mixed states is not so well understood (e.g. the open problem of \(\text{LOCC}\) interchangeability for mixed states), although some important conclusions can be drawn: i) for two qubits systems the entanglement is a monotone function of the concurrence or negativity, and therefore can be properly quantified, and ii) for particles living in higher-dimensional Hilbert spaces the negativity yields the amount of free entanglement detected by the PPT criterion.

1.4. Continuous variable entanglement

When the Hilbert state is no longer finite, the pure states are usually described by wavefunctions defined in the continuous phase-space. The study of Continuous Variable (CV) entanglement encounters many difficulties in infinite-dimensional systems (see, for instance, [27, 28]), but an enormous simplification is found if we consider the special set of Gaussian quantum states. This set encompasses the most important states of the quantum harmonic oscillator, such as thermal states and the coherent states describing the Electromagnetic (EM) field of a coherent light source (e.g. a Light Amplification by Stimulated Emission of Radiation (LASER)), just to name a few. Gaussian states of CV systems are fundamental in experimental Quantum Optics [42, 43, 44, 45]. They are known to be invariant under the action of linear optical devices (beam splitters, phase shifts, etc.), and can be used to securely send/receive information, carry quantum error correction and teleport [46, 47, 48]. In the following, we review the main results of the theory of bipartite entanglement of Gaussian states (for a detailed survey of the subject the reader is referred to [49, 50]).

1.4.1. Preliminaries

In order to set up the basic definitions and introduce the sympletic group, let us focus onto systems made of \(n\) bosons (these could represent \(n\) modes of the EM field, the positional degrees of freedom of \(n\) atoms in a lattice, etc.). The Hilbert space is \(\mathcal{H} = \bigotimes_{k=1}^{n} \mathcal{F}_k\), where \(\mathcal{F}_k\) is the infinite dimensional Fock space spanned by the number basis \(\{|m\rangle_k\}_{m \in \mathbb{N}}\) (i.e. the eigenstates of the number operator \(n_k := a_k^\dagger a_k\), with \([a_k, a_k^\dagger] = \delta_{kk'}\)). Considering, for the moment, all the modes having the same
1.4. Continuous variable entanglement

frequency and \( \omega_k \hbar = 1 \), the free Hamiltonian reads,

\[
H_0 = \sum_{k=1}^{n} \left( a_k^\dagger a_k + \frac{1}{2} \right).
\]  

(1.63)

The position- and momentum-like operators of each mode are defined through the canonical Cartesian decomposition,

\[
a_k = \frac{1}{\sqrt{2}} (X_k + iP_k), \quad a_k^\dagger = \frac{1}{\sqrt{2}} (X_k - iP_k).
\]  

(1.64)

Introducing the vector of operators \( \mathbf{O} = (X_1, P_1, ..., X_n, P_n)^T \) living in the phase-space \( \Gamma = \mathbb{R}^{2n} \), the canonical commutation relations \( [X_j, P_k] = i \delta_{jk} \) assume the compact form \( [O_i, O_j] = i \sigma_{ij} \), where we have introduced the sympletic matrix,

\[
\sigma := \bigoplus_{k=1}^{n} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.
\]  

(1.65)

The correlations between the modes are captured by the covariance matrix, \( V_{ij} := \frac{1}{2} \{ \{ O_i, O_j \} \} - \langle O_i \rangle \langle O_j \rangle \). Having all possible correlations in its entries, we shall see that the covariance matrix is the adequate object for the characterization and quantification of the entanglement of Gaussian states.

To acquaint the reader with the notation, we explicitly write the covariance matrix of a canonical thermal state of \( n \) modes with \( \bar{n}_k = 1/ (\exp \beta_k - 1) \) bosons, in average, in each mode:

\[
V_{\text{thermal}} = \bigoplus_{k=1}^{n} \begin{pmatrix} \bar{n}_k + \frac{1}{2} & 0 \\ 0 & \bar{n}_k + \frac{1}{2} \end{pmatrix}.
\]  

(1.66)

The uncertainty principle, stemming from the non-commutativity of quantum observables, \( [O_i, O_j] = i \sigma_{ij} \), also has a compact form in phase space,

\[
V + i \frac{\sigma}{2} \geq 0.
\]  

(1.67)

This inequality is derived from the positivity of \( \rho \) and the uncertainty relations of the operators \( \mathbf{O} \), and is the only condition a \( 2n \times 2n \) symmetric matrix has to satisfy in order to be a \textit{bona fide} covariance matrix of a physical state \cite{25, 51, 52}.

In Quantum Optics, where one is often interested in photon statistics, it is useful to describe the physics via the characteristic function [or its Fourier transform (the quasiprobability function)] from which all statistical quantities can be predicted \cite{42, 44, 45, 53}. The most interesting states of canonical systems of many modes are fully determined by their covariance matrix; these are the so-called Gaussian states. We would like to define a Gaussian state more carefully, thus we introduce the displacement operator and the characteristic function of bosonic fields. The displacement operator
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for $n$ bosons is defined as \[43, 54\],

$$D(\lambda) = \bigotimes_{k=1}^{n} \exp \left( \lambda_k a_k^+ - \lambda_k^* a_k \right) ,$$

(1.68)

with $\lambda \in \mathbb{C}^n$. The quasi-classical (coherent) states of the EM field are obtained from the vacuum through the action of the displacement operator $|\alpha\rangle = D(\alpha)|0\rangle$. This operator displaces the vacuum to another point of the phase-space (i.e. populates it with bosons) preserving the uncertainty of the canonical operators (see Fig. 1.4). Hence, the covariance matrix is the same as for the vacuum: $V_{ij} = \frac{1}{2} \delta_{ij}$. The set of displacement operators is complete in the sense that every operator $O$ on $\mathcal{H}$ can be written as,

$$O = \int_{\mathbb{C}^n} \frac{d^{2n} \lambda}{\pi^n} \text{Tr}[OD(\lambda)]D^\dagger(\lambda) .$$

(1.69)

The previous formula is due to Glauber and

$$\chi[O](\lambda) := \text{Tr}[OD(\lambda)].$$

(1.70)

is the characteristic function of the operator $O$ [54].

\textbf{Definition.} A state $\rho$ of a CV canonical system with $2n$ degrees of freedom is Gaussian if its characteristic function (or equivalently, its quasiprobability distribution) is Gaussian, i.e.

$$\chi[\rho](\lambda) = \chi[\rho](0)e^{-\lambda^T \Sigma \lambda + d^T \lambda},$$

(1.71)

where $\Sigma$ is a $2n \times 2n$ matrix and $d \in \mathbb{R}^{2n}$.

From its definition, a Gaussian state is completely characterized via its first and second moments (higher moments can be obtained by taking partial derivatives of $\chi$, see [50] for instance). The formal link to the vector of operators of the modes $O$ and the covariance matrix $V$ is,

$$d = \sigma^T \text{Tr}[O\rho]$$

(1.72)

$$\Sigma = \sigma^T V \sigma.$$

(1.73)

The quantum correlations of a Gaussian state are encoded in the second moments only, for $d$ can be trivially set to zero with unitary transformations of the individual modes. In alternative, we can also consider the quasiprobability distribution, $W[\rho](O)$, in phase-space, $\Gamma = \mathbb{R}^{2n}$, associated with the state $\rho$. However, we must have some care when interpreting it as a classical probability distribution, for in Quantum Mechanics the expected value of observables have an intrinsic uncertainty (ultimately due to vacuum fluctuations), and the notion of phase-space cannot be pushed too far. Nevertheless, we can always postulate the properties of such distribution and use it solely as a tool to compute statistics of observables. The price to pay is that a quantum distribution must have some defect as a phase-space in a classical fashion does not exist; in particular, it may become negative or ill-behaved.
1.4. Continuous variable entanglement

The field acquires \( n = \langle a^\dagger a \rangle = |\alpha|^2 \) photons and non-zero quadratures: \( X = \text{Re}[\alpha] \) and \( P = \text{Im}[\alpha] \). Right - The Wigner function \( W(q,p) \) is plotted (before and after displacement of vacuum).

(hence the name "quasiprobability"). Bertrand and Bertrand showed that one postulate is enough to define the quasiprobability function \[ W(O) \] is a joint probability distribution for the operators \( O = (X_1, P_1, \ldots) \) (by bearing in mind that simultaneous determination of non-commuting observables, such as \( X_1 \) and \( P_1 \), is not possible). The marginal distributions yield the positions or the momenta distributions,

\[
P(X_1, \ldots, X_n) := \int_{\mathbb{R}^n} \prod_k dP_k W(p) \langle X_1, P_1, \ldots, X_n, P_n \rangle \tag{1.74}
\]
\[
P(P_1, \ldots, P_n) := \int_{\mathbb{R}^n} \prod_k dX_k W(p) \langle X_1, P_1, \ldots, X_n, P_n \rangle. \tag{1.75}
\]

In the literature, one can find several functions \( W[p] \) obeying the above equations (see \[45\] for an introduction to the phase-space methods). The most famous is the Wigner function, which for the single-mode case \( n = 1 \) reads \[53\],

\[
W(q,p) = \frac{1}{2\pi} \int_{\mathbb{R}} dx e^{ipx} \left( q - \frac{x}{2} \right)^2 |\rho| q + \frac{x}{2}. \tag{1.76}
\]

The Wigner function of the vacuum is displayed in Fig. 1.4. In it, we see the action of the displacement operator [Eq. (1.68)] for the one-mode \( D(\alpha = (q) + i\langle \rho \rangle) \). The fluctuations are kept to its minimum value — the so-called Zero-Point Fluctuations (ZPF) — but the quadratures of the \( \text{EM} \) field no longer have a zero mean-value, \textit{i.e.} the vacuum is coherently populated with photons. Gaussian states — like the coherent states — play a notable role, both in view of their conceptual importance and their relevance in experimental Quantum Optics. They are the states more easily prepared and controlled in the laboratory, and have been successfully employed in quantum cryptography \[47\] and quantum teleportation protocols \[46, 48\]. Moreover, it turns out that, when properly

![Figure 1.4:](image-url)
endowed with *symplectic transformations*, the complex problem of finding entanglement monotones for generic mixed states becomes much easier for Gaussian states.

### 1.4.2. Symplectic local invariants of Gaussian states

With the basic definitions established, we now review a fundamental class of transformations known for a long time in classical mechanics that makes the connection between unitary transformations $U$ and its counterpart at the phase-space level; the symplectic transformations. The Hamilton equations of motion for the canonical variables $\mathbf{R} = (q_1, p_1, \ldots, q_n, p_n)^T$ have a compact form in the symplectic formalism,

$$
\dot{\mathbf{R}}_i = \sigma_{ij} \partial_j H.
$$

A transformation of coordinates ($\mathbf{R} \rightarrow S\mathbf{R}$) leaves the form of the previous equation invariant iff $S\sigma S^T = \sigma$.

**Definition.** The *symplectic group* $Sp(2n, \mathbb{R})$ is the set of $2n \times 2n$ real matrices $S$ satisfying

$$
S\sigma S^T = \sigma.
$$

This group has dimension $n(2n + 1)$, and its elements are called canonical or symplectic transformations.

In Quantum Mechanics the elements of $Sp(2n, \mathbb{R})$ preserve the commutation relations, and all mode transformations generated by linear and bilinear interactions are symplectic. Interestingly, the opposite is also true: every symplectic transformation is generated by a bilinear Hamiltonian. This relation between unitary operations and symplectic transformations is a consequence of the Stone-von Neumann theorem: every symplectic transformation ($S$) in the $2n$-dimensional phase space $\Gamma = \mathbb{R}^{2n}$ has its counterpart at the Hilbert space level $\mathcal{H}$ via an unitary transformation ($U$) [52]. The table 1.1 summarizes the main differences between the description of physical states within the realm of the Hilbert space and that of the phase-space.

| | Hilbert space $\mathcal{H}$ | Phase-space $\Gamma$ |
|---|---|---|
| dimension | $\infty$ | $2n$ |
| structure | $\otimes$ | $\oplus$ |
| description | $\rho$ | $V$ |
| physical states | $\rho \geq 0$ | $V + \frac{1}{2}\sigma \geq 0$ |
| spectrum | $0 \leq p_i \leq 1$ | $1/2 \leq \lambda_i < \infty$ |

Table 1.1.: The Hilbert space versus phase-space description of physical states.

The symplectic theory turns out to be the proper playground for the study of entanglement in CV states. This originates from the fact that the covariance matrix can always be brought to a suitable form by applying local unitary operations $U_A \otimes U_B \leftrightarrow S_A \oplus S_B$ (which, as we have seen in the Sec. 1.3...
do not affect the amount of entanglement shared by two parties), and that a necessary and sufficient condition for separability of Gaussian states exists that can be easily expressed within the sympletic framework. In order to see this, we recall an important theorem due to Williamson and explore its implications for Gaussian states.

**Theorem.** [Williamson, 50] Given \( V \in M(2n, \mathbb{R}) \) satisfying \( V^T = V \) and \( V > 0 \) there exists a sympletic transformation \( S \in S_p(2n, \mathbb{R}) \) and a diagonal matrix \( D \in M(n, \mathbb{R}) \) positive definite such that,

\[
V = S^T \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix} S.
\]

(1.79)

The matrices \( S \) and \( D \) are unique, up to a permutation of the elements of \( D \). The eigenvalues of \( D \) are called sympletic eigenvalues.

We conclude that every Gaussian state \( \rho \) can be obtained from a thermal state \( \Xi \), with covariance matrix given by Eq. (1.66), through an adequate unitary transformation \( U_S \) associated with the sympletic matrix \( S \):

\[
\rho = U_S \Xi U_S^\dagger.
\]

(1.80)

This is a direct consequence of the Williamson theorem [Eq. (1.79)], which will be very useful to discuss separability of bipartite states. Due to its relevance in what will follow, we focus on the particular case of two-mode Gaussian states, \( O_{AB} = (X_A, P_A, X_B, P_B)^T \). With all generality, we can write the covariance matrix in the 2 \( \times \) 2 block form,

\[
V = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix},
\]

(1.81)

In it, \( A \) (\( B \)) and \( C \) are 2 \( \times \) 2 matrices containing the information about the reduced state of \( A(B) \) and the correlations between the two subsystems, respectively. Local invariants with respect to \( S_p(2, \mathbb{R}) \otimes S_p(2, \mathbb{R}) \) can be straightforwardly derived by considering the action of the generic local sympletic transformation \( S_A \otimes S_B \), with \( S_A, S_B \in S_p(2, \mathbb{R}) \), on \( V \),

\[
A \rightarrow S_A \text{AS}_A^T
\]

(1.82)

\[
B \rightarrow S_B \text{BS}_B^T
\]

(1.83)

\[
C \rightarrow S_A \text{CS}_B^T.
\]

(1.84)

The determinant of every block will not change under the action of sympletic transformations \( S_p(2, \mathbb{R}) \otimes S_p(2, \mathbb{R}) \subset S_p(4, \mathbb{R}) \): \( \det A, \det B, \det C \) and \( \det V \) are sympletic invariants. Theorem (1.79) allows to perform a sympletic diagonalization of matrices \( A \) and \( B \) by a proper choice of \( S_A \) and \( S_B \),
1. Introduction

respectively,

\[ S_A S_A^T = D_A := a 1_2, \]
\[ S_B S_B^T = D_B := b 1_2. \]  \(1.85\)

We make a final simplification of Eq. (1.81) by noting that matrices \(C\) and \(C^T\), being \(2 \times 2\) real matrices, admit diagonalization by a proper orthogonal matrix \(O_{AB}\) (naturally not affecting \(D_A\) and \(D_B\) being proportional to the identity matrix):

\[ V = \begin{pmatrix}
    a & 0 & c_1 & 0 \\
    0 & a & 0 & c_2 \\
    c_1 & 0 & b & 0 \\
    0 & c_2 & 0 & b
\end{pmatrix}. \]  \(1.87\)

The covariance matrix \(1.87\) is said to be in its normal form, and the three independent sympletic invariants now read: \(\det A = a^2\), \(\det B = b^2\) and \(\det C = c_1 c_2\). These invariants provide us an handy way to get the sympletic eigenvalues of the covariance matrix \([52, 56]\):

\[ \sqrt{2} d_{ \pm} = \sqrt{\Sigma[V] \pm \sqrt{[\Sigma[V]]^2 - 4 \det V}}, \]  \(1.88\)

with \(\Sigma[V] := \det A + \det B + 2 \det C\). Note that \(d_{ \pm}\) are the eigenvalues of \(D\) [Eq. (1.79)] and that the Williamson form of Eq. (1.87) is simply:

\[ V = S^T \begin{pmatrix}
    d_+ & 0 & 0 \\
    0 & d_- & 0 \\
\end{pmatrix} \oplus \begin{pmatrix}
    d_+ & 0 & 0 \\
    0 & d_- & 0 \\
\end{pmatrix} S. \]  \(1.89\)

1.4.3. The separability of Gaussian states

We would like to use the phase-space picture to say about the degree of non-separability of quantum states in \([CV]\). Like in \([PPT]\) for density matrices [Eq. (1.55)], we should start with a well-defined criterion for separability. Simon’s approach to this problem is based on the observation that transposition (of a density matrix) is equivalent to a mirror reflection in the \([CV]\) scenario: \(O \rightarrow \Lambda O\) with \(\Lambda = \text{Diag} (1, -1, \ldots, 1, -1)\), as the transposition of a Hermitian matrix corresponds to complex conjugation, and this, in its turn, amounts to time reversal in the Schrödinger picture \([25]\). Another way of seeing this is to take the Wigner distribution [Eq. (1.76)] and make the transposition of the density matrix elements. For a bipartite system, \(\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B\), partial transposition with respect to system \(A\) will be rendered on the phase space through the action of the matrix,

\[ \Lambda_A = \Lambda \oplus 1. \]  \(1.90\)
1.4. Continuous variable entanglement

According to what we have learned in Sec. 1.3, a necessary condition for separability is then that partial transposition still yields a semi-positive defined operator (i.e. a physical state) [Eq. (1.67)],

$$\Lambda_A V \Lambda_A + \frac{i}{2} \sigma \geq 0,$$  \hspace{1cm} (1.91)

This is the Simon’s criterion for \carbon{CV} separability. It is instructive to recast the above inequality in an intrinsically $S_p(2, \mathbb{R}) \otimes S_p(2, \mathbb{R})$ invariant form. To this end, we take advantage of the Williamson decomposition for two-mode states [Eq. (1.89)] and write the positivity condition for physical states [Eq. (1.67)] as function of the sympletic eigenvalues: $d_- \geq 1/2$. This expression has a straightforward physical meaning: the product of the variances of canonical conjugate operators cannot be below the ZPF. Hence, when performing partial transposition of a separable state, the vacuum still yields the absolute lower bound for the uncertainties (recall that $V_{\text{vacuum}} = \frac{1}{2} \mathbb{1}$),

$$d_- := d_-(\Lambda_A V \Lambda_A) \geq \frac{1}{2}.$$  \hspace{1cm} (1.92)

The partial transposition $(\Lambda_A V \Lambda_A)$ affects only the off-diagonal blocks ($c_2 \rightarrow -c_2$), and hence a single sympletic invariant: $\det C \rightarrow -\det C$. Using the explicit sympletic invariant formula for $d_-$ [Eq. (1.88)] the following criterion is obtained:

$$\det A + \det B + 2|\det C| \leq \frac{1}{4} + 4 \det V.$$  \hspace{1cm} (1.93)

Before partial transposition, the covariance matrix already obeys the above inequality with $|\det C| \rightarrow \det C$. The inclusion of the absolute value operation above, leads then to a more restrictive separability condition. It should be noted that the above criterion is valid for any \carbon{CV} (Gaussian or not). The bottom line for Gaussian states [Eq. (1.71)] separability is the remarkable conclusion that Simon’s criterion $>[1.91][1.93]$ is also necessary:

**Theorem.** <Simon, [25]> The PPT is a necessary and sufficient condition for separability, for all bipartite Gaussian states.

In the same spirit as the $2 \otimes 2$ and $2 \otimes 3$ cases where PPT is sufficient and necessary, the quantification of entanglement of Gaussian states is conveniently given by the logarithmic negativity [Eq. (1.59)]. For the bipartite scenario, it is a decreasing function of the smallest sympletic eigenvalue $d_-$.  \hspace{1cm} (1.94)

Here, for pedagogical reasons, we apply Simon’s criterion to the two-mode squeezed thermal state. This state arises when a pair of bosonic modes, $a = (X_A + iP_A)/\sqrt{2}$ and $b = (X_B + iP_B)/\sqrt{2}$, interact via an Hamiltonian of the form $H = gab + g^* a^\dagger b^\dagger$. The production and detection of squeezed states represent one of the major topics of Quantum Optics [57, 58]; the name "squeezed" was appropriately adopted since, under evolution through the squeezing operator, $S_I(z) = \exp(za^2 - z^* a^\dagger z^2)$, with $z = \ldots$
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The single-mode EM radiation sees one of its quadratures, say $X_1$, going below the ZPF level:

$$
S_1^+(z)aS_1^-(z) = \cosh(r)a + e^{i\theta}\sinh(r)a^\dagger
$$

(1.95)

$$
S_1^+(z)a^\dagger S_1^-(z) = \cosh(r)a^\dagger + e^{-i\theta}\sinh(r)a.
$$

(1.96)

This is a manifest quantum phenomenon, and it can be easily checked that the above equations effectively squeezes the variances of the quadratures [Eq. (1.64)] maintaining the product of the variances $\Delta X_1\Delta P_1$ unchanged.

Likewise, we define the two-mode squeezed vacuum as $S_2^+(z)|0,0\rangle_{A,B}$, where

$$
S_2^+(z) = \exp\left(zab - z^*a^\dagger b^\dagger\right).
$$

(1.97)

If instead of vacuum we had a thermal state of the modes, we would get the two-mode squeezed thermal state,

$$
\Xi_{AB}(\bar{n}, r) := S_2^+(r)\Xi_A(\bar{n}) \otimes \Xi_B(\bar{n})S_2^-(r).
$$

(1.98)

Once more the squeezing is nicely captured in the Heisenberg picture,

$$
S_2^+(z)aS_2^-(z) = \cosh(r)a + e^{i\theta}\sinh(r)b^\dagger
$$

(1.99)

$$
S_2^+(z)b^\dagger S_2^-(z) = \cosh(r)b^\dagger + e^{-i\theta}\sinh(r)a,
$$

(1.100)

yielding the following change quadrature’s transformations: $O_{AB} \rightarrow \Omega(z)O_{AB}$. The correlations of the thermal state $\Xi_A \otimes \Xi_B$ will change in agreement,

$$
V \rightarrow \Omega(z)V\Omega^T(z),
$$

(1.101)

where $V(\bar{n})$ is the covariance matrix of the two-mode thermal state $\Xi_A(\bar{n}) \otimes \Xi_B(\bar{n})$ without squeezing, that is [see Eq. (1.66)]:

$$
V(\bar{n}) = \bigoplus_{k=A,B} \begin{pmatrix} \bar{n} + \frac{1}{2} & 0 \\ 0 & \bar{n} + \frac{1}{2} \end{pmatrix}.
$$

(1.102)

The $4 \times 4$ sympletic matrix $\Omega$ encodes the two-mode squeezing,

$$
\Omega(z) = \begin{pmatrix} \cosh \frac{r}{2} & \sinh \frac{r}{2} R(\theta) \\ \sinh \frac{r}{2} R(\theta) & \cosh \frac{r}{2} \end{pmatrix}, \quad R(\theta) = \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix}.
$$

The possibility for entanglement can be investigated via inequality Eq. (1.93). This is accomplished by computing the determinant $V$ [Eq. (1.101)] and the determinant of its $2 \times 2$ blocks (namely, $A$, $B$...
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We find,
\[
\text{det} V = \frac{1}{16} (1 + 2\bar{n})^4
\]  
\[
\text{det} A = \text{det} B = \frac{1}{4} (1 + 2\bar{n})^2 \cosh (2r)^2
\]  
\[
\text{det} C = -(1 + 2\bar{n})^2 \cosh (r)^2 \sinh (r)^2
\]

The important case of the two-mode squeezed vacuum ($\bar{n} = 0$) yields a violation of Eq. (1.93) for any $r > 0$. This means that any finite squeezing will generate entanglement from the vacuum. This makes all sense as $S^{(z)}_2(0,0)^\perp_{A,B}$ is highly non-local in the Fock basis [44],
\[
S^{(z)}_2(0,0)^\perp_{A,B} = \frac{1}{\sqrt{\cosh r}} \sum_{n=0}^{\infty} \left( e^{i\theta \tanh r} \right)^n |n,n\rangle_{A,B}.
\]

The case $\tanh r = 1$ corresponds to infinite squeezing (like in the original EPR pair) giving rise to a maximally entangled state $\sim \sum_n |n,n\rangle$ with diverging entanglement entropy [Eq. (1.44)]. The log-negativity [Eq. (1.94)] for the two-mode squeezed thermal state can be computed using Eqs. (1.103)-(1.105) together with the expression for the sympletic eigenvalue $\tilde{d}$ [Eq. (1.92); see also Eq. (1.88)] and yields
\[
E_N(\Xi_{AB}) = \max [0, 2r - \ln (2\bar{n} + 1)].
\]

When the vacuum is populated with photons, i.e. $\bar{n} > 0$, the violation of the separability criterion may still happen, but the amount of entanglement decreases according to the formula above. This should be no surprise, as "mixing" usually destroys entanglement (Sec. 1.3). Hence, like in the Heisenberg magnet (see Fig. 1.3), there is a critical temperature $\bar{n}_c$ defined by: $\exp (-2r) (2\bar{n}_c + 1) = 1$.

In the next chapter, we will show the first evidence of an ideal macroscopic system capable of sustaining bipartite entanglement at high temperature (compared to typical energy scales) by allowing one part of the system to be initialized in a pure state, rather than a thermal state. A similar phenomenon had been reported before for an EM mode interacting with a two-level atom [59], and we will see it remains true in the macroscopic domain by exploiting the vastness of the Hilbert space.
1. Introduction
2. Macroscopic entanglement at finite temperatures: an ideal scenario

This chapter is based on the following publication by the author:

Macroscopic thermal entanglement due to radiation pressure, AIRES FERREIRA, A. Guerreiro, and V. Vedral, Phys. Rev. Lett. 96, 060407 (2006).

2.1. Overview

The mind-puzzling question of the quantum-to-classical transition is not yet fully understood despite all the effort made in that direction, since the very birth of Quantum Mechanics [60, 61, 62]. Does the center-of-mass motion of macroscopic bodies obey the Schrödinger equation? Many condensed matter physicists would answer positively to this question; it is known that superconducting quantum interference devices allow for the superposition of a clockwise and anti-clockwise current consisting of billions of electrons [63, 64]: a genuine superposition of macroscopic states!

Nothing in the principles of standard Quantum Mechanics says it would be different with, let us say, the center-of-mass motion of an apple provided that the degrees of freedom of the macroscopic object are sufficiently decoupled from the environment (as first noted by Caldeira and Leggett [65]). Although this might seem clear for some, it is still a question of great debate and, despite the recent technological and experimental advances in such direction, no experiment capable of testing such limits has been performed so far.

Within the Quantum Optics community, a few opto-mechanical experiments have already been proposed endeavoring to reach the quantum-classical boundary from top to bottom. For instance, in [66] (like in the original Schrödinger-cat gedanken experiment [67]) an entangled photon state induces quantum superpositions of a mirror, and in [68] multi-component cats of the EM field are created in the interaction of a cavity mode with a moveable tiny mirror. All these proposals have the common feature of considering special states of light (e.g. Fock states, squeezed states, etc.) to create superpositions involving macroscopic subsystems. If there is no "collapse" of the wave function of the macroscopic object, then one would be able to measure its interference with a photon in the spirit...
Opto-mechanical systems represent a natural candidate to test the quantum-to-classical transition for several reasons. To begin with, mechanical oscillators resemble a prototype of “classical” systems, and thus any genuine quantum signature would constitute a major progress. From the experimental side, a fine control of the EM field is possible in the laboratory, and high quality mechanical oscillators can be manufactured with state-of-the-art microfabrication techniques.

The interaction of light with mechanical oscillators was well studied throughout the last century, mainly because of detection of gravitational waves [70]. As the waves travel, their energy impinges a very weak force onto the mechanical oscillator, thus requiring an unprecedented level of precision in monitoring the oscillator’s position: the Standard Quantum Limit (SQL). For a mechanical oscillator with mass $m$ and natural frequency $\omega_m$, the SQL equals the uncertainty in the position due to vacuum fluctuations, i.e. $\Delta x_{\text{SQL}} = \sqrt{\hbar/2m\omega_m}$.

The seminal work on single quantum measurements by Braginsky [70] has taught us that the actual conditions to observe quantum signatures in a mechanical oscillator depends on the details of the specific experiment due to the quantum back action of the measurement device. As a consequence, the common cited criterion for an oscillator to behave quantum mechanically,

$$k_B T \leq \frac{\hbar\omega_m}{2},$$

has to be corrected depending on the measurement time and the oscillator’s relaxation time (we refer the reader to Appendix A.1 for more details on the SQL). While the quantum-classical transition has been observed in microscopic systems and even in mesoscopic systems [71] [72], for a macroscopic mechanical oscillator (with $\omega_m$ typically in the Mhz range) achieving the quantum realm requires extremely low temperatures (a rough estimate is provided by the above criterion: $T \sim 1\mu\text{K}$).

The temperature is indeed the main obstacle in most of the proposals, but not the only one, though. For instance, in the Penrose experiment, the back-action of the environment (by friction) rapidly destroys the coherence of the macroscopic superpositions — a particular case of a phenomenon traditionally referred to as decoherence in the context of open quantum systems (see [73] [74] [75] for a quantitative description of the difficulties of such experiments).

Inspired by the fundamental difference between classical and quantum correlations discussed in Chap. [1], we will tackle the aforementioned problem by asking the question of the quantum-to-classical transition in a slightly different way; can a macroscopic system be entangled with another system? We know that teleportation of photons [5] [6] [7] is possible due to maximal polarization entanglement created by a standard Quantum Optics phenomenon: the so-called parametric-down conversion [76]. In this process, a photon interacts with a non-linear medium producing two entangled photons with half of the frequency of the original photon. In general, however, there are no generic processes leading to entanglement between other degrees of freedom, but interactions can
2.1. Overview

Figure 2.1.: A photon carrying momentum $\mathbf{P} = E/c$ meets a totally reflective mirror attached to a vibrating spring with natural frequency $\omega_m$. A very feeble momentum ($= 2P$) is transferred to the mirror which starts to oscillate. A correlation between the EM field quadratures and the mirror canonical observables develops in time. Can we speak about genuine quantum entanglement in this case?

always be "designed" so that the resulting wave function is entangled. Photons are known to carry a momentum given by its frequency, $\mathbf{P} = h\omega/c$, and we may feel tempted to think that, due to the ponderomotive interaction, the quadratures of a EM field consisting of many photons could actually become entangled with the positional degree of freedom of a massive oscillator. If the latter is true, then we could speak about **macroscopic entanglement** (see Fig. 2.1).

In what follows, we present a very simple heuristic calculation in favor of the idea expressed in the previous paragraph. Indeed, let us consider two mirrors mounted in a Fabry-Perot geometry, and allow the end mirror to move under radiation pressure (see the details in Fig. 2.2). A single mode of the EM field is prepared in a superposition of Fock states, $|\psi(0)\rangle = |0\rangle + |1\rangle$, and we let the system evolve unitarily. If the temperature is negligible, $T \approx 0$, one can approximate the initial state of the mirror by the vacuum state, $|0\rangle_m$. By confining the EM field into a sufficiently small cavity, we expect an instantaneous displacement of the mirror due to radiation pressure. We can then describe the coherent evolution of the coupled system by,

$$
(|0\rangle + |1\rangle) \otimes |0\rangle_m \rightarrow |0\rangle \otimes |0\rangle_m + f(k,t)|1\rangle \otimes |\phi(t)\rangle_m,
$$

(2.2)

where $k$ is the strength of the radiation pressure interaction in units of the initial wave packet size, $f(k,t)$ is an unknown function and $|\phi(t)\rangle_m$ describes the state of the mirror after the momentum of the EM field has been transferred. We require the wave function of the mirror to preserve its Gaussian character and, hence describe it as a coherent state. We take the displacement of the mirror to be proportional to the radiation pressure coupling, $\phi(t) \sim k$, and, by noticing that the amplitude of a coherent state is proportional to $\text{Re}[\phi(t)]$, define,

$$
\phi(t) \equiv k\eta(t).
$$

(2.3)
2. Macroscopic entanglement at finite temperatures: an ideal scenario

The unitary evolution will make the mirror to oscillate coherently. This implies a few restrictions on the properties of the unknown functions: \( \eta(0) = \eta(2\pi/\omega_m) = 0 \) and \( f(k,t) = e^{i\theta(t)} \) with \( \theta(t) \in \mathbb{R} \).

\[
|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left( |0\rangle \otimes |0\rangle_m + e^{i\theta(t)} |1\rangle \otimes |k\eta(t)\rangle_m \right).
\]

(2.4)

In the above formula, \( |k\eta(t)\rangle_m \) describes a coherent state obtained from the mirror’s vacuum through the action of the displacement operator \( D(z) = \exp \left( za^\dagger - z^* a \right) \) [with \( a \) and \( a^\dagger \) being standard bosonic operators satisfying \( [a, a^\dagger] = 1 \) and \( z \in \mathbb{C} \) — see also Eqs. (1.68) and (A.10)] according to,

\[
|k\eta(t)\rangle_m = D_m(k\eta(t)) |0\rangle = e^{-|k\eta(t)|^2/2} \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} (k\eta(t))^n |n\rangle.
\]

(2.5)

The last equality is straightforwardly obtained by factorizing the displacement operator \( D_m(k\eta(t)) \) with the Baker-Campbell-Hausdorff formula [42, 45]. The entanglement present in such bipartite system, being pure, is determined by the partial states. The Schmidt decomposition (1.40) guarantees that the eigenvalues spectrum of the mirror and cavity are the same [Eq. (1.42)], and hence we conveniently choose to compute the partial state of the cavity field due to its low dimensionality.

Arranging the result in a matrix in the Fock basis, \( \{|0\rangle, |1\rangle\} \), we have,

\[
\rho_{\text{cav}}(t) = \text{Tr}_m[|\psi(t)\rangle\langle \psi(t)|] = \frac{1}{2} \begin{pmatrix}
1 & e^{i\theta(t)} e^{-|k\eta(t)|^2/2} \\
e^{-i\theta(t)} e^{-|k\eta(t)|^2/2} & 1
\end{pmatrix}.
\]

(2.6)

The density matrix \( \rho_{\text{cav}}(t) \) determines the full dynamics of the EM field quadratures. The entropy of entanglement [Eq. (1.45)] is directly obtained from its eigenvalues.

\[
E(|\psi(t)\rangle) = -x_+(t) \ln x_+(t) - x_-(t) \ln x_-(t)
\]

(2.7)

\[
x_\pm(t) = \frac{1 \pm e^{-|k\eta(t)|^2/2}}{2}.
\]

(2.8)

The entanglement shared by two parties is maximal when the reduced states have no information, \textit{i.e.} the partial state is maximally mixed [Eq. (1.15)] and \( E = \ln 2 \). The latter happens for large coupling and \( t \in [0, 2\pi/\omega_m] \) as \( k\eta(t) \gg 1 \) implies \( x_\pm(t) \simeq 1/2 \). For \( t = 0, 2\pi/\omega_m, 4\pi/\omega_m, \ldots \) the system returns to its initial state and the wave function displays no entanglement.

### 2.2. Towards high-temperature macroscopic entanglement

In this section we will study the interaction of a tiny mirror with a coherent state of the EM field, and show for the first time that macroscopic bipartite entanglement can persist at finite temperatures. When referring to macroscopic entanglement, we mean that at least one of the subsystems has many
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internal degrees of freedom or a macroscopic mass\(^1\). In either case, the systems are allowed to exchange large amounts of energy due to an intrinsic large Hilbert space, in opposition to single photons interacting with two-level atoms, for instance (i.e. microscopic systems).

Our results will lead us to the conclusion that the standard criterion for a macroscopic oscillator to behave quantum mechanically (2.1) can be surpassed, and that in fact the quantum behavior of two coupled systems can survive at moderately high temperatures. This clearly paves the way to a realistic experiment aiming to test the limits of quantum mechanics, and we shall discuss such possibility with more detail in Chap. 3 by computing the critical temperature above which no measurable entanglement is expected in a realistic scenario.

Our motivation is the naive optimistic result expressed in Eq. (2.8): at zero temperature, the entanglement between the mirror and the cavity field, \(|0\rangle + |1\rangle\), is large when the coupling between the photon and the mechanical oscillator is high enough, \(k > 1\). Generally, the effect of temperature unavoidably destroys entanglement, for mixing together pure states corresponds to entanglement dilution (compare with the entanglement reduction by temperature in the Heisenberg magnet, Fig. 1.3). Nevertheless, it can happen that the radiation-pressure mechanism is robust enough to attain entanglement even at high-temperatures in some physical regime exploiting the vastness of the Hilbert space of a macroscopic system. In order to see whether this turns out to be true, a more sophisticated calculation is needed, which is able to take into account the important issue of temperature and the possibility of preparing the cavity with many photons. The drawback of this approach is that one will not be able to compute the exact entanglement as for the simple case of Eq. (2.4); but still, the most important question addressing the possibility of macroscopic entanglement will be answered.

We start by studying more carefully the interaction of the cavity field with a movable mirror (see Figure 2.2). In a quantum treatment, the mirror is modeled by an harmonic oscillator with operators \(b\) and \(b^\dagger\) acting in the Fock space of phononic occupation. The full opto-mechanical Hamiltonian includes all the modes of the cavity as they can be excited by the motion of the mirror. A rigorous derivation of the interaction non-relativistic Hamiltonian was given in \[77\]. Here, instead, we will derive it heuristically for the case of interest: the adiabatically driven mechanical oscillator, i.e. \(\omega_m \ll \omega_c\). Typically, the resonant frequencies of an optical cavity and mechanical oscillator are of the order of \(10^{12} - 10^{15}\) Hz and \(10^6\) Hz, respectively, which is well inside the mentioned limit. This simplifies very much the treatment, as photons do not get scattered to higher modes. The free Hamiltonian of the system simply reads,

\[
H_0 = \hbar \omega_c a^\dagger a + \hbar \omega_m b^\dagger b,
\]  

(2.9)

where \([a, a^\dagger] = 1\) and \([b, b^\dagger] = 1\) are the standard commutation rules of bosonic operators (see the table 2.1 for the relation between these operators and the quadratures of the fields).

\(^1\)A criterion to decide whether or not a given mass is macroscopic could be that its mass is above the Planck scale, \(m > m_{\text{Planck}} \approx 4\mu g\).
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Figure 2.2.: At equilibrium the Fabry-Perot cavity consists of two mirrors separated by a distance $L$. Hence, the cavity has resonance frequencies given by $\omega_n = n\omega_c$ (with $n \in \mathbb{N}$ and $\omega_c = \pi c / L$) and the mirrors are assumed to be perfect reflective. The end mirror is able to move under radiation pressure (experimentally this can be done by placing the mirror on a oscillator cantilever), and as soon as a large coherent field is prepared inside the cavity (for instance, by a pumping laser) the mirror starts to oscillate with natural frequency $\omega_m$ and amplitude larger than the ZPF.

|                | Position ($Q$)                                                                 | Momentum ($P$)                                                                 |
|----------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------|
| mechanical mode| $q = \sqrt{\frac{\hbar}{2m\omega_m}} (b + b^\dagger)$                       | $p = \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar m\omega_m}{2}} (b - b^\dagger)$   |
| cavity field   | $X = \frac{1}{\sqrt{2}} (a + a^\dagger)$                                   | $Y = \frac{i}{\sqrt{2}} (a - a^\dagger)$                                   |

Table 2.1.: This table summarizes the relation between the canonical bosonic operators and the generalized coordinates (or quadratures) of the mechanical mode and the cavity field, respectively.

At equilibrium, the lowest frequency of the cavity reads $\omega_c(L) = \pi c / L$ where $L$ is the length of the cavity. For small displacements of the mirror, $q \ll L$, the frequency $\omega_c$ can be Taylor expanded around the equilibrium position, $\omega_c(q) \simeq \omega_c(1 - q / L)$, and the adiabatic interaction Hamiltonian can be immediately written,

$$H_{int} = -\frac{\hbar \omega_c}{L} a^\dagger a q = -\frac{\hbar \omega_c}{L} x_{ZPF} a^\dagger (b + b^\dagger) = -\hbar g a^\dagger a (b + b^\dagger).$$

(2.10)  
(2.11)  
(2.12)

The radiation pressure coupling can be written as function of the ZPF $[x_{ZPF} = \sqrt{\hbar / 2m\omega_m}]$ of the mechanical oscillator. The intuitive idea expressed in the previous section that a sufficiently small cavity leads to large couplings is then confirmed,

$$g = \frac{\omega_c}{L} \sqrt{\frac{\hbar}{2m\omega_m}}.$$  
(2.13)
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Each resonant photon transfers momentum to the mirror in each of the reflection it undergoes causing the enhancement of the mechanical effects of light. The full Hamiltonian reads,

\[ H = \hbar \omega_c a^\dagger a + \hbar \omega_m b^\dagger b - \hbar g a^\dagger (b + b^\dagger) . \]  

(2.14)

Some comments on the validity of an unitary evolution under Hamiltonian (2.14) are in order. As mentioned before, the derivation is strictly valid in the adiabatic limit, where the resonant frequency of the mirror is much smaller than the free-spectral range of the cavity, \( \omega_m \ll \pi c/L \). In this limit, the coupling between different cavity field modes (leading to the Casimir effect, etc.) can be neglected as the single mode picture captures all the relevant physics.

In practice, perfect cavities do not exist, and the photons have some probability to leak out destroying unitarity. However, for cavities with very high quality factor \( Q \) (defined as the number of average photon round trips inside the cavity), the damping is negligible, as it occurs on a time scale much longer than it takes for the photons to perform several round trips. As long as photon leakage is the most relevant source of decoherence, the unitary evolution under Hamiltonian (2.14) is expected to be a good description of the problem for times \( t \ll QL/c \). The effect of the cavity damping and a finite viscosity (the main sources of decoherence in a realistic scenario) will be taken in account in Chap. 3. In what follows, we discuss the unitary evolution of a thermalized mirror and its entanglement dynamics with the cavity mode. A summary of the main features of optical cavities is given in Appendix B.1.

The evolution operator associated with the Hamiltonian (2.14) has a closed formula and it was derived in [78], using the Campbell-Baker-Hausdorff formula for the Lie algebra, and in [68], using operator algebra methods:

\[ U(t) = e^{-i\omega_c a^\dagger a t} e^{i k^2 (a^\dagger a)^2 \Lambda(t)} D_m(\eta(t) k a^\dagger a) e^{-i\omega_m b^\dagger b t} . \]  

(2.15)

In the above formula, \( \Lambda(t) = \omega_m t - \sin(\omega_m t) \), \( \eta(t) = 1 - e^{-i\omega_m t} \), \( k = g/\omega_m \) and \( D_m(\eta(t) k a^\dagger a) = e^{k a^\dagger a(\eta(t)b - \eta(t)^*b)} \) is the displacement operator of the mirror, \( D_m(\gamma)|0\rangle = |\gamma\rangle \). It is pedagogical to apply the evolution operator to the simple example of the Cat-like state considered above, \( |\psi(0)\rangle = (|0\rangle + |1\rangle) \otimes |0\rangle_m \). The evolution operator consists of two free evolution phases, a Kerr-like non-linear phase and a displacement operator whose amplitude depends upon the photon pressure \( \sim a^\dagger a \). They yield for the "Cat-like" state,

\[ (|0\rangle + |1\rangle \otimes |0\rangle_m \rightarrow |0\rangle \otimes |0\rangle_m + e^{f(t)} |1\rangle \otimes |k\eta(t)\rangle_m . \]  

(2.16)

Since \( f(t) = k^2 \Lambda(t) - \omega_c t \) is a phase, we have exactly recovered the heuristic result derived earlier (2.4): the interaction term of the Hamiltonian has the potential to entangle the cavity field modes with the vibrational modes of the mirror for intermediate times [Eq. (2.8)]. The entanglement results from the evolution of the term \(|1\rangle \otimes |0\rangle_m \), which can be interpreted as the transference of momentum
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from the photon $|1\rangle$ to the mirror $|0\rangle_m$, as the photon kicks the mirror. Though the Cat-like state of light, $|0\rangle + |1\rangle$, is easy to produce experimentally, the radiation pressure in this case is so small that it is virtually impossible to detect any entanglement using present day technology. However, we will see in this chapter, that a detectable amount of thermal entanglement is expected when the cavity is initially in a coherent state with sufficiently high amplitude, \emph{i.e.} when many photons are considered instead of just one.

The EM field is prepared in a coherent state of the light, $|\alpha\rangle = D(\alpha)|0\rangle$, using a driving LASER tuned to resonance with the cavity mode, whereas the mirror is considered to be initially in a Gibbs state with temperature $T$. Expressing the thermal state of the mirror in the coherent state basis (see Appendix A.2), the composite state of the system reads,

$$\rho(t_0) = \frac{1}{\bar{n}} \int_{\mathbb{C}} \frac{d^2z}{\pi} e^{-|z|^2/\bar{n}} |\alpha\rangle \langle \alpha| \otimes |z\rangle \langle z|,$$

(2.17)

where $\bar{n} = 1/\left(e^{\hbar \omega / kT} - 1\right)$ is the mean number of phononic excitations and $z \in \mathbb{C}$ represents all the possible coherent states of the mirror. The density matrix $\rho(t_0)$ evolves according to $\rho(t) = U(t)\rho(0)U^\dagger(t)$ and it can be readily obtained as soon as the evolution of a pure coherent state \(|\alpha\rangle_m\), for any population of the cavity $|n\rangle$, is written in a suitable basis. From Eq. (2.15) we have,

$$U(t)|n\rangle \otimes |z\rangle_m = e^{-i\phi_n(t)}|n\rangle \otimes |ze^{-i\omega_0 t} + kn\eta(t)\rangle_m,$$

(2.18)

with $\phi_n(t) = n\omega_c - k^2 n^2 \Lambda(t)$. The amplitude $z$ in (2.18) is displaced by the evolution operator depending on radiation pressure ($\sim a^\dagger a$) exactly as we found before [Eq. (2.16)]. A coherent state of the mirror will evolve according to,

$$U(t)|\alpha\rangle \otimes |z\rangle_m = e^{-|\alpha|^2/2} \sum_{n \in \mathbb{N}_0} e^{-i\phi_n(t)} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \otimes |ze^{-i\omega_0 t} + kn\eta(t)\rangle_m.$$

(2.19)

Finally, the evolution of the density matrix is obtained by averaging the latter expression with the corresponding Boltzmann’s weights [see Eq. (2.17)]. Here we express $\rho(t)$ in the Fock basis,

$$\rho(t) = \sum_{\mu, \nu, n, m=0}^\infty \rho_{\mu\nu mn}(t)|n\rangle \langle m| \otimes |\mu\rangle \langle \nu|,$$

(2.20)

where the Latin indexes refer to the radiation and the Greek indexes refer to the mirror. It is useful to define the following functions,

$$\Phi_{\mu\nu mn}(t) := \alpha^m \alpha^* n \exp\left[i\Lambda(t)(n^2 - m^2) - i\phi_m(n - m) - |\alpha|^2/(n!m!\mu!\nu!t)^{1/2}\right]$$

(2.21)

$$K_{nm}(z) := |F_n(z)|^2/2 + |F_m(z)|^2/2 + |z|^2/\pi,$$

(2.22)

where $F_n(z) = z + kn\eta(t)$. With these definitions the elements of the density matrix read (see
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Appendix A.3 for a detailed derivation):

\[
\rho_{\mu\nu\eta\xi}(t) = \Phi_{\mu\nu\eta\xi}(t) \int_{\mathbb{C}} \frac{d^2 z}{\pi n!} \bar{F}_\nu(z) \mu \bar{F}_\eta(z) \nu e^{-K_{\mu\nu}(z)}.
\]  

(2.23)

This integral can be analytically solved (see Appendices A.2 and A.3 for the integration techniques for bosons). Up to a normalization constant it yields [Eq. (A.40)],

\[
\rho_{\mu\nu\eta\xi}(t) = \Phi_{\mu\nu\eta\xi}(t) e^{-k_2 |\eta(t)|^2} \left[ \prod_{a,b} \bar{G}_{nm}(a,b,\bar{n},k,t) \right]_{(a=0,b=0)}
\]  

(2.24)

\[
G_{nm}(a,b,\bar{n},k,t) : = \exp \left[ \frac{\bar{n}}{\bar{n}+1} G_{1nm}(a,-t) G_{1nm}(b,t) + G_{2nm}(a,b,t) \right],
\]  

(2.25)

where \(G_{1nm}(X,t) = X - \eta(t)k(n+m)/2\) and \(G_{2nm}(a,b,t) = akn(t) + bk\eta(-t)\). These equations contain all the physics of the cavity-mirror problem for the initial condition [Eq. (2.17)] and will be the basis of our discussion for the rest of the present chapter.

For infinite dimensional density matrices, the separability problem is solved for pure states [through the entropy of entanglement Eq. (1.45)] and for Gaussian states (see Sec. 1.4). However, the state (2.25) is neither pure (except for \(\bar{n} = 0\)) nor Gaussian, and thus we have to study entanglement by less standard means — note that even for the pure state (\(\bar{n} = 0\)) it is non-trivial to get the eigenvalues of the matrix (2.20). Quantifying entanglement in mixed states is generally a difficult problem, unless the Hilbert dimension is sufficiently small\(^2\). Encouraged by the study of the entanglement between a two-level atom and the EM field by Bose et al. [59], in this thesis we develop a method inspired by Boses’s approach that will allow us to discuss entanglement for arbitrary temperatures — we will refer to it as (discrete variable) projection method. The projection method consists of two steps:

1. projecting the original density matrix (2.22) into subspaces of low dimensionality,

\[
\rho(t) \rightarrow P\rho(t)P;
\]

2. computing entanglement markers and monotonies for the projected subspaces,

\[
E(P\rho(t)P).
\]

The projection (1) into a subspace of lower dimension corresponds to a local action [Eq. (1.37)], thus not increasing the global amount of entanglement, \(E(\rho(t)) \geq E(P\rho(t)P)\), as guaranteed by the fundamental law of QI as it applies to LOCC actions [Eq. (1.51)]. Thus, if succeed in showing the existence of entanglement in the smaller subspaces, we will have proven the existence of genuine quantum correlations among the EM field and the mechanical oscillator. In other words, the non-separability within the projected subspaces implies non-separability of the full density matrix (2.25).

\(^2\)Recall that for 2 \(\otimes 2\) and 2 \(\otimes 3\) systems, PPT and separability are equivalent [Eq. (1.55)].
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and thus an evidence of quantumness of the coupled system. Finally, we remark that, by using this simple method, lower bounds for the entanglement can be obtained from the study of the smaller subspaces.

2.2.1. Zero-Temperature analysis

For the sake of simplicity, we begin our analysis by projecting the density matrix into the smallest possible subspace capable of attaining bipartite entanglement, that is a $2 \otimes 2$ subspace. Let $P_{nm\mu\nu} = P_{nm} \otimes P_{\mu\nu}$ be the projection operator onto the subspace spanned by $n, m$ excitations of the cavity field and $\mu, \nu$ excitations of the mirror, with:

$$P_{ab} := |a\rangle\langle a| + |b\rangle\langle b|.$$ (2.26)

The subspace spanned by the Fock states $\{|n\rangle, |m\rangle\} \otimes \{|\mu\rangle, |\nu\rangle\}$ will be denoted by $[n, m; \mu, \nu]$ and the expression "lowest subspace" will be used to mean that the Fock states we are looking at are close to the ground state of the system — i.e. the vacuum ($|0\rangle$) and a single excitation of the fields ($|1\rangle$).

In the system’s ground state, the density matrix (2.25) is pure ($\rho^2 = \rho$) and it is advantageous to use a specific entanglement monotone — the so-called tangle — rather than the negativity [Eq. (1.57)].

The tangle is a full entanglement monotone for bipartite pure states $\rho_{AB}$ in $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ defined as [24],

$$\tau(\rho_{AB}) := 4 \det \rho_{A(B)}.$$ (2.27)

where $\rho_{A(B)}$ denotes the (normalized) partial state of subsystem $A(B)$ — recall that Schmidt spectrum of a pure state is common to both partial states [Eqs. (1.41)-(1.42)].

Like the entanglement entropy, the tangle is valid for bipartite pure states, but with the advantage of being much easier to calculate. Let us focus momentarily on the lowest subspace, that is $[0, 1; 0, 1]$; the $4 \times 4$ elements of the density matrix projected onto this subspace, $\rho_{AB}$, are computed from Eqs. (2.24)-(2.25) by choosing the adequate values of $n, m, \mu$ and $\nu$. With this notation $A$ refers to the cavity field and $B$ to the mirror. Arranging the result in a matrix in the Fock basis: $\{|0\rangle \otimes |0\rangle, |1\rangle \otimes |0\rangle, |0\rangle \otimes |1\rangle, |1\rangle \otimes |1\rangle\}$, we have,

$$\rho_{AB} = \frac{1}{1 + |\alpha|K(t)H(t)} \begin{pmatrix}
1 & \alpha^* K(t) & 0 & \eta(-t)k\alpha^* K(t) \\
\alpha K(t) & |\alpha|^2 K(t) & 0 & \eta(-t)k|\alpha|^2 K(t)^2 \\
0 & 0 & 0 & 0 \\
\eta(t)k\alpha K(t) & \eta(t)|\alpha|^2 K(t) & 0 & 4k^2|\alpha|^2 \sin(\omega_{pt}/2) K(t)^2 \\
\end{pmatrix},$$ (2.28)

with $K(t) := \exp\{-2k^2 \sin(\omega_{pt}/2)^2\}$ and $H(t) = 1 + 4k^2 \sin(\omega_{pt}/2)^2$. The tangle is calculated by tracing one of the subsystems in $\rho_{AB}$ and computing the determinant of the remaining $2 \times 2$ matrix.
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Figure 2.3.: Tangle $\tau$ as a function of the scaled coupling $k = g / \omega_c$ and the scaled time for $\bar{n} = 0$ and $\alpha = 1$. The projection subspace is $[0, 1; 0, 1]$ (Left) and $[1, 2; 1, 2]$ (Right). Only half of the evolution is plotted $t \in [0, \pi/\omega_m]$ as the system possesses reflection symmetry around $t = \pi/\omega_m$.

When the mirror is maximally displaced from its equilibrium position ($t = \pi/\omega_m$), it reads,

$$
\tau(\pi/\omega_m) = \frac{16k^2|\alpha|^2 e^{4k^2}}{(e^{4k^2} + 1 + 4k^2)|\alpha|^2}. \tag{2.29}
$$

It is apparent that a large mean number of photons ($|\alpha|^2$) does not favor entanglement; there exists an optimal value of $\alpha$ in every $2 \otimes 2$ subspace. We will briefly explain why this is so. From this behaviour, however, it cannot be inferred that preparing a cavity with a quasi-classical state, $\alpha \gg 1$, in pursuit of genuine quantum phenomena, such as entanglement, is inadequate (note that no conclusions can be drawn about the overall entanglement contained in $\rho(t)$ by peculiar phenomena occurring in low dimensional subspaces). The crucial role played by $\alpha$ in the entanglement of the overall density matrix will be discussed later, in Sec. 2.2.3.

The projected subspaces give us important hints about the entanglement performance of this simple opto-mechanical system: Fig. 2.3 shows the tangle as function of time $t$ for two different subspaces. The tangle reaches higher values in the lowest subspace as a null temperature will favor the low occupation numbers. Thus, is not surprising that by moving upwards from subspace spanned by $\{\ket{0}, \ket{1}\} \otimes \{\ket{0}, \ket{1}\}$ to the subspace spanned by $\{\ket{1}, \ket{2}\} \otimes \{\ket{1}, \ket{2}\}$ we loose most of the entanglement. The figure also shows a curious dynamical transition from one regime where the maximal entanglement is achieved for maximum displacement of the mirror, to a regime where the maximum of the tangle is achieved faster.

For small $k$ the system reaches the maximum of entanglement at $t = \pi/\omega_m$, simultaneously with the maximum displacement of the mirror (Fig. 2.3). For $k$ above a critical value, say $k_c$, the maximum of entanglement is achieved before $t = \pi/\omega_m$. Clearly, the time of maximum entanglement depends on
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the balance between the interaction time $t_{int} \sim 1/g$, i.e. the time scale of the interaction term in the Hamiltonian, and the time of oscillation of the mirror, $t_m \sim 1/\omega_m$.

It is worth understanding the importance of the amplitude of the coherent state, $\alpha$, in establishing the value of $k_c$. Naively, we would expect that increasing $\alpha$ would decrease $k_c$ because more photons interact with the mirror, for larger $\alpha$, resulting in a larger effective coupling ($\sim g \langle a^\dagger a \rangle$). Curiously, this is not the case: the value of $k_c$ increases with $\alpha$! This can be understood as follows; the ratio between the weight of the $|n+1\rangle$ number state and the weight of $|n\rangle$ number state in the expansion of the coherent state [Eq. (A.9)], being given by $\alpha/\sqrt{n+1}$, increases with $\alpha$, weakening the entanglement generated after interaction with the mirror [hence explaining the tangle dependence on $\alpha$, see Eq. (2.29)]. Regarding entanglement, the best situation occurs when the weights of the states are the most equally distributed [Eq. (1.45)]. Hence, a higher coupling helps the entanglement generation to have the same efficiency when $\alpha$ is increased.

For completeness, we give the explicit formula of $k_c$ for the subspace $[1,2;1,2]$:

$$-1 + 14k_c^2 + 24k_c^4 = 2\alpha^2(1 + 4k_c^2 + 96k_c^4)e^{-12k_c^2} \geq 0. \quad (2.30)$$

The right-hand side of equation (2.30) is non-negative resulting in a restriction for $k_c$, i.e. $k_c$ is lower bounded. Also, it can be deduced from equation (2.30) that $k_c$ increases with $\alpha$. This confirms, at least for this subspace, that a higher coupling is necessary for reaching the maximum of entanglement before $t = \pi/\omega_m$ if the amplitude of the cavity field is increased. Although the actual value of entanglement differs from subspace to subspace (Fig. 2.3), there are quite universal characteristics; for example, the asymptotic behavior of the tangle at $t = \pi$ as function of $\alpha$ is always

$$\tau(\pi/\omega_m) = \begin{cases} \sim |\alpha|^2, & \alpha \ll 1 \\ \sim |\alpha|^{-2}, & \alpha \gg 1 \end{cases} \quad (2.31)$$

2.2.2. Finite temperature entanglement

In practice, unless very low temperatures are considered, any mirror will be populated with thermal phonons (even if few), and the previous results should be seen as the limiting case $\bar{n} \simeq 0$. At $T > 0$ the system is in a mixed state and the entanglement must be investigated by other means than the tangle. It can be inferred from the plots of the negativity [Eq. (1.57)] that increasing the temperature transfers the correlations to higher subspaces as higher excitations get populated by thermal phonons, while the peak of negativity is reduced compared to the $T = 0$ case; also, it can be deduced that $k_c$ increases slowly with the temperature (at least for the subspaces of Fig. 2.3), and hence thermal fluctuations make it more difficult to achieve maximum entanglement before the mirror being maximally displaced from its equilibrium position ($t = \pi/\omega_m$).

We introduce a convenient marker of entanglement based on PPT which is valid for projected
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subspaces with arbitrary dimensionality. In going to larger subspaces we will be able to strength our conclusions about the nature of the entanglement generated by radiation pressure and, especially, conclude about its robustness against thermal fluctuations. First, we introduce the marker,

\[ \Upsilon(\rho) := -\det[(\Lambda_A \otimes 1_B)\rho]. \] (2.32)
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The subspaces considered are: [0,2;0,2] (Top-Left), [1,2;2,3] (Top-Right), [1,4;1,4] (Bottom-Left) and [1,5;0,1] (Bottom-Right). In these plots, the temperature varies such that $x$ lies in the range $[0.5, 1] \leftrightarrow \bar{n} \in [1, \infty]$. The coupling and time assume any value as $y \in [0, \infty]$. For a given temperature and coupling $(x,k)$, by going downwards in the $y$ axis we can imagine that we are decreasing time while fixing $k$ $[y = 2k|\sin(\omega_m t/2)|]$ in the interval $t \in [0, \pi/\omega_m]$. The white regions witness the presence of entanglement in the respective projected subspaces, whereas the grey regions correspond to separable projected states. The most important feature common to all the plots is the existence of a critical temperature above which, no matter the value of $k$, entanglement completely vanishes in the projected subspaces.

From PPT [Eq. (1.55)] it is clear that $\Upsilon(\rho) > 0$ implies non-separability, since at least one eigenvalue of the partial transposed matrix $(\Lambda_A \otimes 1_B)\rho$ is negative. A careful inspection shows that, for the cases under study, this marker is equivalent to the existence of entanglement as the partial transposed matrix has at most one negative eigenvalue (it never happens that two negative eigenvalues exist,
in which case, of course, the marker would not detect entanglement). Defining \( x := \bar{n}/(\bar{n} + 1) \), the marker for the lowest subspace reads,

\[
\Upsilon[0, 1; 0, 1] = F(\alpha, t, k, x) \left( e^{i k \eta(t)} x^2 (x - 2)^4 |k\eta(t)|^4 - 16 \left( 1 + e^{i k \eta(t)} x^2 \right)^2 x^3 \right),
\]

where \( F(\alpha, t, k, x) \) is a positive function, and thus not relevant to our discussion. By setting \( \bar{n} = 0 \) \( (\Leftrightarrow x = 0) \) in the above expression, we get \( \Upsilon[0, 1; 0, 1] = 16 |k\eta(t)|^4 F(\alpha, t, k, x) \) which is positive for every \( t \) (except for \( t = 2p\pi/\omega_m \) with \( p \in \mathbb{N}_0 \)), hence detecting entanglement; in accordance with the result derived earlier [see Eq. (2.29)]. For other subspaces, the marker gets cumbersome but its sign is a function of just \( x \) and

\[
y(t) := |k\eta(t)| = 2k |\sin(\omega_m t/2)|. \tag{2.34}
\]

In Fig. 2.4 the marker is plotted for various subspaces as function of \( x \) and \( y \). A curious feature of \( \Upsilon \) in \( 2 \otimes 2 \) subspaces is the fact that its sign does not depend on \( \alpha \), meaning that the role played by the amplitude of the coherent state will be in determining the exact amount of entanglement of the complete density matrix (this will be confirmed in Sec. 2.2.3 by an explicit calculation).

So far we have discussed entanglement in subspaces equivalent to two spin-1/2 particles (qubits) and neglected all the entanglement shared between branches corresponding to different number occupations. In doing so, we have found (see Fig. 2.4) that sometimes a thermal occupation as low as \( \bar{n} = 2 \) is surprisingly enough to destroy the quantum correlations within the low dimensional Fock subspaces. A more realistic lower bound to entanglement, and consequently stronger conclusions, however, can be obtained by enlarging just a bit the projected subspace. Indeed, let us investigate the entanglement dynamics for subspaces of dimension \( d = 6 \), concretely in Hilbert spaces of the form \( \mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^3 \).

In the line with the projection method, we define the projector operator to be now,

\[
P = P_{nm} \otimes P_{\mu\nu\epsilon}, \tag{2.35}
\]

with \( P_{\mu\nu\epsilon} = |\mu\rangle \langle \mu| + |\nu\rangle \langle \nu| + |\epsilon\rangle \langle \epsilon| \) and denote the respective projected subspace by \( [n, m; \mu, \nu, \epsilon] \).

The Fig. 2.6 shows two plots — at the left-hand side the negativity for the subspace \([0, 1; 3, 4, 5]\) and at the right-hand side the respective marker. Is is apparent from these results that for some couplings the entanglement persists at arbitrary high-temperatures (even if in a very small quantity). This is at odds with what we have found in subspaces with \( d = 4 \) and it may seem an anomalous result [we have learned in the Introduction that increasing the temperature too much unavoidably destroys entanglement (see, for instance, the comments in Fig. 1.3 or the explicit calculation of Sec. 1.4.3)]. This is explained by the fact that the cavity is prepared in a pure state; the purity of the subsystem works as an enforcer of entanglement. This was first discovered by Bose et al. in [59] for one EM field mode interacting with a two-level atom in a thermal state and here we find a similar phenomenon. An even more curious peculiarity of this system will be disclosed by studying
2. Macroscopic entanglement at finite temperatures: an ideal scenario

Figure 2.5.: This figure illustrates the "subspace renormalization" procedure discussed in the text; the opto-mechanical state is projected onto the state having 0 and 1 excitations of the cavity EM field and $\mu$, $\nu$, ... excitations of the mirror. If for a given temperature and $k$ the subspace $[0, 1; \mu, \nu, ...]$ is able to support entanglement, then the subspace $[0, s; \mu, \nu, ...]$ will attain entanglement for the smaller coupling defined by $k_s := k/s$ [see Eq. (2.36)].

The density matrix [Eq. (2.23)] has a pattern regarding the matrix elements of the cavity; $k$ always appears multiplied by $n$ or $m$. This follows directly from photon conservation (the number operator $\hat{n} = a^\dagger a$ commutes with the Hamiltonian [Eq. (2.14)]). Bearing this in mind, and denoting by $\Upsilon_{[0,s]}$ the marker for the subspaces spanned by the Fock states $\{|0\rangle, |s\rangle\}$ of the cavity (whereas the specific projection on the side of the mirror is arbitrary), then it is straightforward to verify that $\Upsilon_{[0,s]}$ is proportional to $\Upsilon_{[0,1]}$ if, in the latter, the coupling $k_s = k/s$ is chosen. This has an immediate important consequence: if we choose a large $k$ capable of producing entanglement in the cavity subspace $[0, 1]$, then there must be entanglement in the subspace $[0, s]$ for coupling constant $k_s := k/s$, even though $k_s$ might not lead to entanglement in the subspace $[0, 1]$. For instance, in the right-hand side plot of Fig. 2.6 entanglement actually survives for the parameter region concerning the bottom-left corner, provided a proper choice of the projection subspace $[0, s]$ is made. The grey region at the top-right is not as important, since we can always, with fixed $k$, move downwards in the $y$-axis by decreasing time (recall that $y = 2k |\sin(\omega_m t/2)|$). Mathematically, this can be expressed as follows,

$$|\alpha|^{-2s}!\Upsilon_{[0,s]}(k_s) = |\alpha|^{-2}\Upsilon_{[0,1]}(k).$$

(2.36)

This result implies that for a given Fabry-Perot geometry and mirror — characterized by its own natural frequency and mass — the existence of entanglement in a suitable $2 \otimes 3$ subspace of (2.20) is guaranteed for any temperature, even for small coupling $k = g/\omega_m$, provided we choose a sufficiently high subspace (Fig. 2.5). Inspired by this result, we put forward the following conjecture,

**Conjecture 1.** The opto-mechanical system consisting of a thermalized mechanical oscillator interacting via radiation pressure with a cavity EM field, initially prepared in a large coherent-state, supports macroscopic entanglement.
2.2. Towards high-temperature macroscopic entanglement

The entanglement in the $2 \otimes 3$ subspaces is more robust against temperature. In fact, it persists at arbitrary high-temperatures for some couplings (right-hand plot). The condition in $k$ can even be relaxed if we choose sufficiently high cavity excitations (see text and Fig. 2.5). Left - The negativity is plotted as function of coupling $k$ and $x = \bar{n} / (1 + \bar{n})$ for the subspace $[0, 1; 3, 4, 5]$ with $\alpha = 1$ and $t = \pi / \omega_m$. In the range considered, the peak of the negativity happens for $x = 0.9 \land k = 0.2$, yielding $N \simeq 3 \times 10^{-4}$. This value can be improved by a proper choice of parameters. Right - The marker, $\Upsilon$, for the same subspace, as a function of $(2 / \pi) \arctan(y)$ and $x$. The white regions witness the presence of entanglement, $\Upsilon > 0$.

2.2.3. Macroscopic thermal entanglement

At this point, fair criticism to the projection method is in order. In Sec. 1.3.2, we have learned that the maximal amount of entanglement in a $d \otimes d$ dimensional density matrix is precisely $\ln d$. In QI, by comparison with the entanglement entropy of the singlet, one speaks about $\ln d / (\ln 2)$ e-bits (i.e. entanglement bits) in honour of Schumacher’s seminal work on quantum communication with qubits. In the macroscopic limit, we have a diverging number of e-bits in a maximally entangled state [Eq. (1.44)]. The presence of entanglement in the $2 \otimes 3$ subspaces is not a guarantee of macroscopic entanglement as these subspaces support a maximum of just $\simeq 2.6$ e-bits. The relevant question that should be asked is then; does a finite amount of thermal entanglement in the low dimensional subspaces imply a macroscopic amount of quantum correlations in the complete density matrix? We have conjecture that, indeed, the answer is positive, since the particular entanglement structure shows that entanglement survives in many subspaces $\Upsilon$. Thus, at least in principle, one could distill a detectable amount of e-bits when adding up the contribution of each subspace.

$\Upsilon$The marker will actually detect entanglement in infinitely many subspaces, at least for small temperatures (despite only a small subset will yield a detectable amount of negativity). This can be seen as follows: for a given set of parameters ($\delta$, $t$, and $\alpha$) consider a subspace of the form $[0, 1; ...]$ leading to non-zero negativity for couplings $k$ and $\tilde{k} := k \ast p$, with $p$ an integer. That is, the subspace of the mirror fulfills $\Upsilon_{0,1}(k) > 0 \land \Upsilon_{\bar{0},1}(\tilde{k}) > 0$ — an example is provided in Fig. 2.6 for $x \lesssim 0.7$. Then, by virtue of the renormalization procedure [Eq. (2.36)], the subspace $[0, p; ...]$ entails: \[ \Upsilon_{[0,p]}(k_{p} = \tilde{k}/p) = \Upsilon_{[0,p]}(k) \sim \Upsilon_{[0,1]}(\tilde{k}). \] Hence, $\Upsilon_{[0,p]}(k) > 0$, for every $p$ since $\Upsilon_{[0,1]}(\tilde{k}) > 0$. 69
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Further insight can be made by studying the mutual information [Eq. (A.50)] between the cavity field and the mirror. This quantity, with roots in classical statistical theory, has two clear operational meanings in the context of quantum systems: it equals the minimum amount of randomness required to erase all the correlations shared by two subsystems (in a many copy scenario like the one discussed in Sec. 1.3 [79], and is equivalent to the relative entropy between $\rho_{AB}$ and the separable state from the partial states: $\rho_A \otimes \rho_B$. That is,

$$I(\rho_{AB}) = S(\rho_{AB}|\rho_A \otimes \rho_B). \tag{2.37}$$

Indeed, $I(\rho_{AB})$ measures how much information the compound system $A' + B'$ has more than the respective partial states. The connection of $I(\rho_{AB})$ to entanglement is clear for the amount of non-separability of a state $\rho_{AB}$ can be thought as the distance of $\rho_{AB}$ to the closest separable state $\sigma \equiv \sigma_A \otimes \sigma_B$ (Fig. 1.1). For pure states it equals twice the von Neumann entropy of the reduced state, and therefore is an entanglement measure. For mixed states it quantifies entanglement no more, but can still be used to speak about the total amount of correlations shared between two parties.

Here, we consider a related quantity (which we will refer to as the normalized mutual information; see Appendix A.4) detecting non-classical correlations directly. For practical reasons, we adopt the linear entropy [Eq. (1.11)] as our measure of mixness. Defining $\phi_{nm}(t) := \Phi_{00nm}(t)$ [see (2.21)], the partial states of the density matrix read (see Appendix A.2),

$$\rho_{cav}(t) = \sum_{nm} \phi_{nm}(t)e^{-|k\eta(t)|^2(n-m)^2(2+\bar{n})/4}|n\rangle\langle m|, \tag{2.38}$$

$$\rho_{m}(t) = \sum_{n} \phi_{nn}(t) \int_{C} \frac{d^{2}z}{\bar{n}\pi} e^{-|z|^2/\bar{n}}|z+k\eta(t)\rangle\langle z+k\eta(t)|. \tag{2.39}$$

The entropy is invariant under unitary evolution, and hence the linear entropy of the compound system, $S_{\mathcal{L}}(t) = 1 - \text{Tr}[\rho(t)^2]$, can be evaluated at $t = 0$, taking advantage of the state being separable there [Eq. (2.17)]:

$$S_{\mathcal{L}}(t) = 1 - \frac{1}{2\bar{n}+1}. \tag{2.40}$$

The entropy of the partial states can be obtained through the same methods leading to the partial entropies,

$$S_{\mathcal{L},cav}(t) = 1 - e^{-2|\alpha|^2} \sum_{p,q} \frac{\alpha^{2(p+q)}}{p!q!} e^{-|k\eta(t)|^2(p-q)^2(2+\bar{n})/2}, \tag{2.41}$$

$$S_{\mathcal{L},m}(t) = 1 - \frac{1}{2\bar{n}+1} e^{-2|\alpha|^2} \sum_{p,q} \frac{\alpha^{2(p+q)}}{p!q!} e^{-|k\eta(t)|^2(p-q)^2g(\bar{n})/2}, \tag{2.42}$$

with $g(\bar{n}) = x^2/(1+x)$ and $x = \bar{n}/(1+\bar{n})$ as before. The normalized mutual information (A.51)
2.2. Towards high-temperature macroscopic entanglement

![Figure 2.7:](image)

Figure 2.7.: Left - The normalized mutual information averaged through one period of the mechanical oscillator [Eq. (2.44)] as function of the average number of phonons, $\bar{n}$, for a cavity prepared with a small coherent state (one photon in average, red curve) and a relative large amplitude (one hundred photons in average, blue curve). The classical upper bound on correlations [Eq. (A.52)] is represented by the dashed curve. We see a clear signature of macroscopic quantum correlations for the larger coherent state. In both plots the coupling was chosen to be one (in units of the mirror’s natural frequency). Right - Various linear entropies are plotted for a mirror at very low-temperature ($\bar{n} = 1$) and $\alpha = 1$ as function of the scaled time $t \omega / \pi$ (only half of the evolution is plotted): $S_L(t)$ (thick, blue), $S_m(t)$ (dashed, black), $S_{cav}(t)$ (dashed, black) and the average linear entropy of the subsystems (green line). The latter is a signature of entanglement every time it exceeds the global entropy $S_L(t)$, which happens in the interval $1.69 \gtrsim \omega_m t / \pi \gtrsim 0.31$.

guarantees the presence of quantum correlations whenever $\mathcal{I} > 1/2$. It reads,

$$\mathcal{I}(t) = 1 - \frac{S_L(t)}{S_{L,cav}(t) + S_{L,m}(t)}.$$  \hfill (2.43)

From the above equations, we can infer that $\mathcal{I}$ increases with $\alpha$ initially and that then it stabilizes; the quantum correlations emerging from the radiation-pressure mechanism should therefore increase with $\alpha$, at least in the range where $\mathcal{I}$ increases monotonously above the classical upper bound [Eq. (A.52)]. Within this range, a detectable amount of entanglement is expected.

We finish the present chapter giving a numerical value for the averaged normalized mutual information over a period of oscillation of the mirror,

$$\mathcal{I}_{av} := \frac{1}{2\pi} \int_0^{2\pi} I(\tau) d\tau.$$  \hfill (2.44)

We choose a strong mirror-light coupling $k \simeq 1$, a low (but not too low) thermal occupancy $\bar{n} = 10$, and a relative small cavity amplitude $\alpha \simeq 10$. With these values, the averaged normalized mutual information yields $\mathcal{I}_{av} \simeq 0.52 > \mathcal{I}_c$, which should be interpreted as an indicator of quantum
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How does the temperature affect entanglement in the total density matrix? According to Fig. 2.7, the correlations become totally classical after a few thermal photons ($\bar{n} \sim 10$) have populated the mirror — a careful study, though, shows that this behavior is little sensitive to the radiation pressure coupling and even $\alpha$; an indicator that the linear entropy does not capture all the subtleness of the correlations from the radiation pressure interaction.

2.3. Concluding remarks

We have seen that entanglement between the motion degree of freedom of a mechanical oscillator and the EM quadratures of light does exist at any temperature in low dimensional subspaces of the density matrix, although it may be very feeble for very high temperatures. The findings of Sec. 2.2 show the coexistence of entanglement in many subspaces; the radiation-pressure mechanism is robust, in the sense that small opto-mechanical couplings, leading to little or no entanglement in a given subspace, attain entanglement in suitable subspaces, as implied by the subspace renormalization condition [Eq. (2.36)].

Our results provide the first plausible evidence for macroscopic entanglement in opto-mechanical systems in the experimental relevant regime, $k_B T \gtrsim \hbar \omega_m$. To our knowledge this was the first time that entanglement (and therefore the quantum behavior) was shown to survive at finite temperatures in bipartite macroscopic systems. This has confirmed Bose’s expectation about the capability of macroscopic compound systems to attain entanglement when one of the subsystems is initialized in a pure state $|59, 80\rangle$. A complementary argument validating this conclusion will be given in the following chapter, where the important issues of mirror’s friction, damping of the cavity and especially decoherence will be added to Hamiltonian (2.14).

Our findings hence suggest a way to explore the quantum-classical boundary in mesoscopic and macroscopic mechanical oscillators by coupling them to a confined EM field. The reason why opto-mechanical systems are a laboratory for quantum effects stems from the radiation-pressure mechanism; the thermal phonons of the mirror are coherently displaced in phase space by virtue of the interaction term (2.15) in a manner that is only sensitive to the number of photons,

$$\langle b(t) \rangle = k \eta(t) |\alpha|^2.$$  

By monitoring the position of the mirror, we actually perform a Quantum Non-Demolition (QND) measurement of the resonator’s energy as first envisaged by Braginsky [81] (as can be seen by the latter equation); a measurement of $\langle b(t) \rangle$ gives information about the cavity energy $E_{cav} = \hbar \omega_m |\alpha|^2$ up to any desired accuracy (recall that $[a^\dagger a, H_{\text{int}}] = 0$), when the adiabatic limit is considered. In the line of Penrose’s proposal, an equivalent setup has been considered recently in the pursuit of
2.3. Concluding remarks

Macroscopic superpositions of a tiny mirror \[66\]. There, they consider the effect of a single photon, and hence the entanglement generation is too feeble to survive at any realistic low-temperature \[75\]. Here we have showed that one increases substantially the chances to probe quantum macroscopic behavior by considering a coherent \(\text{EM}\) field, instead of a single photon\[4\]. The applications of the simple radiation-pressure mechanism are numerous; they comprise detection of gravitational waves and the study of the quantum-to-classical transition.

The present chapter has shed some light on the celebrated radiation-pressure mechanism in a cavity quantum electrodynamics setup. This was essentially done by solving for the system density matrix in an exact way and taking advantage from the already well-established tools of the young field of \(\text{QI}\) science. Many questions are still open, though. The exact dependence of the entanglement with the radiation pressure coupling (an thus the mirror’s mass, for instance) was not addressed satisfactorily — only qualitative conclusions can be drawn by the study of the linear entropy of the subsystems as argued in Sec. 2.2.3. Also, our method does not provide an entanglement measure (see Sec. 1.3.3) for the total density matrix.

These questions will be partially answered in the following chapter; others we leave as possible research topics: can the spectrum of the density-matrix [Eq. (2.23)] be obtained, and, therefore, the mutual information (based on the von Neumann entropy rather than the linear entropy)? Even more importantly, perhaps, would be, not to assume the somewhat artificial initial state [Eq. (2.17)],

\[
\rho_{ab}(t_0) = |\alpha\rangle\langle\alpha| \otimes \Xi(\beta),
\]

(where \(\Xi(\beta)\) is a thermal state of the mirror), but a more realistic initial condition. This can be accomplished by considering that an external coherent source populates a cavity initially with no photons (which is a good approximation even at room temperature given the high energy of optical photons),

\[
\rho_{abc}(t_0) = (|0\rangle\langle0| \otimes \Xi(\beta)) \otimes |\alpha\rangle\langle\alpha|,
\]

which then would evolve via the total Hamiltonian,

\[
H = \hbar \omega_c a^\dagger a + \hbar \omega_m b^\dagger b + \hbar \omega_0 c^\dagger c - \hbar g a^\dagger a (b + b^\dagger) + \hbar (Gac^\dagger + G^*a^\dagger c),
\]

where \(c\) and \(c^\dagger\) are the bosonic operators of the driving source photons with frequency \(\omega_c\) and \(G\) their coupling to the intra-cavity field. The density operator would be computed by performing the partial trace of the driving photons,

\[
\rho_{ab}(t) = \text{Tr}_c [U(t) \rho(t_0) U^\dagger(t)].
\]

\[4\] This could seem ironic since coherent states are “quasi-classical” states of light (they resemble a classical \(\text{EM}\) wave due to their small uncertainty around the classical values). Nevertheless, photons still are quantum in nature and their interaction with a free-standing mirror, for instance, will be characterized by Hamiltonian [Eq. (2.14)] in the adiabatic limit. Surprisingly, as we have seen in the present chapter, these photons get strongly entangled with the mirror as each one of them contributes to a sort of macroscopic net effect.
2. Macroscopic entanglement at finite temperatures: an ideal scenario

The main challenge is to solve for the evolution operator in a closed fashion. If we were able to do so, then the same method leading to the analytical solution of equations \((2.38)\) and \((2.39)\) could be used to compute \(\rho_{ab}(t)\). This would strength the validity of our conclusions since a more realistic initial condition, breaking down the renormalization procedure, would be considered. Nevertheless, this unitary approach, although introducing mixness in the reduced state, does not take into account decoherence as a real active surrounding bath unavoidably leads to. We study the effect of such bath in the next chapter when proper assumptions are made about the dynamics of the system.
3. Stationary opto-mechanical entanglement at moderately high temperatures

This chapter is based on the following publications by the author:

- Macroscopic thermal entanglement due to radiation pressure, AIRES FERREIRA, A. Guerreiro, and V. Vedral, Phys. Rev. Lett. 96, 060407 (2006).

- Optomechanical entanglement between a movable mirror and a cavity field, D. Vitali, S. Gigan, AIRES FERREIRA, et al., Phys. Rev. Lett. 98, 030405 (2007).

3.1. Overview

In the previous chapter, we have learned that the radiation pressure mechanism is able to entangle the center-of-mass motion degree of an object consisting of many particles and the EM quadratures of light itself. The ideal scenario — with no dissipation and no active environment (i.e. no thermal and quantum noise) — was considered through a global unitary evolution of the opto-mechanical system. Based on solid arguments, we conjectured that a macroscopic mirror, at one end of an optical cavity, shares genuine quantum correlations, at finite temperature, if a sufficiently large coherent state of the light is prepared inside the cavity. However, in the laboratory, the unavoidable sources of noise, diffraction and imperfections in the mirror break down the simple unitary description. Moreover, we expect that only very moderate temperatures will accommodate a finite amount of entanglement as the interaction with an active bath of quantum oscillators (a real environment) will destroy entanglement above some critical temperature. This phenomenon is referred to as decoherence, and many people believe that eventually it is the responsible for the quantum-to-classical transition observed many times in nature. Nevertheless, whether decoherence is the actual mechanism explaining classicality or not, it gives an appropriate description of the results of experiments and can be analyzed within several frameworks, namely,

1. the master equation (Schrödinger picture);
3. **Stationary opto-mechanical entanglement at moderately high temperatures**

2. the Fokker-Planck equation (phase space);

3. the quantum Langevin equation (Heisenberg picture).

Decoherence is enhanced with temperature and the system size and, in most of the cases, is so fast that quantum interference is never observable; every bipartite system (or any system for that matter) gets entangled with the environment causing entanglement dilution within the degrees of freedom of the system. Very generally it manifests as a suppression of the off-diagonal entries of the reduced density matrix and it is present even at zero-temperature.

Indeed, opto-mechanical entanglement between a massive mirror and the EM field will only be observable if two conditions are met, namely that the temperature is not high enough as to suppress quantum coherence, and that the radiation pressure coupling, $g$, is sufficiently robust compared to energy scales associated with noise. We already gave arguments in favor of the last point, but our unitary approach gives little clues about the former.

The thermal robustness of entanglement in this system is paramount in order to achieve an experimental demonstration, since all types of ground-state cooling techniques encounter many difficulties making the regime $k_B T \lesssim \hbar \omega_m$ prohibitive even with state-of-the-art technology. Some promising experiments have been performed in this direction but no real quantum behavior of the mechanical oscillator was probed so far [82, 83, 84, 85, 86, 87, 88]. Recent advances in theory of opto-mechanical cooling [89, 90, 91, 92] have raised the interest in opto-mechanical systems, either as a way to test the quantum-classical boundary, or due to their potential to enhance the sensitivity of displacement measurements (which is crucial for many applications being the detection of gravitation waves the most famed). Interestingly, the radiation-pressure mechanism by itself is able to cool the motion of the mirror when the cavity field is pumped by LASER radiation [92, 93] — the so-called dynamical back-action cooling or simply self-cooling — in a spirit very close to what we have already seen in atomic and molecular physics (e.g. with cold atoms, ion traps, etc.). The opto-mechanical cooling is a very interesting and fast-developing field of theoretical and experimental physics.

An experimental demonstration of entanglement in these systems may be reachable after a sufficient experimental improvement is achieved in the physics of opto-mechanical cooling. In what follows, we review the dynamics of driven optical cavities and compute the stationary entanglement taking into account the most relevant sources of dissipation and decoherence. The reader unfamiliar with Langevin equations and the input-output formalism of Quantum Optics will find some guidance in short appendices. The results of this chapter will settle on quite solid grounds the preceding conclusions about macroscopic entanglement and, together with the recent effort in understanding and reaching the quantum regime in the laboratory [82, 83, 84, 85, 86, 87, 88, 89, 92, 95, 96, 97], open a very promising direction in the endeavour to bring quantum effects to the macroscopic domain.
3.2. The dynamics of a driven cavity

In the past two decades, the study of small systems interacting with the EM field of an optical cavity had been a fertile ground producing many outstanding results, especially in the so-called cavity quantum electrodynamics experiments. Among many experimental demonstrations, we find the energy quantum jumps between Fock states of a cavity field [98], and the quantum coherent control of atomic collisions inside a cavity, just to name a few (see [99] for a review). The reason why cavities are so special is because they intrinsically impose boundary conditions on the EM field leading to a discrete energy spectrum. This not only amplifies the radiation pressure coupling as we have seen in Sec. 2.2, but it also introduces a myriad of new physics (e.g. the modification of the spontaneous emission rate of atoms [100]).

According to the results of Chap. 2, a large coherent-state of the EM field must be prepared inside the optical resonator if one hopes to reach a detectable amount of entanglement. In fact, this represents no problem at all, for it became a standard enterprise in Quantum Optics the preparation of coherent-states of light by means of a pumping coherent-source, i.e. LASER light. Harder experimental constraints, however, come about when we make the requirement that the life-time of photons is large enough as to enhance the momentum-transfer to the mirror. Discarding decoherence effects on the mechanical oscillator, and if no photons leak out of the cavity (perfect reflecting mirrors), the EM excited mode of the cavity will essentially follow an unitary evolution under the Hamiltonian of Eq. (2.14). Real cavities, though, have many modes beside the resonant ones, and hence an unitary description will not apply; they are characterized by a finite photon life-time, $\tau$. A poor optical finesse [Eq. B.8] will blur the effectiveness of the radiation pressure-mechanism and thus one must guarantee that a high-quality cavity is used in a real experiment.
3. Stationary opto-mechanical entanglement at moderately high temperatures

In order to study how a finite finesse and a damped mirror will affect the entanglement (and hence, genuine quantum effects) of the opto-mechanical system, we must study the non-unitary evolution of the system due to dissipation and decoherence, even at zero temperature. This is easier to accomplish with the Langevin equations of motion, which are often used in Quantum Optics when quantum and thermal noise must be taken into account. A master equation approach for the full density-matrix, in the same spirit as Leggett and Caldeira [65, 101], would raise many difficulties (for instance, in finding the exact low-temperature limit of the master equation of quantum friction [73, 74, 75]). Following tradition, we adopt the Heisenberg equations of motions for the fields as the starting point to the study of the dynamics (and later the entanglement). Hence, a study of quantum correlations in the spirit of Chap. 2 will not be possible. This is, however, not a problem at all, since the CV approach of the present section will yield all the relevant information in order to reconstruct the covariance matrix in the relevant regimes.

We consider a single mechanical mode of the mirror only, which can be modeled as an harmonic oscillator with natural frequency $\omega_m$. The notation is essentially the same as of Chap. 2 but now with dimensionless position and momentum operators satisfying $[q, p] = i$. This is obtained from the canonical conjugate operators [see table 2.1] through the transformation,

$$
q \rightarrow \sqrt{\frac{m\omega_m}{\hbar}} q, \quad (3.1)
$$

$$
p \rightarrow \sqrt{\frac{1}{m\hbar\omega_m}} p. \quad (3.2)
$$

The Heisenberg equations of motion for the operators will therefore contain parameters with dimensions of frequency. This will simplify the study of the covariance matrix as all its entries become dimensionless and allow an easier investigation of entanglement through the parameter region. We model the driving coherent-source as a classical field with strength $E$ and frequency $\omega_0$, and hence the Hamiltonian reads [102, 103],

$$
H = \hbar\omega_0 a^\dagger a + \frac{\hbar\omega_m}{2} (p^2 + q^2) - \hbar g a^\dagger a q + i\hbar E (e^{-i\omega_0 t} a^\dagger - e^{i\omega_0 t} a), \quad (3.3)
$$

The extra term describes the effect of adding photons by a driving coherent source. The amplitude $E$ is related to the input LASER power $P$ by $|E| = \sqrt{2P\kappa/\hbar\omega_0}$, where $\kappa$ is the decay rate of the cavity. The radiation-pressure coupling $g$ [Eq. (2.13)] gets renormalized by a factor of $\sqrt{2}$ due to the transformation above and reads,

$$
g = \frac{\omega_0}{L} \sqrt{\frac{\hbar}{m\omega_m}}. \quad (3.4)
$$

Although several degrees of freedom, which have different resonant frequencies, will be excited by the motion of the mirror, the single-mode description of Eq. (3.3) will capture the physics as long as mode-mode coupling is negligible. This happens in the so-called adiabatic regime (Sec. 2.2), where
3.2. The dynamics of a driven cavity

the frequency of the mirror is much smaller than the free-spectral range of the cavity,

$$\omega_m \ll \Delta \omega_c = \frac{\pi c}{L}. \quad (3.5)$$

We are well inside this limit as typically $$\Delta \omega_c \sim 10^{12} - 10^{15} \text{ Hz}$$ for optical cavities, and $$\omega_m \sim 10^5 - 10^7 \text{ Hz}$$ for macroscopic mirrors — please refer to Appendix [B.1] for an outline of the physical parameters controlling the operation of an optical resonator. From the detection side, a single frequency mode can also be addressed via a bandpass filter in the detection scheme [104]. This, together with the discussion of Sec. 2.2 on the derivation of the radiation-pressure interaction, give the grounds for the use of Hamiltonian (3.3).

The dynamics of the cavity field will be strongly influenced by the motion of the mirror as any slightly change in the mirror’s position changes the cavity length and thus the mode spectrum (Fig. B.1). The Heisenberg equation of motion for the operators assume a more elegant form when written in the frame rotating at frequency $$\omega_0$$. This corresponds to write $$a$$ and $$a^\dagger$$ in the interaction picture with respect to $$\hbar \omega_0 a^\dagger a$$:

$$a_I(t) := e^{i\hbar \omega_0 a^\dagger a} e^{-i\hbar \omega_0 a^\dagger a} = e^{i\omega_0 t}. \quad (3.6)$$

The equation of motion for $$a_I$$ is $$\dot{a}_I = \partial_t a_I + (i/\hbar) [H, a_I]$$ and the Hamiltonian has no time dependence in the rotating frame (i.e. when written in terms of $$a_I$$ and $$a_I^\dagger$$). The transformation $$a \rightarrow a_I$$ corresponds to a local unitary action, thus not changing the correlations properties whatsoever. In what follows, we drop the subscript $$I$$ by bearing in mind that we are in the rotating frame. The equations of motion read

$$\dot{q} = \omega_m p, \quad (3.7)$$

$$\dot{p} = -\omega_m q + g a^\dagger a, \quad (3.8)$$

$$\dot{a} = -i\Delta_0 a + i g a q + E, \quad (3.9)$$

where $$\Delta_0 = \omega_c - \omega_0$$ is the source-cavity detuning. The coupled dynamics is entailed by the non-linear term proportional to the radiation-pressure coupling, $$g$$ and its classical orbits display a multitude of rich phenomena (e.g. static bistability [105] and dynamical multistability leading to self-induced oscillations [106]).

The mirror and the cavity are not isolated from the rest of the world, and thus the above equations are not the full story yet. The two main sources of noise must be taken into account. They are,

1. the dissipative effects affecting the mirror, which in the absence of radiation-pressure would essentially follow a Brownian quantum motion (even at zero temperature);

2. the damping of the cavity dynamics due to photon leakage (no perfect reflective mirrors do exist).
3. Stationary opto-mechanical entanglement at moderately high temperatures

The interaction of the cavity EM field with its environment is correctly described by the input-output theory due to Gardiner and Collett [107, 108]. The Appendix B.2 contains the essential of this theory for the present study. Finally, the derivation of the Langevin equations for the mechanical oscillator is outlined in Appendix B.3.

We denote the mechanical and cavity damping rates by $\gamma_m$ and $\kappa$, respectively. Indeed, the Langevin equations for the opto-mechanical system read,

$$\dot{q} = \omega_m p,$$  \hspace{1cm} (3.10)

$$\dot{p} = -\omega_m q - \gamma_m p + ga^\dagger a + \xi,$$  \hspace{1cm} (3.11)

$$\dot{a} = -(\kappa + i\Delta_0)a + igaq + E + \sqrt{2\kappa}a_{in},$$  \hspace{1cm} (3.12)

Consistently with Eq. (B.21), we have introduced the vacuum radiation input noise, $a_{in}$, whose only nonzero correlation function is [Eq. (B.26)]

$$\langle a_{in}(t)a_{in}^\dagger(t') \rangle = (\bar{n}(\omega_c) + 1) \delta(t-t'),$$  \hspace{1cm} (3.13)

and the Hermitian Brownian noise operator $\xi$ [with correlation function given by Eq. (B.34)]. The quantum Langevin equations [Eqs. (3.10)-(3.12)] very much resemble the long-established Langevin equation from classical physics. Remarkably, however, the quantum Brownian motion is not a Markovian process in general [Eq. (B.33)]. Quantum effects, on the other hand, are only achievable by using oscillators with a large mechanical quality factor $Q := \omega_m/\gamma_m \gg 1$. In this limit, $\xi(t)$ becomes delta-correlated [see Eq. (B.40) and comments therein]:

$$\langle \xi(t)\xi(t') \rangle \simeq \gamma_m (2\bar{n} + 1) \delta(t-t'),$$  \hspace{1cm} (3.14)

where $\bar{n} = (\exp\{\hbar\omega_m/k_BT\} - 1)^{-1}$ is the mean thermal excitation number of the mirror, and one recovers a Markovian process.

The noise auto-correlation function (3.13) can be significantly simplified by noting that optical photons are very energetic ($\sim 1\text{eV}$) and thus thermal occupation is insignificant even at room temperature: $\bar{n}(\omega_c) \simeq 0$. Although these simplifications constitute reasonable progress, the Langevin equations [Eqs. (3.11) and (3.12)] are a non-linear dynamical system and, hence, do not admit a simple general solution. We are interested in the steady-state regime, however. In this case an analytical solution can be bound following the tradition in Quantum Optics [89, 109, 110] of considering small fluctuations around the steady-state.

Indeed, we rewrite each Heisenberg operator as a $c$-number steady state value plus an additional fluctuation operator with zero mean value, $a = a_s + \delta a$, $q = q_s + \delta q$, $p = p_s + \delta p$. By inserting these expressions into the Langevin equations [Eqs. (3.10), (3.11) and (3.12)], these latter decouple into a set of nonlinear algebraic equations for the steady state values and a set of quantum Langevin
3.2. The dynamics of a driven cavity

Equations for the fluctuation operators \[109, 110\]. The steady state values are given by,

\[ p_s = 0, \]
\[ q_s = \frac{g}{\omega_m} |\alpha_s|^2, \]
\[ \alpha_s = \frac{E}{\kappa + i(\Delta_0 - gq_s)}. \]

The latter equation is, in fact, a nonlinear equation determining the stationary intra-cavity field amplitude, \( \alpha_s \), since the effective cavity detuning, \( \Delta \equiv \Delta_0 - gq_s \), including radiation pressure effects, is given by \( \Delta = \Delta_0 - g^2 |\alpha_s|^2/\omega_m \), and thus depends on \( \alpha_s \). Given our conjecture (Sec. 2.2.2), we expect the parameter regime relevant for generating opto-mechanical entanglement is that of a very large input power \( P \), i.e. \( |\alpha_s| \gg 1 \). In this case, one can safely neglect the nonlinear terms \( \delta a^\dagger \delta a \) and \( \delta a \delta q \), and one gets the linearized Langevin equations,

\[ \delta \dot{q} = \omega_m \delta p, \]
\[ \delta \dot{p} = -\omega_m \delta q - \gamma_m \delta p + G\delta X + \xi, \]
\[ \delta \dot{X} = -\kappa \delta X + \Delta \delta Y + \sqrt{2} \kappa X_{in}, \]
\[ \delta \dot{Y} = -\kappa \delta Y - \Delta \delta X + G\delta q + \sqrt{2} \kappa Y_{in}, \]

where we have re-written the cavity operators as function of the cavity field quadratures (see table 2.1): \( \delta X \equiv (\delta a + \delta a^\dagger)/\sqrt{2} \) and \( \delta Y \equiv (\delta a - \delta a^\dagger)/i\sqrt{2} \). The corresponding Hermitian input noise operators read \( X_{in} \equiv (a_{in} + a_{in}^\dagger)/\sqrt{2} \) and \( Y_{in} \equiv (a_{in} - a_{in}^\dagger)/i\sqrt{2} \). The most important aspect of the linearized Langevin equations is that the quantum fluctuations of the field and the oscillator are now coupled by the much larger effective opto-mechanical coupling,

\[ G \equiv g\alpha_s \sqrt{2}. \]

The latter can be very large by increasing the intra-cavity field amplitude and a significant amount of entanglement will be possible as we shall see in a moment. For the sake of simplicity, in what follows we choose the phase reference of the cavity field so that \( \alpha_s \) is real. Its amplitude reads,

\[ \alpha_s = \sqrt{\frac{P\kappa}{2\hbar\omega_0(\kappa^2 + \Delta^2)}}. \]

When the system is stable it reaches a unique steady state, independently of the initial condition. Since the quantum noises \( \xi \) and \( a_{in} \) are zero-mean quantum Gaussian noises and the dynamics is linearized, the quantum steady state for the fluctuations is a zero-mean bipartite Gaussian state, fully characterized by its \( 4 \times 4 \) correlation matrix [Eq. 1.4],

\[ V_{ij} = \langle u_i(\infty)u_j(\infty) + u_j(\infty)u_i(\infty) \rangle / 2, \]
3. Stationary opto-mechanical entanglement at moderately high temperatures

where \( u^T(\infty) = (\delta g(\infty), \delta p(\infty), \delta X(\infty), \delta Y(\infty)) \) is the vector of fluctuation operators at the steady state \( (t \to \infty) \). Defining the vector of noises \( n^T(t) = (0, \xi(t), \sqrt{2\kappa X_{in}(t)}, \sqrt{2\kappa Y_{in}(t)}) \) and the matrix,

\[
A = \begin{pmatrix}
0 & \omega_m & 0 & 0 \\
-\omega_m & -\gamma_m & G & 0 \\
0 & 0 & -\kappa & \Delta \\
G & 0 & -\Delta & -\kappa
\end{pmatrix},
\]

(3.25)

This matrix determines the dynamical stability of the physical system, and it also provides a measure of the correlations between its two subsystems, the intra-cavity field and the mirror. Eqs. (3.18)-(3.21) can be now written in compact form as

\[
\dot{u}(t) = Au(t) + n(t),
\]

(3.26)

whose formal solution is

\[
u(t) = M(t)u(0) + \int_0^t dsM(s)n(t-s),
\]

(3.27)

with \( M(t) = \exp\{At\} \). The system is stable and reaches its steady state when all the eigenvalues of \( A \) have negative real parts so that \( M(\infty) = 0 \). The stability conditions can be derived by applying the Routh-Hurwitz criterion \(^{[111]}\), yielding the following two nontrivial conditions on the system parameters

\[
\mathcal{S}_1 = 2\gamma_m\kappa \left[ \Delta^4 + \Delta^2(\gamma_m^2 + 2\gamma_m\kappa + 2\kappa^2 - 2\omega_m^2) \right. \\
+ \left. (\gamma_m\kappa + \kappa^2 + \omega_m^2)^2 \right] + \omega_m G^2 \Delta (\gamma_m + 2\kappa) > 0,
\]

(3.28)

\[
\mathcal{S}_2 = \omega_m^2 (\Delta^2 + \kappa^2) - \omega_m G^2 \Delta > 0.
\]

(3.29)

A careful stability analysis of this system is found in \(^{[112]}\). From now on we will consider the above conditions to be satisfied. When the system is stable Eq. (3.24) becomes,

\[
A V + VA^T = -D.
\]

(3.32)

The latter is a linear equation for \( V \) containing the linearized dynamics of the full system. The linearized dynamics of the system can be studied in all the parameter region obeying inequalities (3.29).

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and (3.30). The analytic expression for \( V \) can be straightforwardly derived either from Eq. (3.32) or from the Fourier transform \( \mathcal{F} \) of the Langevin equations,

\[
-i\omega (\mathcal{F}u)[\omega] = A(\mathcal{F}u)[\omega] + n[\omega],
\]

by expressing all the correlation functions in the frequency domain. For instance,

\[
V_{11} = \langle \delta q(\infty) \delta q(\infty) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega |\mathcal{F}(\delta q)[\omega]|^2.
\]

The exact form of \( V \) in the whole parameter region is complicated and not very enlightening. Indeed, we just present the analytic solution for the mirror’s reduced covariance matrix (containing the mirror’s correlations) at zero-detuning (\( \Delta = 0 \)), where the system is stable everywhere [see equations (3.29) and (3.30)]. We find \( V_{12} = V_{21} = 0 \), and

\[
V_{11} = \frac{1}{2} + \bar{n} + \frac{G^2 (\kappa + \gamma_m)}{2\gamma_m (\kappa^2 + \kappa\gamma_m + \omega_m)^2}
\]

\[
V_{22} = \frac{1}{2} + \bar{n} + \frac{G^2 \kappa}{2\gamma_m (\kappa^2 + \kappa\gamma_m + \omega_m)^2}.
\]

Recalling that the effective temperature of the mirror (and thus the effective phononic occupation number, \( n_{\text{eff}} \)) is determined by the average of the fluctuations undergoing Brownian motion, \( i.e. \)

\[
\hbar \omega_m \langle (\delta p(\infty))^2 + (\delta q(\infty))^2 \rangle = \hbar \omega_m \left( n_{\text{eff}} + \frac{1}{2} \right),
\]

we conclude that, in the zero-detuning case, the mirror is in a squeezed thermal state with an effective thermal occupation number given by

\[
n_{\text{eff}} = \bar{n} + \frac{G^2 (2\kappa + \gamma_m)}{4\gamma_m (\kappa^2 + \kappa\gamma_m + \omega_m^2)}.
\]

This shows the heating of the mirror above its environmental temperature (\( n_{\text{eff}} > \bar{n} \)) for \( \Delta = 0 \). Whether this results in detectable entanglement or not, will depend on the particular statistics of the cavity field. \(^{\text{1}}\)

\(^{\text{1}}\) Recall that in the unitary evolution scenario the heating of the mirror was a signature of quantum correlations only when the partial sate of the cavity field was sufficiently mixed, see Fig. [2.7] after some time has passed the partial entropies, \( S_{\text{cov}} \) and \( S_m \), are sufficiently high producing a violation of the classical bound [Eq. (A.52)]. \( S_{\text{cov}} + S_m > 2S \), where \( S \) is the total entropy of the system. In this case, also, the effective temperature of the mirror increases, in agreement with the increase of the linear entropy. In fact the mirror’s effective phononic occupancy can be derived quite easily from the evolution operator [Eq. (2.15)]:

\[
\langle (b^\dagger b)(t) \rangle = \langle U^\dagger(i)b^\dagger bU(i) \rangle = \langle U^\dagger(i)b^\dagger U^\dagger(i)bU(i) \rangle = \langle (b^\dagger + k\eta (1 - i) a^\dagger) (b + k\eta (1 + i) a^\dagger) \rangle = \bar{n} + k^2 |\eta| (|a|^2 + 1 - |a|^2),
\]
3. Stationary opto-mechanical entanglement at moderately high temperatures

Figure 3.2.: Left - The entanglement [Eq. (3.41)] is plotted as function of the rescaled detuning, $\Delta/\omega_m$, for a cavity with $L = 1 \text{ mm}$ and optical finesse [Eq. (B.8)] $F = 1.07 \times 10^4$ (corresponding to a damping rate of $\simeq 88 \text{ MHz}$) and $T = 0.4 \text{ K}$ (corresponding to a thermal occupancy of $\bar{n} \simeq 832$). The cavity is driven by a Laser with wavelength $\lambda = 810 \text{ nm}$ and power $P = 50 \text{ mW}$. The mirror has quality factor [Eq. (B.39)] $Q = 10^5$ and natural frequency $\omega_m/2\pi = 10 \text{ MHz}$. Right - The effective phononic occupation number, $n_{\text{eff}}$, is plotted for the same physical parameters. We clearly see a giant suppression of the thermal fluctuations of the mirror as soon as $\Delta > 0$; an effective self-induced cooling has lowered the phononic occupation of the mechanical oscillator and enhanced the quantum correlations of the compound system.

In the following section, we will see that, in fact, stationary entanglement is strictly null for $\Delta = 0$ and that the situation is radically different for non-zero detuning $\Delta > 0$ as the mirror is effectively cooled down to its ground state.

3.3. Approaching stationary entanglement

In order to establish the conditions under which the optical mode and the mirror vibrational mode are entangled, we consider the logarithmic negativity, $E_N$, a quantity that correctly quantifies entanglement for Gaussian bipartite states. The nature of the correlations described by $V$ depends only on the smallest sympletic eigenvalue of the partial transposed covariance matrix, $\tilde{d}_- \equiv d_- (\Lambda_A V \Lambda_A)$ [Eq. (1.88)],

$$\tilde{d}_- \equiv 2^{-1/2} \left[ \tilde{\Sigma}(V) - \left[ \tilde{\Sigma}(V)^2 - 4 \det V \right]^{1/2} \right]^{1/2}$$  \hfill (3.39)

with $\tilde{\Sigma}(V) \equiv \det A + \det B - 2 \det C$, and we have used the $2 \times 2$ block form of the covariance matrix,

$$V \equiv \begin{pmatrix} A & C \\ C^T & B \end{pmatrix}.$$  \hfill (3.40)

from which we confirm the heating of the mirror for $t \neq 2n\pi/\omega$ (with $n \in \mathbb{N}_0$).
3.3. Approaching stationary entanglement

A Gaussian state is entangled if and only if $\tilde{d} - \frac{1}{2} < 0$, which is equivalent to Simon’s necessary and sufficient transpose criterion for Gaussian states (Sec. [1.4]). The entanglement of a Gaussian bipartite state is properly quantified via the logarithmic negativity [Eq. (1.94)],

$$E_N = \max[0, -\ln 2\tilde{d}] .$$

(3.41)

As mentioned in the previous section, we can show that $\tilde{d} - \frac{1}{2} \geq 0$ for $\Delta = 0$, at any temperature, and thus no genuine quantum correlations are shared by the photons and the phononic mode of the mirror. On the contrary, by a proper choice of detuning, we can reach a steady state with entanglement: Fig. [3.2] shows that a detectable amount of steady-state entanglement is expected for $\Delta \sim \omega_m$ at environmental temperatures much above the mirror’s ground state for state-of-the-art experimental parameters. For the parameters values of Fig. [3.2] the effective coupling, $G$, varies between $10^7$ and $10^8$ (in units of frequency). This large effective coupling leads to the establishment of bona fide macroscopic entanglement at relatively high-temperature ($T = .4$ K $\leftrightarrow \bar{n} \simeq 832$). Curiously, the effective temperature of the mirror suffers an abrupt change as soon as $\Delta > 0$ (see the right-hand side of the figure).
3. Stationary opto-mechanical entanglement at moderately high temperatures

plot in Fig. 3.2). We find a mirror’s effective thermal occupancy as low as \( n_{\text{eff}} \approx 0.75 \) for a mirror of mass \( m = 5 \text{ ng} \) and \( \Delta = 2\omega_m \), which is in deep contrast to the situation found for \( \Delta = 0 \) [Eq. (3.38)]. A careful study in the stable parameter region shows that entering in the low coupling regime \( (G \lesssim \omega_m) \), completely destroys the quantum correlations even at low temperatures (see Fig. 3.3).

It is apparent from these results that the usual criterion on temperature for quantum behavior [Eq. (A.6)] is misleading in the context of complex open quantum systems. Braginsky found a similar situation for an oscillator measured for a short time compared to its own relaxation time [see Appendix A.1 and Eq. (A.7)]. Indeed, the rigid condition \( k_B T \lesssim \hbar \omega_m / 2 \) can be very much relaxed when we look carefully to all the physical scales playing role in a given setup. Ultimately, with optimal experimental conditions, our results predict stationary entanglement up to \( \bar{n} \approx 10^4 \Leftrightarrow T \approx 20 \text{ K} \) (for a mirror with \( m = 5 \text{ ng} \) and \( \omega_m / 2\pi = 10^7 \text{ Hz} \)).

In our case, the mechanism by which we beat the naive \( k_B T \lesssim \hbar \omega_m / 2 \) criterion has no direct correspondence with the presence of a measuring apparatus in the Braginsky calculation. But still we can relate the quantum behaviour at high-temperature we found to the low entropy continuously flowing into the cavity, which enhances the effective coupling, thus making particularly efficient the radiation-pressure mechanism [for \( P \gg 1 \) we can have \( \alpha_s \gg 1 \), and hence \( G \gg g \), see Eqs. (3.22) and (3.23)]. The functional dependence of entanglement with all parameters is rather complicated but Fig. 3.3 shows the general trends: increasing the mass suppresses entanglement, as decreasing the cavity optical finesse, for instance; the plots also indicate that steady-state entanglement is much more sensitive to the mirror’s frequency, the detuning or the optical finesse rather than the mirror’s mass or its quality factor.

3.4. Concluding remarks

Opto-mechanical coupling via the radiation pressure mechanism, as Braginsky conceived [70, 113], is a promising approach to prepare and manipulate quantum states of mesoscopic and macroscopic mechanical oscillators. We proposed an experimentally achievable setup to create opto-mechanical entanglement between a light field and a mechanical oscillator (see [103] for the details of covariance matrix detection). This is accomplished by using a bright \( \text{LASER} \) field that resonates inside a cavity and couples to the position and momentum of the moving (micro)mirror.

Our proposal is based on feasible experimental parameters in accordance with current state-of-the-art optics and microfabrication [83], although its practical implementation is not yet within reach (the main obstacle probably being combining in the same experiment all the requirements leading to entanglement, see for instance [87]). The noticeable feature of this proposal is the fact that, in contrast to previous proposals [114, 115], it neither requires non-classical states of light, nor temperatures close to the oscillator’s ground state.
3.4. Concluding remarks

Our calculation was based on two assumptions, namely,

1. the single-mode description justified by the adiabatic limit, \( \omega_m \ll \Delta \omega_c \), and

2. the linearization of the Langevin equations, which is accurate for large intra-field amplitudes, \( \alpha_s \gg 1 \).

The fluctuations of the cavity intra-field around its classical value can be very small (for \( \alpha_s \gg 1 \)), thus making the linearization procedure very accurate and commonly used when dealing with optical cavities. These simplifications allowed to take into full account the quantum Brownian motion of the mirror and the main source of the cavity field decoherence (i.e. leakage through the mirrors). In the linearized regime, the bipartite state (mirror+cavity) is well-described by a Gaussian state. Thus, in resemblance to the cases \( 2 \otimes 2 \) and \( 2 \otimes 3 \), where PPT is a sufficient and necessary condition for separability, we were able to completely characterize entanglement, albeit the Hilbert space being infinite dimensional. This method is to be compared with perturbative approaches based on the master equation for the reduced state of the mirror \[92\] which are only valid in the weak-coupling regime \( G \ll \omega_m \) of little interest for entanglement generation according to our calculation.

Also, we have settled on quite solid grounds the main conclusions of Chapter 2: the radiation-pressure mechanism is extremely robust as it accommodates high-temperature macroscopic entanglement — a phenomenon which we believe is very rare (recall the discussions of Chapters 1 and 2 regarding the damage caused by thermal noise on quantum correlations). Some interesting questions are open, e.g. how does the non-linear regime affect the stability region of our setup and the amount of stationary entanglement? Other questions were already answered at the time of writing this thesis, for instance, the entanglement between the output field (instead of the intra-cavity field) and the moveable mirror was computed recently in Ref. [116].
3. Stationary opto-mechanical entanglement at moderately high temperatures
4. Entanglement mediated by the ground-state of gapped spin chains

This chapter is based on the following publication by the author:

- Analytic results on long-distance entanglement mediated by gapped spin chains, Aires Ferreira, and J. M. B. Lopes dos Santos, Phys. Rev. A 77, 034301 (2008).

4.1. Overview

When macroscopic degrees of freedom are addressed with high precision and the decoherence effect of the environment is sufficiently suppressed, the EM field and a macroscopic mirror can get entangled at high-temperatures — this was the essential conclusion of the previous chapters, where by means of a QI approach the quantum-classical boundary of opto-mechanical systems was studied.

The present and the following chapters are devoted to solid-state systems, where a multitude of many-body quantum behavior is well known for several decades (e.g. the superconductivity or the fractional Hall effect) and new phenomena is discovered regularly (e.g. the exotic physics of graphene). The study of entanglement in many-body physics is a topic in its infancy but already lead to at least two significant contributions, namely:

- strict bounds to the scaling of von-Neumann entropy; area laws have been shown to emerge for the latter quantity in the ground state of quantum lattice systems with short-range interactions (e.g. one-dimensional spin chains, bosonic harmonic lattices, disordered systems, etc.). This says that quantum correlations (entanglement) between a region $R$ and the rest of the lattice $\mathcal{L} \setminus R$ are encoded in the boundary $\partial R$. This remarkable result resembles the black hole entropy and it is at odds with the volume law usually satisfied by regions sharing classical correlations (such those arising in thermal states) — for a complete review see [IT7] and references therein;

- a deeper understanding of numerical methods, in particular their ability in simulating efficiently complex many-body systems. For instance, it was understood that if little entanglement
4. Entanglement mediated by the ground-state of gapped spin chains

Figure 4.1.: Schematic of two probe particles, \( a \) and \( b \), initially in a product state \( |\psi_a\rangle \otimes |\psi_b\rangle \), getting entangled after interacting with a quantum many-body lattice, \( \mathcal{L} \), through sites, \( i \) and \( j \), respectively. When the probes are separated by distances of the order of the lattice’s size, we say the lattice has mediated long-distance entanglement between the probes.

is present in the ground state then a matrix-product state yields a good approximation to this ground state [118], a area law would be observed and algorithms such as the Density Matrix Renormalization Group (DMRG) would perform well. By looking to the problem of simulating many-body physics with a QI perspective, the tensor product structure of the Hilbert space of a quantum lattice system could be better manipulated, and powerful new numerical methods, like the multiscale entanglement renormalization ansatz, were proposed capable of reliably simulating one-dimensional (1D) and two-dimensional (2D) systems [119].

Other topics in this field are related to the characterization of the entanglement properties of many-body systems at zero temperature, particularly near quantum phase transitions and also at finite temperatures (see [120] for a review). Although up to our knowledge this approach has not unveiled new properties regarding the phases of matter, it already led to a more complete understanding of physics known for a long time, such that of quantum phase transitions.

The possibility of using quantum many-body systems as quantum channels (systems capable of transporting quantum information), or even as "all-in-one" devices for quantum computation is also a promising subject where entanglement plays an important role. Encouraging works showed that the collective dynamics of the low excitations of the ferromagnetic 1D Heisenberg spin-1/2 model is able to transfer quantum states of a qubit with high fidelity [121], and that finite spin-1/2 chains with "always on" interactions encompass all the features of a processing core model for quantum computation [122].
4.1. Overview

The reason why spin-1/2 chains have been explored in QI is because their particles naturally embody the SU(2) algebra of a qubit, therefore allowing quantum information processing and manipulation along the traditional lines of quantum computing, i.e. via the establishment of quantum gates \cite{26} (see Figure 4.2). Recent DMRG results by Campos Venuti and collaborators \cite{123,124} showed that spin systems can also mediate entanglement between two spin probes separated by large distances. This possibility had already been suggested earlier, in the proposal for entanglement extraction from solids by De Chiara \cite{125}, i.e. that entanglement in a many-body system could be "swapped" to neutrons interacting with the bulk during a flight.

The possibility of extracting entanglement from a large system might seem a bit awkward, as generally the coupling to a system with many degrees of freedom usually destroys entanglement very quickly due to suppression of off-diagonal elements of the density matrix \cite{60,61,126}. However, a few notable exceptions do exist; if two qubits, not interacting directly, are coupled in a symmetric way to a bath of harmonic oscillators, their entanglement will partially survive (or even be created if initially their state was separable) during their evolution when these qubits have degenerate energy eigenstates \cite{127,128}, or when the bath has a gap in its spectrum \cite{129}. A considerable quenching of decoherence is also found in bosonic systems, such as two harmonic oscillators interacting with a common bath \cite{130}. A similar phenomenon, where the effect of decoherence is largely avoided, is found, for instance, in quantum computing using the so-called decoherence-free subspaces \cite{131,132}. The present chapter is devoted to the physics of Long-Distance Entanglement (LDE) in the ground-state of gapped quantum lattice systems. In contrast with the references cited in the previous paragraph, our focus will be on situations where all particles involved are spins. We will demonstrate the emergence of quasi-perfect entanglement among the spin probes by tuning their coupling to the "entangler" bulk to very small values.

Since we are mainly interested in the quantum-classical boundary, the concern of our investigation will be on the conditions which make favorable the emergence of LDE as well as its quantification and its robustness against temperature. For qubits interacting with bosonic baths under Markovian and non-Markovian dynamics, the problem is already well understood (see \cite{130} and references therein). For the case of spins systems, the many-body physics is quite complicated and we cannot make exact computations; nevertheless, in the present chapter we will derive some analytical results in perturbation theory strictly valid at $T = 0$. The generalization to stronger probe-bulk coupling and finite temperature will be made in the following chapter with the help of large numerical simulations.

In what follows, we review the basic ideas behind using many-body systems to accomplish QI tasks and outline the main difficulties of computing LDE in these systems. Afterwards, we derive an adequate perturbation theory for the LDE problem. Our main result will be to show that two (or more) uncorrelated qubit probes, separated by large distances, form highly entangled states, when interacting locally with gapped 1D antiferromagnetic systems; a very appealing situation for QI.
4. Entanglement mediated by the ground-state of gapped spin chains

![Figure 4.2](image)

Figure 4.2.: Schematic of a hypothetical solid-state quantum computer. A highly correlated spin system (inside box) serves as a quantum bus. A magnetic field $\vec{B}$ prepares a qubit (blue on top) in a given quantum state. This qubit is dynamically transferred to a particle within the quantum bus (the blue spin). In the bottom array, long-range order among two spins is used to prepare a SWAP gate: the fundamental gate of quantum information (see [26] for a review). The latter simply swaps the $z$-th component of the spin state of a bipartite system (blue spins on bottom), $U_{SWAP}|\chi_a, \chi_b\rangle = |\chi_b, \chi_a\rangle$. This gate together with single qubit operations (rotations) encompasses universal quantum computing.

4.2. Many-body quantum channels (main ideas and difficulties)

Feasible mechanisms of entanglement extraction from real solid state and their ability to transfer entanglement between distant parties are of crucial importance for the implementation of QI protocols, such as teleportation, information transfer, quantum secure protocols, or superdense coding [26].

Regarding information transfer, for instance, there are two ways of implementing it in many-body systems: a) by unitary dynamical evolution, and b) via bulk ground states (or another equilibrium state), either with or without the need of special measurements (in one or more particles). In the former scheme, one particle is prepared in a superposition of states, say,

$$|\psi_i\rangle = \frac{1}{\sqrt{2}} (a|0\rangle + b|1\rangle), \quad (4.1)$$

(with $a, b \in \mathbb{C}$ and $\{|0\rangle, |1\rangle\}$ denoting an orthogonal basis). Afterwards, the compound state (particle + system) is let to evolve unitarily; in suitable systems, after some time has passed, the particular superposition of Eq. (4.1) will be transferred with high fidelity to another particle in the system. That is, the overlap between the partial state of a distant particle $\rho_j$ (at time $t'$) and the fiducial particle $i$ (in the state $|\psi_i\rangle$ at time $t = 0$) will be nearly maximal,

$$\langle \psi_i | \rho_j (t') | \psi_i \rangle \approx 1. \quad (4.2)$$
4.2. Many-body quantum channels (main ideas and difficulties)

The time elapsed $\Delta t = t^* - t$ depends on the velocity of the excitations; in some spin systems this could be the spin-wave velocity. The study of capabilities and limitations of information transfer via dynamical evolution is a rapidly developing field; the interested reader is referred to the introduction to quantum communication via spin chains by Bose [133]; a study of entanglement and state transfer via dynamical evolution of harmonic spin chains and the $XY$ spin chain can be found in references [134, 135]. Regarding possibility b), here we just mention that bipartite entanglement works as a figure of merit for the capabilities of a physical system towards quantum information processing. Thus, all that is found on mediation of entanglement in spin lattices (such as LDE) will tell us about performance in quantum processing via a "quantum bus" in equilibrium. For these reasons, we focus on the fundamental issue of quantification of LDE rather presenting particular consequences for QI protocols (specific implementations may be found in many texts, see for instance [124]).

Finally, systems of spins have also been suggested to integrate QI tasks and accomplish quantum computation in a single processing core, although many questions regarding their robustness against temperature and decoherence remain open. Among the DiVicenzo’s requirements to achieve quantum computation, the ability to generate rapid elementary gates between well-characterized qubits is central [136]. Due to significant technical difficulties in switching on direct interactions between qubits, various proposals have been put forward where a quantum sub-system usually denominated as bus is used to mediate the fundamental universal gates. The physical embodiment of such bus could be, for instance, the phononic mode of cold ions in the famous ion-trap quantum computer [137], or the magnetic degrees of freedom of a quantum spin chain in "all-in-one" solid state device (see [138] and references therein).

Central to the discussion of LDE and nearly all QI enterprise is the understanding how bipartite entanglement is distributed in typical solid-state systems and how it is rearranged in the presence of two (or more) probes. Coffman et al. were the first to grasp the complexity of this issue by considering pure states of three-qubits: entanglement cannot be distributed arbitrarily but obeys the so-called monogamy relations [139]; one consequence is the impossibility of a spin-1/2 in a singlet state to form a singlet with a third spin — the frustration mechanism well-known in condensed matter physics. Interestingly, restrictions from entanglement theory are even stronger implying, in the particular case of 3 qubits, for instance, that a singlet (being a maximal entangled state) does not even allow one of its particles to be partially entangled with a third system.

We are then led to the conclusion that, unlike classical correlations, entanglement cannot be freely distributed among the parties. How does nature distribute entanglement among the tiny magnetic moments constituting a solid-state system? It is known that in systems with short-range interactions, entanglement between two particles usually decays quickly with distance between them [140, 141], in opposition to the usual classical correlations which can persist for large distances. As a pedagogical example, think about the paradigmatic model of antiferromagnetism: the AF spin-1/2 Heisenberg
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chain, whose Hamiltonian reads

\[ H_{AF} = J \sum_{i=1}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1}, \]  \hspace{1cm} (4.3)

where \( \vec{S}_i := (1/2) \vec{\sigma}_i \) are spin-1/2 operators \([\vec{\sigma}^a] \) denotes Pauli matrices, see Eq. (1.19). The spin-spin correlations in the thermodynamic limit read, \( \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \sim (-1)^r \ln r/r \) \( [142] \). The form of the partial state of the \( i \)-th and \( j \)-th spins, \( \hat{\rho}_{ij} \), is trivially fixed by the global \( SU(2) \) symmetry of the Hamiltonian,

\[ \hat{\rho}_{ij} = \frac{1}{4} + C_{ij} \hat{O}_{ij}, \]  \hspace{1cm} (4.4)

where \( \hat{O}_{ij} = (4/3) \vec{S}_i \cdot \vec{S}_j \) is the only \( SU(2) \) invariant (besides the identity) for the two spins, and \( C_{ij} := \langle \vec{S}_i \cdot \vec{S}_j \rangle \) is the spin-spin correlation function. From the above formula, one can show (for instance, via PPT, see Sec. [1.3]) that asymptotic correlations are entirely classical. As a matter of fact, in the thermodynamic limit, only next-neighbor spins are entangled as it can be concluded by the study of the exact correlations for this model. Take for instance, the nearest-neighbor correlator,

\[ C_{i,i+1} = \frac{\partial E_0}{\partial J} = -\frac{1}{4} + \ln 2 \simeq -0.44, \]

where \( E_0 \) is the energy per site (derived via Bethe ansatz by Hulthén \([143]\)). The latter value is low enough that correlations are quantum (recall that two spins-1/2, \( i \) and \( j \), display entanglement iff \( C_{i,j} < -1/4 \) — see Sec. [1.2]). In this case, each spin is entangled with its nearest neighbors but the specific form of the many-body wave-function entails a very short entanglement correlation length, despite the chain being critical and correlations decaying slowly.

In other spin chains, entanglement can persist at larger distances (for instance reaching next-nearest-neighbors, see \([140]\)), but generally decaying much faster than correlations. On the other hand, entanglement between a block of spins and the rest of the chain can be very large in critical chains, reflecting that spin-spin entanglement is just one facet of quantum correlations in ground-state of many-body systems \([117]\).

The fact that bipartite spin-spin entanglement is highly restrained in spin chains make us questioning about the possibility of establishing entanglement between distant particles. However, as mentioned in the previous section, numerical studies show that certain spin chains are able to establish LDE between probes to which they couple, without the need of an optimal measurement strategy onto the rest of the spins \([123]\), raising the question: which classes of strongly correlated systems are able to produce LDE?

4.3. A perturbation theory for long-distance entanglement

In this section we answer the latter question by considering the particular and important case of weakly coupled probes. The other limit, namely that of strongly interacting probes is of little interest
4.3. A perturbation theory for long-distance entanglement

Regarding LDE — this fact can be understood by realizing that if a probe interacts strongly with a given site in the lattice it will develop entanglement with it, avoiding entanglement with the other probe (the frustration mechanism mentioned previously).

Regarding the nature of the quantum many-body system, our choice will be directed to those leading to strongly-correlated ground states with antiferromagnetic correlations. We can anticipate that ground states with strong classical order (ferromagnetism, for instance) will not be able to entangle external particles. Think for instance in a one-dimensional ferromagnet; weakly coupled spin probes would perceive this system as a strong magnetic field and would align producing a product state with well-defined spin directions.

We start by defining LDE at zero-temperature; denoting the ground-state of the total system by $|\psi\rangle$ and the degrees of freedom of the many-body lattice by $\mathcal{L}$, then if the partial state of two probes $a$ and $b$ (not interacting directly),

$$\rho_{ab} = \text{Tr}_{\mathcal{L}}\left(|\psi\rangle\langle\psi|\right),$$

is entangled for distances of the order of the system size, $d_{AB} \sim O(L)$, they are said to display long-distance entanglement. The trace operation in Eq. (4.5) is most of the times impossible to perform analytically as the dimension of $\mathcal{H}$ grows exponentially with the system size. If the quantum systems living on the sites of $\mathcal{L}$ are spin-1/2 particles, then an exact calculation can be carried out for the XY model where a remarkable mapping to a theory of free fermions exists [144]. In other cases, such that of the AF Heisenberg model, we have to address the physics of the probes by other means. Here we use degenerate second-order perturbation theory to derive a quantitative description of the effective Hamiltonian of the probes. This will be sufficient to prove the existence of quasi-perfect LDE in 1D gapped systems and in the next chapter, by means of a different approach, we will quantify the amount of LDE.

The Hamiltonian of the LDE problem has the following form,

$$H = H_0 + V_{m,n},$$

where $H_0$ is the full many-body Hamiltonian of the bulk and $V_{m,n} = V_{a,m} + V_{b,n}$ describes the interaction between the probes, $a$ and $b$, and the bulk through sites $m$ and $n$, respectively. Although the present formalism can be employed to general gapped many-body systems, we focus on one-dimensional spin chains and probes with the same Hilbert space (i.e. $\mathcal{H}_A = \mathcal{H}_B$).

The requirement of weakly coupled probes reads

$$J_p \ll J,$$

where $J_p$ is the interaction strength between the probes and the spin chains, and $J$ is a typical energy scale for the spin system (for instance, a nearest neighbor exchange interaction). When $J_p = 0$ the
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State of the probes becomes totally uncorrelated and the Ground State (GS) of the entire system becomes \( d \times d \) fold-degenerate, where \( d \) is the dimension of the probe’s Hilbert space. In this case we may write \( |\psi\rangle = |\psi_0\rangle \otimes |\chi_a\rangle \otimes |\chi_b\rangle \), where \( |\psi_0\rangle \) is assumed non-degenerate and \( |\chi_\gamma\rangle \) stands for the state of the probe \( \gamma = a, b \). The role of the interaction \( (J_p > 0) \) is to lift this degeneracy causing the probes to develop correlations.

On quite general grounds, this interaction can be recast in the following form,

\[
V = \sum_{a=1}^{p} \left( \gamma_a^O_{m} \otimes A^a \otimes 1_b + \gamma_b^O_{n} \otimes 1_a \otimes B^a \right),
\]

(4.8)

where \( A(B) \) denotes an (vector) operator with components \( \alpha = x, y, z \) acting on the Hilbert space of the probe \( a(b) \) and \( 1_a(b) \) the corresponding identity operators. The many-body system operators on sites \( m \) are represented by \( O^a_m \) and \( \gamma^a \) stand for coupling strengths for each of the terms in \( V \).

A projection on the spin chain ground state, integrating their degrees of freedom, is the key feature of our method and thus it is useful to define the projector onto the states with unperturbed energy \( E_0 \equiv \langle \psi_0 | H_0 | \psi_0 \rangle \):

\[
\mathcal{P}_0 = |\psi_0 \rangle \langle \psi_0 | \otimes 1_a \otimes 1_b.
\]

(4.9)

The projector onto the subspace of higher energy \( E_k > E_0 \) is denoted by \( \mathcal{P}_k \) (with \( k > 0 \)) and thus \( 1 = \mathcal{P}_0 + \sum_{k>0} \mathcal{P}_k \). Using second order degenerate perturbation theory we can determine the probes GS by diagonalizing an effective Hamiltonian in the subspace spanned by \( \mathcal{P}_0 \). This is a familiar concept that finds many applications in condensed matter physics, such as, for instance, in the derivation of the Ruderman-Kittel-Kasuya-Yosida magnetic interaction between local moments in a metal \[145, 146, 147\].

In what follows, we set \( \mathcal{P}_0 H_0 \mathcal{P}_0 \) to zero as it contributes with a constant, and thus not changing the physics. The derivation of the effective Hamiltonian is made in Appendix C.1. It reads

\[
H^{(ab)} = -\sum_{k>0} \langle \bar{V} \mathcal{P}_k \bar{V} \rangle \langle \bar{V} \rangle (E_k - E_0)^{-1} + "local terms",
\]

(4.10)

where the average is taken with respect to the GS of the spin chain, \( \langle \bar{V} \mathcal{P}_k \bar{V} \rangle = \langle \psi_0 | \bar{V} \mathcal{P}_k \bar{V} | \psi_0 \rangle \), \( \bar{V} := V - \langle \psi_0 | V | \psi_0 \rangle \) and constants are absorbed in the local terms whose form we do not make explicit yet.

Entanglement between the probes arises from \( H^{(ab)} \) since it contains non-local terms such as \( V_{a,m} \mathcal{P}_k V_{b,n} \) \[148\]. The probe Hamiltonian can be transformed by straightforward manipulations into an explicit form involving time dependent correlation functions of the spin chain. A similar procedure is used to express cross sections of scattering by many-body systems in terms of its correlation functions.
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We obtain (we set $\hbar = 1$, see Appendix $\text{C.1}$),

$$H^{(ab)} = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{dE}{E} \int_{-\infty}^{+\infty} dt \langle \tilde{V}(t) \tilde{V} \rangle_0 e^{iEt}. \quad (4.11)$$

We now introduce the explicit form of $\tilde{V}$ to arrive at the desired result: $H^{(ab)} = H_L^{(a)} + H_L^{(b)} + H_{NL}^{(ab)}$.

Defining the two-body connected correlation in the usual form

$$\langle O^{\alpha}_{m}(t) O^{\beta}_{n}(t) \rangle_c = \langle \psi_0 | O^{\alpha}_{m}(t) O^{\beta}_{n} | \psi_0 \rangle - \langle \psi_0 | O^{\alpha}_{m}(t) | \psi_0 \rangle \langle \psi_0 | O^{\beta}_{n} | \psi_0 \rangle, \quad (4.12)$$

the term coupling the two probes reads,

$$H_{NL}^{(ab)} = \sum_{\alpha, \beta = 1}^{\beta} \gamma^{\alpha \beta}_{m n} (C_{m\alpha, n\beta} + C_{n\beta, m\alpha}) A^{\alpha} \otimes B^{\beta} \quad (4.13)$$

$$C_{m\alpha, n\beta} = \frac{1}{2i} \int_{-\infty}^{+\infty} dt e^{-0^{+}|t|} \text{sign}(t) \langle O^{\alpha}_{m}(t) O^{\beta}_{n}(0) \rangle_c. \quad (4.14)$$

The form of local terms $H_L^{(a)} + H_L^{(b)}$ will not be given since they play no role in the systems of our interest, i.e. those with full rotational symmetry. The coupling between the probes can be expressed in terms of the response function (or adiabatic susceptibility) $\chi_{m\alpha, n\beta}(t) = -i \langle [O^{\alpha}_{m}(t), O^{\beta}_{n}] \rangle (t)$, where $\theta(t)$ is the Heaviside step function. Using the Lehman representation at $T = 0$ one can show that

$$\tilde{\chi}_{m\alpha, n\beta}(0) = C_{m\alpha, n\beta} + C_{n\beta, m\alpha}, \quad (4.15)$$

where $\tilde{\chi}_{m\alpha, n\beta}(\omega)$ is the time Fourier transform of $\chi_{m\alpha, n\beta}(t)$ (Appendix $\text{C.2}$). This formula says that any interaction mediated by the spin chain will be encoded in the response function. Usually, the study of external perturbations requires the knowledge of the susceptibility $\chi(t)$ for all times, but since we are interested in the equilibrium physics an integration in the time domain emerges in our equations. The fact that we are able to write the effective couplings in this language will be central later on, when specializing for concrete spin chains.

Some comments about the validity of perturbation theory are in order: the effective Hamiltonian [Eq. (4.13)] lifts the degeneracy of the GS level of the uncoupled system ($J_p = 0$) and, as long as the couplings appearing in $H_{NL}^{(ab)}$ are small, compared to typical energy scales of the spin chain, like the gap to first excited state, $\Delta$, the low energy physics of this system, $E \ll \Delta$, with no real excitations of the spin-chain, will be well described by $H_{NL}^{(ab)}$. This condition limits the strength of the chain-probe interaction, but is shown by numerical results to be the appropriate limit to maximize LDE [123] (stronger couplings will be studied in Chapter $5$).

1 Systems with magnetic field, for instance, will produce local terms in the effective Hamiltonian which reduces the amount of entanglement (compare with the effect a local magnetic field on the Heisenberg magnet considered in the introduction, see for instance Fig. [1.3].

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4.3.1. Quasi-perfect LDE in the spin-1/2 Heisenberg chain

Neutron-scattering experiments reveal that the low energy physics of many magnetic compounds is described by the Heisenberg model \[150\]. The same model emerges as the effective low-energy Hamiltonian in strongly correlated systems, such as the Hubbard model at half-filling \[151\]. For these reasons this model has been the basis of many studies in condensed matter physics for many years. On the other hand, the Heisenberg model is also very important in \[QI\]. The reason is twofold; spin chains are candidates for quantum computers (Sec 4.2), and recent advances in the field of atomic and molecular physics, namely in optical cooling, made it possible to engineer (via the Coulomb coupling of neighboring ions) effective short-range Hamiltonians acting on internal degrees of freedom of trapped ions — a laboratory to investigate typical condensed matter phenomena in different physical scenarios (the interested reader is referred to \[152\] for an extensive review on cold atoms in optical lattices and their applications in \[QI\]).

For the aforementioned reasons, we start by addressing the Heisenberg antiferromagnetic spin chain and its capacity towards \[LDE\]. It is useful to write Eq. (4.13) in terms of spin operators \(\vec{S}_m\) for the spin chain and \(\vec{\tau}_{a(b)}\) for the probes. Considering that the probes couple with the spin chain via an Heisenberg interaction, the most common situation,

\[
V_{m,n} = J_a \vec{S}_m \cdot \vec{\tau}_a + J_b \vec{S}_n \cdot \vec{\tau}_b,
\]

(4.16)

the connection with the previous notation becomes straightforward (see table 4.1). The effective Hamiltonian becomes simply,

\[
H^{(ab)} = J_{\text{eff}} \vec{\tau}_a \cdot \vec{\tau}_b,
\]

(4.17)

where \(J_{\text{eff}} = J_a J_b \tilde{\chi}_{m(n)}(0)\). The effective Hamiltonian in the general form (4.17) already involves

| generic quantum lattice | spin chain |
|-------------------------|-----------|
| many-body operators     | \(O^\alpha_m\) | \(S^\alpha_m\) |
| probe operators         | \(A^\alpha(B^\alpha)\) | \(\tau^\alpha_{a(b)}\) |
| couplings               | \(\gamma^\alpha_{a(b)}\) | \(J_{a(b)}\) (isotropic) |

Table 4.1.: Connection between the generic quantum lattice notation and the spin chain notation.

the important conclusion that for a correct choice of signs of \(J_a\) and \(J_b\) any spin chain is a potential entangler for the probes as long as the susceptibility is finite and sufficiently small, so that one remains well inside perturbation theory limits. To see if this is the case in the \[AF\] Heisenberg chain, we have to compute explicitly the effective coupling. The Hamiltonian of an \[AF\] Heisenberg chain with \(L\) spins reads

\[
H_0 := J \sum_{i=1}^{L-1} \vec{S}_i \cdot \vec{S}_{i+1},
\]

(4.18)

with \(J\) standing for the exchange coupling (in this chapter, without any loss of generality, we set
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Our formalism only applies to the finite chain which has gapped excitations although its size can be arbitrarily large. The effective Hamiltonian Eq. (4.17) will preserve the full SU(2) symmetry of the interaction Hamiltonian $H_0 + V_{m,n}$, i.e. no local terms will give additional contribution to $H^{(ab)}$. From now on, we assume that the probes couple to the spin chain with the same strength, $J_a = J_b = J_p$. Hence, the effective Hamiltonian, $H_{\text{eff}}$, takes the very compact form

$$H_{\text{eff}} = J_p \tilde{\tau}_a \cdot \tilde{\tau}_b = J_p \tilde{\chi}_{\text{mczc}}(0) \tilde{\tau}_a \cdot \tilde{\tau}_b. \quad (4.19)$$

The partial state, $\rho_{ab}$, will correspond to a quasi-perfect singlet-state as long as $\tilde{\chi}_{\text{mczc}}(0) > 0$ is bounded and $J_p$ is chosen such that $J_p^2 \tilde{\chi}_{\text{mczc}}(0) \ll \Delta$, where $\Delta$ is the gap to the first excited state of $H_0$. Given the above result, one could be tempted to conclude that $\rho_{ab}$ is in fact a perfect singlet state since the GS of Hamiltonian (4.19) is precisely the single-state for the probes. However, due to the perturbative nature of our formalism with expansion parameter $J_p/\Delta$ (Appendix C.1), the inspection of the perturbed wave-function shows that the negativity (or any other entanglement monotone) will deviate from the value of maximal entanglement (the singlet state) with corrections of the order of $(J_p/\Delta)^2$, which can be very small for weakly interacting probes, i.e.

$$E(\rho_{ab}) = 1 - O(J_p^2/\Delta^2). \quad (4.20)$$

The impossibility of perfect LDE is in agreement with the intuition that tracing out the degrees of freedom in the bulk (in general) introduces mixedness, which in its turn reduces the amount of entanglement even at $T = 0$ (Sec. 1.3); this represents no limitation from the point of view of QI applications, since entanglement extraction procedures do exist that convert partial entangled states in maximally entangled pairs (Fig. 1.2).

In Chapter 5, we will see that equilibrium averages of operators $\tilde{\tau}_a(b)$ computed directly from Eq. (4.19) must be renormalized, explaining why $\rho_{ab}$ does not follow directly from $H_{\text{eff}}$. As a consequence, Eq. (4.20) is in fact a particular case of a more general situation encompassing gapped systems with different characteristics. For the moment, however, we do not attempt to quantify the amount of entanglement but rather focus on the LDE capability of one-dimensional AF systems, where corrections can be so small that quasi-perfect LDE [Eq. (4.20)] is guaranteed.

### 4.3.1.1. Computation of correlation functions from conformal theory

To calculate the GS time-dependent correlation functions, $\langle S^a_m(t)S^b_n(0) \rangle_c$, necessary for the computation of the adiabatic susceptibility, we will use the conformal invariance of the critical infinite chain ($L \to \infty$) since its time-dependent correlations are enough to extract the effective coupling $J_{ab}$ for the finite chain. The reason why we adopt this method (rather than trying to solve for $\tilde{\chi}$ directly in the finite size scenario) is because the conformal character of the infinite chain can be used to relate the physics in distinct geometries, as we will briefly see.
4. Entanglement mediated by the ground-state of gapped spin chains

General results for correlations of critical spin-1/2 chains are known from bosonization theory (e.g. the asymptotic behavior of time-dependent correlations [153]), but how can the physics of these systems be mapped to the physics of a gapped (non-critical) spin chain? The basic idea is to generalize the scale invariance of a classical system at criticality to encompass a broader class of transformations than the usual rotations, changes of scale, etc.

We outline the basic notions of the so-called conformal mapping; the reader is referred to the review by Cardy for more details [154]. We introduce some notation; let \( \phi_i \) denote the fields of a given theory defined in a lattice (assumed critical) and \( b \) be a scale transformation \( r'_i = b^{-1} r_i \). The critical behavior of the theory entails the following scaling transformation law,

\[
\langle \phi_1(r_1) \ldots \phi_n(r_n) \rangle = b^{-\mu_1} \ldots b^{-\mu_n} \langle \phi_1(r'_1) \ldots \phi_n(r'_n) \rangle,
\]

where \( \langle \ldots \rangle \) is an equilibrium average of the fields defined in lattice \( \mathcal{B}(\mathcal{B}') \) and \( \{\mu_i\} \) denote the scaling dimensions of the operators \( \phi_i \). A trivial example of such scaling transformation is a classical critical spin model whose lattice spacing \( a \) is shrunk by a constant factor \( \gamma \); its correlations, such as the two-body correlator,

\[
\langle \phi_1(r_1) \phi_2(r_2) \rangle \sim \left( \frac{1}{r_1 - r_2} \right)^2 \mu,
\]

will change according to

\[
\langle \phi_1(r_1) \phi_2(r_2) \rangle \rightarrow \gamma^{2\mu} \left( \frac{1}{r_1 - r_2} \right)^2 \mu = \gamma^{2\mu} \langle \phi_1(r_1) \phi_2(r_2) \rangle,
\]

which clearly agrees with the transformation law (4.21) with \( \mu_1 = \mu_2 = \mu \). This result is not surprising as we would not expect that changing the lattice spacing \( a \) would modify the asymptotic physics if the underlying model is the same; after all, critical models look the same in all scales, a fact encoded in the power-law behavior of their correlators.

What is surprising though is that this transformation law holds to all conformal transformations (i.e. the transformations preserving locally the angles between a triplet of points). In 3D these are just rotations, changes of scale and translations which do not produce essentially different lattices (hence the correlators having similar structures). However, in 2D the group of conformal transformations is a much larger class! The latter stems from the well-known fact in complex analysis that any analytic transformation \( f(z) \) of the plane (\( z \) being a complex coordinate) is conformal. Accordingly, we can generalize (4.21) by considering all transformations \( f(z) \) preserving locally the metric of \( \mathcal{B} \):

\[
\langle \phi_1(z_1, \bar{z}_1) \ldots \phi_n(z_n, \bar{z}_n) \rangle = \left| f'(z_1) \right|^{\frac{\mu_1}{2}} \ldots \left| f'(z_n) \right|^{\frac{\mu_n}{2}} \langle \phi_1(z'_1 = f(z_1)) \ldots \phi_n(z'_n = f(z_n)) \rangle.
\]

This method is very powerful for it relates the physics of lattices with different geometries simply by finding the appropriate analytic function \( f(z) \) mapping the points in \( \mathcal{B} \) to points in \( \mathcal{B}' \). The physical motivation behind generalization (4.24) is the following; if the Hamiltonian contains only local
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Figure 4.3.: The conformal transformation $w(z) = \sigma + ir$ maps every point $(v_F \tau, x)$ in the plane into the strip geometry ($\sigma \in [-\infty, \infty]$, $r \in [-L/2, L/2]$) with periodic boundary conditions along the $r$ direction (see Appendix C.4).

terms (such the Heisenberg model) then, in principle, conformal transformations will not change the asymptotic physics as they are (locally) just simple rotations, rescalings or translations.

4.3.1.2. Adiabatic susceptibility of the Heisenberg AF spin-1/2 chain

Let us apply conformal mapping methods to the critical Heisenberg AF chain so to extract $\chi_{mzn}(0)$ for the ring geometry. It is convenient to express the correlations in terms of the staggered magnetization, $M^z_j$:

$$G^R_{mn}(t) := -i\langle [M^z_m(t), M^z_n(\tau)] \rangle \theta(\tau),$$  \hspace{1cm} (4.25)

from which the response function can be obtained simply by a sign exchange [Eq. (C.35)] and compensating the $\pi$ phase change: $\chi_{mzn}(t) = (-1)^{|m-n|+1} G^R_{mn}(t)$. In its turn, using conformal mapping, the retarded Green’s function can be obtained from the asymptotic Matsubara Green’s function of the critical chain. The latter is defined as $G(x, \tau) := \langle \hat{T}_\tau M^z_m(x_m, \tau) M^z_n(x_n, 0) \rangle$ where $\hat{T}_\tau$ is the imaginary time-ordering operator [Eq. (C.58)] and $\tau \in [0, \beta]$ the imaginary time variable. In the limit $|x_m - x_n| \gg 1$, we may take $x = |x_m - x_n|$ as a continuum variable, and the Matsubara function for gapless spin-1/2 chains reads [153,155]

$$G(x, \tau) = \frac{\nu_F}{(v_F^2 \tau^2 + x^2)^{K/2}},$$  \hspace{1cm} (4.26)
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where is an amplitude (from bosonization theory), for the chain and stands for the Fermi velocity of excitations. This result embodies a divergent ; a direct consequence of a zero gap and a signal of the critical nature of the spin chain at — external perturbations in such systems are not described by linear response theory anymore.

The mapping of the infinite chain to the finite chain is achieved by the following analytic transformation (see Fig. 4.3): where is an amplitude (from bosonization theory), for the finite chain with periodic boundary conditions in the spatial coordinate and stands for the Fermi velocity of excitations. This result embodies a divergent ; a direct consequence of a zero gap and a signal of the critical nature of the spin chain at — external perturbations in such systems are not described by linear response theory anymore.

Setting the branch cut of the logarithm in the negative real axis (Fig. C.2), we get:

The analytic continuation to real time is made by Wick rotation, yielding a time-ordered Green Function. Finally, using standard analytic continuation methods (Appendix C.3) the latter function gives defined in the cylinder (and hence, the susceptibility).

Setting the branch cut of the logarithm in the negative real axis (Fig. C.2), we get:

where and an outline of the main properties of spectral representation of Green’s functions can be found in Appendix C.2.

We now compute the response function at zero frequency according to Eq. (C.53), . To this end, we define and separate the integral in many parts using for with (we omit, for the moment, multiplicative constants and denote the integral by ).

where we have defined . The next step is to perform the summation over [the
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Figure 4.4.: Left - The integration of the adiabatic susceptibility is done by thinking of the variable $y$ [Eq. (4.31)] as living on the circle. Then Eqs. (4.30)-(4.33) simply subtract the grey area on the top (with plus sign in the figure and weight proportional to $\epsilon_0 + y$) from the grey area on the bottom (with minus sign in the figure and weight proportional to $\epsilon_0 + (2\pi - y)$). This procedure is repeated many times as $y$ crosses the same points in the circle. At the end, the limit of $0^+ \to 0$ is done to get Eq. (4.34). Right - The absolute value of the response function at zero frequency for the finite antiferromagnetic Heisenberg chain. We have assumed $r \gg 1$, so that the results from bosonization theory are accurate. Only $r/L \in [0, 1/2]$ is represented, since boundary conditions imply $\tilde{\chi}_{r/L}(0) = \tilde{\chi}_{1-r/L}(0)$.

substitution $0^+ \to 0$ is made only at the end to assure convergence (see Figure 4.4 - Left):

$$\tilde{\chi} = \frac{1}{1 - e^{-2\pi y}} \left( \int_x^\pi dy - \int_0^{\pi - x} dy \right) \frac{e^{0^+ y}}{\sqrt{\cos(x) - \cos(y)}}, \quad (4.32)$$

$$= \frac{1}{1 - e^{-2\pi y}} \int_x^\pi dy \frac{e^{-0^+ y} - e^{0^+ (2\pi - y)}}{\sqrt{\cos(x) - \cos(y)}}, \quad (4.33)$$

$$= 0^+ - 0 \int_x^\pi dy \frac{1 - y/\pi}{\sqrt{\cos(x) - \cos(y)}}. \quad (4.34)$$

This shows that the AF ring has a finite $\tilde{\chi}_{m;n}(0)$, as expected for a gapped chain ($\Delta \sim J/L$); conformal theory [Eq. (4.24)] could effectively be used to calculate correlation functions in a different geometry. Gathering all the constants, we finally reach to the desired result,

$$\tilde{\chi}_{m;n}(0) = c_{mn} \int_{2\pi r/L}^\pi d\tau \frac{\tau/\pi - 1}{\sqrt{\cos(2\pi r/L) - \cos(\tau)}}, \quad (4.35)$$

with $c_{mn} = (-1)^{m-n}/(\sqrt{2v_F})$. Figure 4.4 (Right) shows the plot of the absolute value of the rescaled response function at zero frequency ($|\tilde{\chi}_{m;n}(0)/c_{mn}|$) demonstrating the existence of quasi-perfect LDE for a wide range of values of $r/L$. Note that $\tilde{\chi}_{m;n}(0)$ diverges logarithmically at the origin. Our perturbative approach cannot be applied unless $J^2 p \tilde{\chi}_{m;n}(0) \ll \Delta \sim J/L$, and will fail
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in the thermodynamic limit \((L \rightarrow \infty)\) for fixed \(r\). The numerical results of Ref. [123] show probes almost completely entangled only for small values of coupling \((J_p \sim 0.1)\), for a finite chain \(L = 26\). This value is well estimated by the limit of validity of our perturbative approach, for \(r/L \sim O(1)\), namely, \(J_p \ll J/\sqrt{L}\).

These results strongly suggest that the conditions for \(LDE\) are coincident with the conditions for validity of the perturbative approach; weakly coupled probes get maximally entangled by the effective antiferromagnetic interaction mediated by the spin chain. We are led then to put forward the following conjecture:

**Conjecture 2.** \(The ground states of many-body gapped systems with no symmetry breaking and dominant long-distance antiferromagnetic correlations mediate quasi-perfect \(LDE\) between sufficiently weakly coupled spin-1/2 probes.**

There is a simple physical picture behind the latter conjecture; if a spin system has a finite adiabatic susceptibility, then sufficiently weakly coupled probes will not perturb its ground state very much (therefore preserving the character of asymptotic correlations). On the other hand, their perturbation, though very feeble, will be perceived by each other, being weakly coupled to the bulk. Indeed, they will necessarily form either a quasi-perfect singlet or a triplet plus corrections of order \(J_p^2/J^2\), for their effective Hamiltonian must preserve \(SU(2)\) symmetry. In perturbation theory, we learned that whichever state they eventually form depends on the sign of the adiabatic susceptibility and, therefore, on the nature of the correlations of the spin system. Although these observations seem quite natural, a careful study in the next chapter will show that quasi-perfect \(LDE\) is a peculiarity of one-dimensional \(AF\) systems at \(T = 0\) and that the general picture is more intricate.

### 4.3.2. Quasi-perfect LDE in the AKLT spin chain at \(T=0\)

Is \(LDE\) a phenomenon exclusive of systems with long range (or quasi-long range) \(AF\) order? The conjecture in the previous section says that even when the correlations decay exponentially we may still have \(LDE\) as long as they are antiferromagnetic in nature and a gap separates the ground state energy from the rest of the spectrum. Here we consider a different \(1D\) model of antiferromagnetism: the Affleck-Kennedy-Lieb-Tasaki (AKLT) spin chain — a particular case of the spin-1 \(AF\) chain with biquadratic interactions:

\[
H = \sum_{i=1}^{L-1} \left[ \vec{S}_i \cdot \vec{S}_{i+1} + \beta (\vec{S}_i \cdot \vec{S}_{i+1})^2 \right].
\] (4.36)

In \(1D\) the physics of integer and half-integer spins chains differ very much [151, 156, 157]; the latter model has massive excitations in some phases (even in the thermodynamic limit), a completely different picture than that of spin-1/2 isotropic chains. For \(\beta = 1/3\) it admits an exact solution known as the AKLT spin chain; a picture of its \(GS\) is given by the so-called valence-bond-solid
— each spin-1 is represented by a couple of spins one-half, as long as the antisymmetric state is projected out. The valence-bond-solid state is constructed by forming short-ranged singlets between nearest spin-1/2 and then symmetrizing local pairs to get back $S = 1$ states.

In the thermodynamic limit, the static correlations are very short-ranged $[\xi_{\text{AKLT}} = 1/\ln(3) \cong 0.9]$ [158]. For this reason, we may ask whether two probes are able to get entangled by interaction mediated by the spin-1 chain. We cannot make an exact computation of the adiabatic susceptibility as for the Heisenberg model, since the exact dynamical correlations are not known even for large distances. However, as suggested by Arovas et al. [159], we can apply the single-mode approximation used to deduce the phonon-roton curve in liquid 4He [160, 161], in order to study the excitations in this model. This is done by assuming that a excited state at wave vector $q$ is given by

$$|q\rangle = S_q^z|\psi_0\rangle = N^{-1/2} \sum_i e^{iqr_i} S_q^z |\psi_0\rangle,$$

(4.37)

where $|\psi_0\rangle$ is the exact GS of the AKLT model. Within the single-mode approximation, the dynamical structure factor defined as

$$\mathcal{S}^{\alpha\beta}(q, \omega) = \int dt \int d\omega e^{i(\omega t - qr)} \langle S^\alpha(t) S^\beta_0(0) \rangle$$

(4.38)

is related with the static structure factor defined as $s^{\alpha\beta}(q) = \langle |\psi_0\rangle S^\alpha_q S^\beta_0^\dagger \langle |\psi_0\rangle \rangle$ in the simple way $\mathcal{S}(q, \omega) \cong s(q) \delta(\omega - \omega_q)$. In [159] it was shown that, $\omega_q = E_q - E_0 = (5 + 3 \cos q)/27$, and that $s(q) = (10/27)(1 - \cos q)/\omega_q$. The knowledge of the dynamical structure factor allows us to compute the effective couplings of Eq. (4.14) by inverse Fourier transform. By inverting Eq. (4.38) and make use of the single-mode approximation (SMA), we can derive the effective couplings. Indeed, we consider the right-hand side of Eq. (4.14) and make some manipulations using time translation invariance and rotational symmetry,

$$\tilde{\chi}_{m+rz;mc}(0) = -\frac{1}{27} \int_{-\infty}^{\infty} dt e^{-0 t} |\text{sign}(t)| \left[ \langle S_q^r(t) S_0^r(0) \rangle - \langle S_q^r(0) S_0^r(t) \rangle \right]$$

(4.39)

$$= -\text{Im} \left[ \int_{-\infty}^{\infty} dt e^{-0 t} |\text{sign}(t)| \langle S_q^r(t) S_0^r(0) \rangle \right]$$

(4.40)

$$= -\text{Im} \left[ \int_{-\infty}^{\infty} dt e^{-0 t} |\text{sign}(t)| \int \frac{d\omega}{2\pi} \int \frac{dq}{2\pi} e^{-i(\omega t - qr)} \mathcal{S}^{zz}(q, \omega) \right]$$

(4.41)

$$= 2 \int_0^{\infty} dt e^{-0 t} \int \frac{d\omega}{2\pi} \int \frac{dq}{2\pi} \cos(qr) \mathcal{S}^{zz}(q, \omega)$$

(4.42)

$$= 2 \int_0^{\infty} dt e^{-0 t} \int \frac{dq}{2\pi} \sin(qr) \cos(qr) s(q).$$

(4.43)

The latter expression can be recast into a convenient form by expressing the static structure factor $s(q)$ as function of the excitation energy $\omega_q$. This yields,

$$\tilde{\chi}_{m+rz;mc}(0) = \int_0^{\infty} dt e^{-0 t} \int \frac{dq}{2\pi} \cos(qr) \sin(qr) \left( a + \frac{b}{\omega_q} \right)$$

(4.44)
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with \( a = -2/3 \) and \( b = 80/81 \). The integration in the time domain gives \( 1/\omega_r \), and thus we are left with a one-dimensional integral,

\[
\tilde{\chi}_{m+r\alpha mc}(0) = \int_{-\pi}^{\pi} \frac{dq \cos(qr)}{2\pi \omega_q} \left( a + \frac{b}{\omega_q} \right),
\]

which can be evaluated via contour integration. Indeed, we extend the integral to the interval \([ -\infty, \infty ]\) by means of an appropriate change of variables, \( x = \tan(q/2) \). Let us compute explicitly the term involving \( 1/\omega_q \). Defining \( a_1 = a/(2\pi \ast 25/27) \) and \( a_2 = a/(2\pi \ast 15/27) \),

\[
I_1 := \int_{-\pi}^{\pi} dq \frac{\cos(qr)}{a_1 + a_2 \cos q} = 2 \int_{-\infty}^{\infty} dx \frac{\cos(2r \arctan x)}{(1 + x^2) a_1 + (1 - x^2) a_2}.
\]

We can invert the relation between \( x \) and \( q \) given above to get \( q = i\ln(1 - ix) - i\ln(1 + x) \). Under this relation, the integrand is simplified according to,

\[
2 \cos(2r \arctan x) \rightarrow \left( \frac{1 + ix}{1 - ix} \right)^r + \left( \frac{1 - ix}{1 + ix} \right)^r.
\]

The conditions for the Jordan lemma are verified and thus we can extend the integral to the complex plane:

\[
I_1 = 2 \oint dz \frac{(1 + iz)^r}{(1 + z^2) a_1 + (1 - z^2) a_2}.
\]

This integral has simple poles at \( z = \pm i \sqrt{(a_1 + a_2)/(a_1 - a_2)} \) and a pole of order \( r \) at \( z = -i \). We then conveniently choose to close the contour in the upper half plane. The residues theorem yields \( I_1 = 2\pi \sqrt{(1 - \zeta)/(1 + \zeta)}/\sqrt{a_1^2 - a_2^2} \) with \( \zeta = \sqrt{(a_1 + a_2)/(a_1 - a_2)} \). The calculation of the remaining integral,

\[
I_2 = b \int_{-\pi}^{\pi} dq \frac{\cos(qr)}{\omega_q^2},
\]

is similar and thus will not be reproduced. Adding both contributions we arrive at,

\[
\tilde{\chi}_{m+r\alpha mc}(0) = \frac{1}{\Delta} (-1)^{r+1} \left( 1 + \frac{4r}{3} \right) e^{-\frac{r}{\pi \Delta 17}},
\]

where \( \Delta = \omega_r \) is the gap of the chain in units of the exchange interaction. The sign of the interaction mediated by the AKLT spin chain changes according to the distance between the probes. This comes from the fact that the static correlations in this spin chain have a similar alternation. Since the effective coupling is given by \( J_p^2 \tilde{\chi}_{m+r\alpha mc}(0) \), we conclude that at \( T = 0 \) the probes get entangled whenever their distance corresponds to an odd number of sites.

What happens at \( T > 0 \)? The effective interaction vanishes so rapidly with the distance [see Eq. (4.50)] that any finite temperature will "thermalize" the probes: their partial state will be an uncorrelated mixed state in \( 2 \otimes 2 \). We can give an estimate of the critical temperature above which no LDE is expected; to do so, we restrict ourselves to temperatures much below the gap (remark that the
opposite limit would necessarily wash out the antiferromagnetic order and thus LDE. In this case, we do not expect real excitations of the spin chain to be present: only the subspace of states described by $\hat{H}_{\text{eff}}$ [Eq. (4.19)] will be populated and then we may calculate the correlations between the probes using

$$\rho_{ab} \simeq e^{-\beta J_{mn} \tau_a \cdot \tau_b} \frac{\text{Tr}[e^{-\beta J_{mn} \tau_a \cdot \tau_b}]}{\text{Tr}[e^{-\beta J_{mn} \tau_a \cdot \tau_b}]} \tag{4.51}$$

with $\beta^{-1} = k_B T$. This defines a temperature, $T^* \equiv 1/(k_B \beta^*)$, above which entanglement disappears. PPT yields: $\beta^* J_{mn} \simeq 0.27$ where $J_{mn}$ is the effective coupling of probes interacting with sites $m$ and $n$ and $|m-n|$ is an odd integer. This corresponds to a very low temperature because $J_{mn} \sim (J_p^2/\Delta) f_{mn}$ is exponentially suppressed for large distances, $f_{mn} \simeq |m-n| \exp(-|m-n|/\xi_{\text{AKLT}})$. Thus, quasi-perfect LDE will be present at $T \ll \Delta$, more precisely when

$$k_B T^* \ll \frac{J_p^2}{\Delta} e^{-r/\xi_{\text{AKLT}}} \tag{4.52}$$

This is to be compared to the AF half-integer spin chain of the previous section for which the criterion on temperature for quasi-perfect LDE reads,

$$k_B T^* \ll \frac{J_p^2}{\Delta} \chi_0 / L \tag{4.53}$$

The latter is a weaker constraint since $\chi$ is very large for $r/L < O(1)$ (Fig. 4.4). We then conclude that, at realistic temperatures (even if much smaller than $\Delta/k_B$), distant probes will display more entanglement when weakly coupled to the $S = 1/2$ spin chain. This situation should be rather insensitive to the actual microscopic model of the spin bus for the fast decay of correlation functions of gapped systems reflects into the large distance behaviour of the susceptibility $\chi$. On the other hand, having a large intrinsic gap, the AKLT chain allows to consider larger couplings and yet being well inside perturbation theory limits. It is in the interplay between a large gap (and thus the possibility of considering higher $J_p$) and a large DC susceptibility (and thus the possibility of quasi-perfect LDE) that a better performance may be achieved. At temperatures strictly zero both spin chains will mediate quasi-perfect entanglement for $J_p^2 \ll \Delta/\chi_{m+zmc}(0)$, which is the main result of the present chapter.

4.4. Concluding remarks

In this chapter we have learned that 1D spin chains are able to entangle two distant spin-1/2 probes which did not interact directly. At $T = 0$ this entanglement is nearly maximal, an attractive situation for quantum communication and computation. This was done by implementing an adequate perturbation theory and holds whenever the following conditions are met:
4. Entanglement mediated by the ground-state of gapped spin chains

1. the bus-probe coupling is small compared to the relevant energy scales of the many-body system, $J_p \ll J$;
2. the effective coupling is small compared to the gap, $J_p^2 \tilde{\chi}_{mc;zz}(0) \ll \Delta$;
3. the system is effectively at zero-temperature, $k_B T \ll \Delta$;
4. the system’s correlations are asymptotically antiferromagnetic so that $\tilde{\chi}_r(0) > 0$, for large $r$.

We have considered $SU(2)$ systems with full rotational symmetry for they generally lead to larger amounts of LDE even at $T = 0$. As an example of a system without full $SU(2)$ symmetry, think about the Heisenberg spin-1/2 chain in field:

$$H_0 = \sum_{i=1}^{L-1} \vec{S}_i \cdot \vec{S}_{i+1} + h \sum_{i=1}^{L} S^z_i.$$

This system entails extra terms in the effective Hamiltonian even in first order perturbation theory [see Eqs. (C.6) and (C.15)]. Also, the $SU(2)$ invariance of the second-order term in the effective Hamiltonian is broken:

$$H_{\text{eff}}(h) = J_p^2 \tilde{\chi}_{xx}(0) \left( \tau^i_a \otimes \tau^i_b + \tau^i_b \otimes \tau^i_a \right) + J_p^2 \tilde{\chi}_{zz}(0) \tau^i_a \otimes \tau^i_b + J_p \langle S^z_i \rangle \left( \tau^i_a \otimes 1_b + 1_a \otimes \tau^i_b \right).$$

The local term above being proportional to $J_p$ dominates for $h$ not to small, yielding aligned (and hence, separable) probes. The case $h \ll J$ will also lead to less probe entanglement because the susceptibilities are not isotropic. The present example, although being a particular case, can be easily extended to other non-rotational invariant spin chains, confirming our argument regarding the importance of spin symmetry.

The present chapter focus on 2 probes that interact with a many-body system. This treatment, however, can be easily extended to include $N > 2$ probes. In the latter scenario, assuming global rotational symmetry and homogeneous probes-system couplings, the effective Hamiltonian [Eq. (4.19)] reads instead,

$$H^{(abc...)} = J_p^2 \sum_{i<j} \tilde{\chi}_{ic;ij}(0) \vec{\tau}_i \cdot \vec{\tau}_j.$$

Within Hamiltonian $H^{(abc...)}$, many multipartite entangled states can be engineered by properly choosing the many-body system and the probes locations. It would be interesting to study the possibility of generating cluster states — these states arise when spins of Ising quantum lattices are initially prepared in a special state $|162\rangle$; their entanglement is very robust in the sense that $N/2$ qubits must be measured (for instance, by the environment) as to completely turn the state separable. Cluster states are very attractive for quantum computation purposes but are very difficult to implement in the laboratory. The alternative of sending probes that would weakly interact with a large system in equilibrium (like those considered in the present chapter), which does not need to be "reset" in a special state, deserves further study.
4.4. Concluding remarks

Still regarding the important case of $N = 2$ some important questions where not answered in the present chapter. Namely,

- What is the specific dependence of entanglement with the relevant physical parameters? How does it vary with the coupling?
- What happens in 2-dimensions where symmetry breaking is known to exist at $T = 0$ for large systems?

Both questions will be addressed in the following chapter. Systems where the gap approaches zero in the thermodynamic limit, accomplish long-range (or quasi-long range) correlations and thus large susceptibilities, but the perturbative regime requires very weak couplings. It turns out that increasing the coupling suppresses LDE very generally because of entanglement monogamy (Sec. 4.2), suggesting that the validity of perturbation theory coincides with the conditions leading to larger LDE. Regarding 2D spin lattices, we can expect LDE to be lessened; models with symmetry breaking in the thermodynamic limit will lead to a finite sub-lattice magnetization, which would be perceived as a local magnetic field by the probes. This should reduce entanglement even in the finite size scenario for sufficiently large lattices. The next chapter will disclose some surprises regarding the role of dimensionality in this problem.

Finally, we make a remark about the distinct roles of the bath in the present problem and the opto-mechanical problem of Chapters 2 and 3: there we had two large systems interacting directly and the continuous monitoring of a bath resulted in a dilution of entanglement, whereas here we have two small particles that not interact directly and get highly entangled via the bath. Indeed, entanglement can arise between two quantum systems which interact directly, but also can be transferred from highly correlated many-body ground states to particles that otherwise would be separable.
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5. Finite temperature entanglement mediated by 2D antiferromagnets

This chapter is based on the following publication by the author:

Emergence of robust gaps in 2D antiferromagnets via additional spin-1/2 probes, AIRES FERREIRA, J. Viana Lopes, and J. M. B. Lopes dos Santos, submitted to PRL (2009).

5.1. Overview

The complex interplay between many degrees of freedom in solid state represents a vast laboratory to test the quantum-classical boundary. In the previous chapter an example of quantum behaviour was studied: entangled ground states of many-body systems induce quantum correlations in qubits — a non-trivial effect that interactions mediated by mesoscopic (and macroscopic) systems can actually produce more than classical correlations between external parties. Apart from the fundamental issues, solid state systems have been exploited for their applications, especially those related to quantum computing and information processing.

Solid state quantum computing relies upon the possibility of generating some kind of entangled state, sufficiently robust not to suffer complete decoherence from local noise or a global environment. One possibility is to use the low-lying energy states of a many-body system as qubits, albeit the decoherence mechanisms are generally very complex and far away from being completely understood in this case.

A good chance of maintaining quantum coherence, though, comes about when the qubits states are separated from the rest of the spectrum by a large gap; when this happens the effect of temperature, and thus decoherence, is highly restrained. In this regards, widespread attention has been paid to carbon-based solid state; for instance, diamond has been shown to be a realistic candidate to quantum computing at room temperature: spins in the vicinity of a single nitrogen-vacancy defect in diamond can be manipulated to the extent of creating entangled states between electron and nuclear spins that lasts for times as large as milliseconds, although no simple method to scale up this system is presently known [97, 163, 164].
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Moreover, a considerable body of work has been devoted to systems of spins-1/2 experiencing nearest-neighbor interactions, since they can be used as models for universal quantum computation meeting (at least partially) the DiVicenzo’s requirements (see Sec. 4.2 and also [122, 165, 166, 167]). Spin chains have been shown to be extremely versatile; for instance, they allow to transfer reliably the state of a single qubit [121] and, as shown by DMRG simulations [123, 124], their ground-states are able to mediate an effective long-distance interaction ultimately entangling distant spin probes.

The LDE phenomenon was the focus of the previous chapter, where we learned that spin-1/2 probes, interacting locally with a large spin system, can get highly correlated if they interact sufficiently weakly as to not destroy completely the bulk’s ground state: a very small quantity of entanglement is extracted from the bulk which is sufficient to force the probes towards a quasi-perfect singlet. Our results constitute the first analytical support for LDE mediated by ground states of large many-body systems and suggest that, like in the case of dynamical evolution of two qubits interacting with a bath of harmonic oscillators [129], the role of the bus gap is crucial.

We have seen that a finite-size gap (in systems where the gap vanishes in the thermodynamic limit) is convenient, whereas in systems with intrinsic massive excitations a large gap results in fast decaying correlations. The latter reduces the effective coupling, and hence the robustness of entanglement at \( T > 0 \). The results of Sec. 4.3 encourage us to consider more general possibilities and investigate with more detail the role of the gap and the non-perturbative regime.

5.2. Non-perturbative theory from adiabatic continuity

In Sec. 4.3 by means of standard condensed matter methods, we computed the effective Hamiltonian of interaction between probes that interact weakly with a gapped many-body system. This was sufficient to conjecture quasi-perfect LDE in the limit of weak coupling, and also to give estimates of critical temperatures above which probes entanglement would vanish [recall Eqs. (4.51)-(4.53)]. However, as we have mentioned, the effective Hamiltonian does not suffice to compute the density matrix (for reasons that will become clear in the course of the present section). Here we overcome this limitation by developing a simple non-perturbative theory describing very faithfully numerical results for LDE.

The problem of computing the partial state of the probes is complex even in perturbation theory; efficient finite temperature methods apply almost exclusively to high-temperatures for any expansion of the partition function, or density matrix, requires \( \beta E \ll 1 \). But in this limit, entanglement in systems endowed with a small Hilbert space, like two spin-1/2 probes, is totally destroyed — high-temperature entanglement (i.e. above natural energy scales of the system) can only be achieved in macroscopic systems or in systems where subpurity is justified, as shown in the first part of this thesis (see Chapters 2 and 3). In \( 2 \otimes 2 \) systems, separability is equivalent to PPT (Sec. 1.3.3) defining a critical temperature \( (T^*) \) above which probes correlations become classical: \( \beta^* J_{ab} \simeq 0.27 \), where \( J_{ab} \)
is the coupling energy between the qubits (Sec. 4.3.2).

We start by considering many-body systems of spins (which we will designate often by bath) with rotational invariant Hamiltonian $H_0$, and a singlet, non-degenerate ground state, $|\psi_0\rangle$. As before, the two probes, $\tau_a$ and $\tau_b$, are coupled to the bath by Heisenberg exchange interaction with strength $J_p := J\alpha$, through sites A and B, respectively,

$$V = \alpha J \left( \hat{S}_A \cdot \tilde{\tau}_a + \hat{S}_B \cdot \tilde{\tau}_b \right),$$

(5.1)

where $J$ denotes an energy scale of the bath (typically its exchange interaction) and $\alpha$ is a dimensionless parameter. We make the simple but crucial assumption that there is a one-to-one map of eigenstates of the uncoupled system ($\alpha = 0$) to the eigenstates of the full Hamiltonian, i.e. we invoke adiabatic continuity [168]. Hence, we define a canonical transformation between the two basis:

$$|\psi_m\rangle \otimes |\chi_{ab}\sigma\rangle = e^{-i\hat{S}}|\Psi_{m,\sigma}\rangle,$$

(5.2)

where $|\psi_m\rangle$ is a bath-only eigenstate, $|\chi_{ab}\sigma\rangle$ a probe state, and $|\Psi_{m,\sigma}\rangle$ an eigenstate for finite $\alpha$. Note that the generator $\hat{S}$ is an operator acting on both probe and bath space. This map has important consequences; the transformed Hamiltonian must have the form of a sum of a probe-only term ($H_p$) with a bath only term ($H'_b$), that is

$$H_S = e^{-i\hat{S}}(H_0 + V) e^{i\hat{S}} = H_p + H'_b,$$

(5.3)

since the corresponding eigenstates are product states. We now add the assumption that the lowest lying states, which map to a probe singlet and probe triplet,

$$|\Psi_{0,s}\rangle = e^{-i\hat{S}}|\psi_0\rangle \otimes |\chi^s\rangle,$$

(5.4)

$$|\Psi_{0,m}\rangle = e^{-i\hat{S}}|\psi_0\rangle \otimes |\chi^m\rangle \quad m = 0, \pm 1$$

(5.5)

are well separated from states which map to excited states of the bath by a "robust gap", $\Delta(\alpha)$. In other words, we assume that the bath+probes system has a low energy manifold isomorphic to the probe space, well separated in energy from the remaining energy spectrum. This could seem a strong restriction, but, on rather general grounds, rotational invariance implies a non-degenerate singlet of total spin, at least in systems with translational invariance as implied by Marshall’s theorems [151]. Our bath+probes problem breaks translation invariance (ultimately due to the probes), but we will see here also the spectrum exhibits a singlet-triplet low energy sector, well separated from the excited

A non-perturbative analytic approach comes with the expense of loss of generality; whereas in the previous chapter we developed a perturbative approach valid for any gapped system, here we will develop a theory that applies to systems with rotational invariance. On the other hand, as we have argued, rotational invariant buses with antiferromagnetic order are precisely the systems potentially attaining large amounts of LDE. Thus, our results will apply in most of the interesting scenarios.
5. Finite temperature entanglement mediated by 2D antiferromagnets

Figure 5.1.: The schematic of the canonical transformed many-body spectrum (at right) under the assumptions of adiabatic continuity and robust gap, $\Delta(\alpha) > 0$. If one succeeds in finding the matrix elements of $\hat{S}$, the low-energy physics of our problem will be described by an effective Hamiltonian containing just the probes canonical singlet and triplet states.

states.

The exact density-matrix of the qubits (the partial state of the probes, $\rho_{ab}$) encodes the full-capabilities of a generic lattice as a quantum bus (in particular, the possibility of LDE):

$$
\rho_{ab} = Z_{ab}^{-1} \text{Tr}_{\mathcal{L}} \left[ e^{-\beta (H_0 + V)} \right].
$$

The trace is made with respect to the degrees of freedom of the bath, $\mathcal{L}$, and

$$
Z_{ab} = \text{Tr}[\exp(-\beta H_0 - \beta V)]
$$

is the system’s partition function. In our case, global $SU(2)$ symmetry implies a very simple form for $\rho_{ab}$,

$$
\rho_{ab} \propto \exp(-\beta J_{ab}(\beta) \mathbf{\tau}_a \cdot \mathbf{\tau}_b),
$$

where $J_{ab}(\beta)$ is the actual effective coupling of the probes (not to be confused with the effective coupling in perturbation theory). As soon as this function is known, bipartite entanglement can be computed directly $\rho_{ab}$ using the negativity [or any other entanglement monotone, see e.g. Eq. (1.57)]. The $SU(2)$ spin symmetry of our problem implies that entanglement will be given directly by the probe correlation:

$$
\langle \mathbf{\tau}_a \cdot \mathbf{\tau}_b \rangle = \text{Tr}[\rho_{ab} \mathbf{\tau}_a \cdot \mathbf{\tau}_b] = \frac{e^{-4\beta J_{ab}(\beta)} - 1}{e^{-4\beta J_{ab}(\beta)} + 1/3}.
$$
5.2. Non-perturbative theory from adiabatic continuity

5.2.1. From renormalized spins to real spins

In the previous chapter we approximated the partial state by $\rho_{ab} \propto e^{-\beta \hat{H}_{\text{eff}}}$, and hence the effective coupling $J_{ab}(\beta)$ was temperature independent [see Eq. (4.51) and Eq. (4.19)], i.e. we have assumed\(^2\) $J_{ab}(\beta) \approx J_p^2 \tilde{\chi}_{ab}^z(0)$ for $\beta \Delta(0) \gg 1$. According to this prescription the probes correlation, $\langle \tau_a \cdot \tau_b \rangle$, for instance, would be computed from $\rho_{ab}$ via,

\[
\langle \tau_a \cdot \tau_b \rangle = \frac{\text{Tr}[e^{-\beta \hat{H}_{\text{eff}}}(\tau_a \cdot \tau_b)]}{\text{Tr}[e^{-\beta \hat{H}_{\text{eff}}}]}, \tag{5.10}
\]

The procedure $\rho_{ab} \propto \exp(-\beta \hat{H}_{\text{eff}})$ only provides a rough estimate to the probes state, even in perturbation theory ($J_p \ll$ energy scales), though. Let us see why using a quick argument based on the zero temperature limit and QI reasoning.

When the probes are antiferromagnetically correlated, $\tilde{\chi}_{ab}^z(0) > 0$, according to the latter approximation, one has,

\[
\lim_{\beta \to \infty} \langle \tau_a \cdot \tau_b \rangle = -3, \tag{5.11}
\]

in which case, their partial state is a perfect singlet with zero linear entropy: $S_L(\rho_{ab}) = 0$ [Eq. (1.11)]. This result does not depend on how accurate is our estimate of the low-temperature limit of $J_{ab}$, for we would obtain the same value provided that $J_{ab} > 0$ is temperature independent. On the other hand, the probes are also correlated (even if weakly) with the spin bath by virtue of the local coupling [Eq. (5.1)]: tracing the degrees of freedom of the bath [Eq. (5.6)] then introduces residual entropy in $\rho_{ab}$, and hence $S_L(\rho_{ab}) > 0$ contradicting Eq. (5.11).

To investigate the roots of this apparent ambiguity, we compute the connected correlation between the probes under the adiabatic assumption and compare it with (5.10) [obtained from the approximation, $\rho_{ab} \propto \exp(-\beta \hat{H}_{\text{eff}})$]. This is achieved by recasting the correlation [Eq. (5.9)] into a form involving the effective Hamiltonian $H_S = H'_b + H_p$. To this end, we make use of the canonical transformation [Eq. (5.2)] to get

\[
\langle \tau_a \cdot \tau_b \rangle = \frac{\text{Tr}[e^{-\beta H_S}(e^{-i\hat{S}} \tau_a \cdot \tau_b e^{i\hat{S}})]}{\text{Tr}[e^{-\beta H_S}]}. \tag{5.12}
\]

From our assumption that the lowest energy sector is mapped to a probe singlet and probe triplet [see Eqs. (5.4)-(5.5)], it is clear that the canonical transformed Hamiltonian must be a scalar in the probes operators, that is $H_p \sim \tau_a \cdot \tau_b$, hence having the same form we found in perturbation theory [$H_{\text{eff}} \sim \tau_a \cdot \tau_b$]. The bottom line comes from the observation that the scalar product entering in $H_S$ (via the term $H_p$) is not the same operator inside brackets [in Eq. (5.12)], for

\[
e^{-i\hat{S}} \tau_a \cdot \tau_b e^{i\hat{S}} = \tau_a \cdot \tau_b - i [\hat{S}, \tau_a \cdot \tau_b] + ... . \tag{5.13}
\]

\(^2\)To simplify notation, from now on, the probe’s susceptibility [Eq. (4.15)] will be simply denoted by $\tilde{\chi}_{ab}^z(0)$. 

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We conclude that, in second order perturbation theory, the correlation computed from Eq. (5.10) will just yield a valid approximation to the exact correlation (5.9) in situations where \( e^{-i\hat{S} \cdot \tau_a e^{i\hat{S}}} \simeq \tau_a \cdot \tau_b + O(\alpha^3) \). In general, however, \( \hat{S} \) (containing bath and probes operators) will give rise to terms not proportional to \( \tau_a \cdot \tau_b \); we can anticipate they will reduce the correlation (5.11) at any temperature and henceforth also diminish the LDE capability of generic spin baths.

In summary, the effective Hamiltonian correctly accounts for the shifts in energy due to the probes and for the possibility of LDE, but, by itself, fails in giving the exact probes partial state; one must take also in consideration the way the operators change (even in perturbation theory). Doing so, one finds that, in the previous chapter, the renormalized spins were taken as being original spins, which is only an approximation.

Further insight on the canonical transformation and its relation with perturbation theory can be found in Appendices D.1, D.2 and D.3. In what follows we analyze the effect of spin renormalization in the partial state of the probes.

5.2.2. The canonical parameters

We learned that the spin operators must be renormalized if one wishes to get averages corresponding to real spin degrees of freedom (that is, spin operators have to be conveniently transformed according to \( \hat{S} \)). This is consistent with perturbation theory (Appendix D.1) for the wave functions also change according to:

\[
|\Psi(S_2)_0\rangle = e^{-iS_2} |\Psi_0\rangle,
\]

where \( S_2 \) is an appropriate generator in second order perturbation theory.

We move gears to the study of the probe correlation (5.12) under the robust gap assumption. Also, connections to previous perturbative results will be made when relevant. We start by introducing new notation for the renormalized spins; we will denote them as \( \tau_{a(b)}^R \) to distinguish from the real spin operators [those appearing in Eq. (5.8)]:

\[
\tau_{a(b)}^R := e^{-i\hat{S}_a} \tau_{a(b)} e^{i\hat{S}}.
\]  

(5.14)

Using symmetry alone, we can relate the scalar product involving real and renormalized spins. The formal derivation is done in Appendix D.2 [see Eqs. (D.34)-(D.44)]; here is sufficient to observe that taking averages with respect to the spin bath GS, \( \langle \psi_0 | \cdots | \psi_0 \rangle_{\text{bath}} := \langle \cdots \rangle_{\text{bath}} \), effectively integrates out the bath and yields the low-energy physics of the probes, when the robust gap assumption is verified [see Eqs. (5.4) - (5.5) and comments therein]. We have,

\[
\langle e^{-i\hat{S} \cdot \tau_a e^{i\hat{S}}} \rangle_{\text{bath}} = \eta \mathbb{1}_{2 \otimes 2} + (1 - \Phi) \tau_a \cdot \tau_b,
\]

(5.15)

with \( \eta = \eta(\alpha) \) and \( \Phi = \Phi(\alpha) \) real and bounded. The reason why other operators do not enter in formula (5.15) is because the canonical transformation \( \hat{S} \) will necessarily produce rotational invariant
5.2. Non-perturbative theory from adiabatic continuity

probe operators (and there are just two in $2 \otimes 2$, namely the identity and the scalar product).

The probes correlation is obtained by averaging the latter equation. It is instructive to consider the zero temperature case,

$$\langle \tau_a \cdot \tau_b \rangle_{T=0} = \langle \Psi_{0,s} | \tau_a \cdot \tau_b | \Psi_{0,s} \rangle$$

(5.16)

$$= \langle \chi', \psi_0 | \tau_a^R \cdot \tau_b^R | \psi_0, \chi' \rangle$$

(5.17)

$$= -3 + \eta + 3 \Phi.$$  

(5.18)

The last equality implies the restriction: $4 \geq \eta + 3 \Phi \geq 0$. The scenario of perfect entanglement, $E(\rho_{ab}) = 1$, requires $\eta + 3 \Phi = 0$. Indeed, considering the approximation of the previous chapter, namely Eq. (5.10), is equivalent to take $\tau^R_a(b) \simeq \tau_a(b)$, which results in quasi-perfect AF correlations for $T = 0$:

$$\langle \tau_a \cdot \tau_b \rangle_{T=0} = \langle \Psi_{0,s} | \tau_a \cdot \tau_b | \Psi_{0,s} \rangle \simeq \langle \chi', \psi_0 | \tau_a \cdot \tau_b | \psi_0, \chi' \rangle = -3.$$  

(5.19)

This approximation is strictly valid when $\eta \simeq \Phi \simeq 0$. We will refer to $\eta$ and $\Phi$ as the canonical parameters (or canonical corrections); they relate the correlation of the renormalized spins and the correlation of real spins:

$$\langle \tau_a \cdot \tau_b \rangle = \eta + (1 - \Phi) \langle \tau_a \cdot \tau_b \rangle_{can}.$$  

(5.20)

The term $\langle \tau_a \cdot \tau_b \rangle_{can}$ is obtained via the Gibbs ensemble constructed directly from $H_p$ and equals the correlations obtained via the approximation (5.10):

$$\langle \tau_a \cdot \tau_b \rangle_{can} = \frac{\text{Tr}_p \left[ e^{-\beta H_p} \tau_a \cdot \tau_b \right]}{\text{Tr}_p \left[ e^{-\beta H_p} \right]} = \frac{e^{-\beta J_{can}} - 1}{e^{-\beta J_{can}} + 1/3}.$$  

(5.21)

where we have employed the definition

$$J_{can} := \langle \Psi_{0,m} | H | \Psi_{0,m} \rangle - \langle \Psi_{0,s} | H | \Psi_{0,s} \rangle.$$  

(5.22)

Contrary to the real effective coupling, $J_{ab}(\beta)$, the canonical coupling, $J_{can}$, is now effectively temperature independent. Its value in second order theory is $J_{ab}/4$ [with $J_{ab} = J_p^2 \tilde{\chi}_{ab}^{zz}(0)$, see for instance Eq. (4.19)]. Equation (5.20) is however more general since it does not depend on the particular perturbation scheme: $J_{can}$ is in fact the gap at any order by construction [see the definition of $H_5$, Eq. (5.3): its energy scale, $4J_{can}$ in our notation, gives directly the gap between the singlet and triplet low-energy sectors; see also Eq. (D.45) and discussion therein].

Adiabatic continuity then entails a curious result: by measuring the correlations of the probes at different temperatures we can derive the many-body gap (in the presence of the probes), which equals the $T = 0$ DC spin response function, $\tilde{\chi}_{ab}^{zz}(0)$, in the weak coupling regime [Eq. (4.15)].

Even in perturbation theory, $\eta$ and $\Phi$ will play a role, and thus Eq. (4.51) is only valid if the canonical corrections are small [see Appendix D.2]. We thus expect quasi-perfect LDE to correspond to a
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very special scenario, that of η + 3Φ ≪ 1. Despite that, as long as the low-lying states are well protected by the remaining spectrum and the canonical corrections are not too large, we can still find a good amount of LDE, especially if the probe triplet is not populated at all, which happens when \( k_B T \ll J_{\text{can}} \).

Finally, we relate the real effective coupling defined by Eq. (5.8) with the canonical parameters. This is accomplished by equaling the right-hand sides of Eqs. (5.9) and (5.20) and solving for \( J_{ab}(\beta) \).

We get,

\[
J_{ab}(\beta) = \frac{1}{4\beta} \ln \left[ \frac{3(\Phi - \eta) + (4 - 3\Phi - \eta) \exp(\beta J_{\text{can}})}{4 - \Phi + \eta + (\Phi + \eta/3) \exp(\beta J_{\text{can}})} \right].
\] (5.23)

We thus have achieved a parameterization of the temperature dependence of \( \rho_{ab} \) as function of three parameters,

\[
\rho_{ab}(\beta) = \frac{1}{4} + \frac{1}{4} \left( \frac{\eta}{3} + (1 - \Phi) \frac{e^{-\beta J_{\text{can}} - 1}}{3e^{-\beta J_{\text{can}} + 1}} \right) \tau_a \cdot \tau_b,
\] (5.24)

which can be easily computed in perturbation theory (Appendix D.3):

\[
J_{\text{can}} \simeq (2J\alpha)^2 \hat{\chi}_{ab}^{zz}(0)
\] (5.25)

\[
\Phi \simeq (2J\alpha)^2 \sum_{m > 0} \left( \frac{1}{E_m - E_0} |\langle \psi_0 | (S_A^z - S_B^z) | \psi_m \rangle| \right)^2
\] (5.26)

\[
\eta \simeq 0 + O(\alpha^4 J^4 / \Delta^4).
\] (5.27)

The states of the spin bath are denoted by \( |\psi_m\rangle \) (with eigenenergy \( E_m \)) and \( \Delta := E_1 - E_0 \). The canonical parameters, for small \( \alpha \), can be computed by diagonalizing the spin bath Hamiltonian, \( H_0 |\psi_k\rangle = E_k |\psi_k\rangle \). This is however only possible in a few models whose analytical solution is known (e.g. the 1D XY model). In general, whether the canonical parameters describe the correlations of the probes accurately, for a given spin model, must be investigated by comparing result (5.20) [or equivalently, (5.23)] with numerical simulations. We recall that these results will only describe accurately LDE of probes interacting with large lattices if adiabatic continuity holds and a robust gap is available. The following section will show an impressive agreement between the canonical theory and simulations in a large family of AF spin systems, which therefore fulfil these two conditions.

A formal derivation of equations (5.26)–(5.27) is found in Appendix D.3; Eq. (5.25) is derived in Appendix D.1 via the canonical formalism. Finally, the renormalization of the spins is explained with detail in Appendix D.2.

5.3. LDE in 2D

Promising advances in the engineering of atomic structures and optical lattices, where finite spin systems are effectively realized in the laboratory, encourage the consideration of more general pos-
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Figure 5.2.: Left - Schematic picture of the opening of a robust gap, $\Delta(\alpha) \gg k_B T$, by two spin-1/2 probes that couple locally to the spin bath with arbitrary strength $\alpha J$. This is observed in all the spin lattices considered in the present section. If adiabatic continuity holds and the singlet is localized near the additional probes, they will be highly entangled even at large distances. In this case the singlet has a protection gap (triplet-singlet energy separation, $J_{\text{can}}$) which determines the robustness of LDE regarding temperature. Right - Schematic of the total system: the probes (blue) interact locally with a 2D lattice through sites A and B. How does the dimensionality of the spin bath will change the entanglement picture?

Possibilities. Indeed, we now consider AF spin systems, ranging from 1D chains to square lattices, and demonstrate the emergence of thermal probe entanglement. We link this phenomenon to the opening of robust gaps in the full many-body spectrum by means of the theory of the previous section. Robust gaps implies negligible thermal occupation of excited bus states in the entire range of temperatures in which the probes are entangled; we will see this allows LDE at higher temperatures than previously considered possible.

As in the previous chapter, we take the probes-bus coupling to be $SU(2)$ invariant (i.e. Heisenberg type). These interactions entail universal quantum computation [138] and are commonly realized in nature (e.g. in the parent compounds of copper-oxide high-temperature superconductors, such as the undoped insulator $La_2CuO_4$ [150]; in electronically coupled quasi-1D chains such as $CuGeO_3$ [169]; in the Mott insulating one-dimensional perovskite, $KCuF_3$ [170,171]; and also more recently in linear chains of $\sim 10$ manganese atoms in engineered structures [172]).

Our systems consist of 2D finite lattices $\mathcal{L}$, with $N = l \times n_c$ spins-1/2 and two extra probes, where $l$ is the number of longitudinal sites and $n_c$ stands for the number of coupled chains, varying from $n_c = 1$ (spin chain) to $n_c = l$ (square lattice), see Fig. 5.2 for a possible geometry. The Hamiltonian of the lattice is

$$H_0 = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j,$$

with $J > 0$. The qubit probes interact with the spins at the boundary of the most central chain (see Fig. 5.2) through an isotropic interaction [Eq. (5.1)]. We expect a significant change in LDE from the
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common one-dimensional scenario analyzed in the previous chapter (and numerically in [123,124]), as the physics of a 2D spin bath is very distinct.

In particular, the 2-leg ladder chain has an Haldane gap [151] which should play against a large $J_{ab}$ since very massive excitations, $\Delta \simeq 0.504 J$, make the correlations die particularly fast [173]. For these systems we are not able to make exact analytic computations. Thus, we will rely on Quantum Monte Carlo (QMC) simulations [174,175,176,177,178] and compare the results with the theoretical prediction [Eq. (5.23)].

We present the results for small probe-bath coupling, $\alpha = 0.05$, before venturing away from perturbation theory. The 1D scenario is of special interest as we have a conjecture in this case [Eq. (4.20)]; our choice of coupling entails, for $L = 20$ and $n_c = 1$: $J_{p}^2/\Delta \simeq 0.015 J$ (with $\Delta$ extracted from the DMRG results of [173]); well inside perturbation limits and thus our conjecture should hold. The numerical results indeed show probes almost maximally entangled (see Fig. 5.5), validating quasi-perfect LDE in the 1D system: the table below shows the canonical parameters for representative lattices when $\alpha = 0.05$.

| System         | Intrinsic (Haldane) gap | The probes gap: $J_{can}$ | $\Phi$ correction | $\eta$ correction |
|----------------|-------------------------|---------------------------|-------------------|------------------|
| spin chain     | no; $\Delta/J \simeq 3.2/L$ [*] | $5.07 \times 10^{-4}J$ | $1.03 \times 10^{-2}$ | $6.23 \times 10^{-4}$ |
| square lattice | no; broken phase for $L \gg 1$ | $3.04 \times 10^{-3}J$ | $1.46 \times 10^{-1}$ | $-1.34 \times 10^{-2}$ |

Table 5.1.: The canonical parameters in representative systems for $\alpha = 0.05$. The canonical parameters are calculated by fitting the QMC data for different temperatures with Eq. (5.20). [*] This expression was taken from Ref. [173].

We observe almost perfect AF correlations in the 1D scenario, since $3\Phi + \eta = O(10^{-2})$ is very small and thus $\langle \tau_a \cdot \tau_b \rangle \simeq -3$ [Eq. (5.11)], and no entanglement mediated by the 2-leg and 4-leg ladders. Regarding these ladders, the numerical results are well-inside what we could expect: the probe correlation is nearly zero in the whole temperature range, a consequence of a very small $J_{can}$ (the fits yield $J_{can} \sim 10^{-5}J$) resulting from an exponentially decaying $\tilde{\chi}_{ab}(0)$ (recall discussion of the gapped AKLT model, Sec. 4.3.2). Indeed, the probes cannot take advantage of the AF coupling mediated by the system: the probes gap, $J_{can}$, is too small so that entanglement survives at finite (even though small) temperatures $T > 0$.

The values in the table show a curious property of the 2D spin system: a remarkable high $J_{can}$ for a system with such a small gap. Moreover, the canonical correction $\Phi$ is sufficiently small as to not delocalize completely the probes singlet. This leads, with the help of a strong $J_{can}$, to more robust LDE against temperature! Let us investigate these issues more carefully.

As an entanglement monotone we adopt the concurrence [see Eq. (1.53) for definition and Ref. [24]].

3These simulations were performed with the library “looper” from the ALPS (Algorithms and Libraries for Physics Simulations) project.

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for a closed expression because it yields an handy expression in systems with rotational symmetry:

\[ E_C = \max [0, |\langle \mathbf{\tau}_a \cdot \mathbf{\tau}_b \rangle|/3 - \langle \mathbf{\tau}_a \cdot \mathbf{\tau}_b \rangle/6 - 1/2] \in [0, 1]. \]  

(5.29)

Using the values of \( \langle \mathbf{\tau}_a \cdot \mathbf{\tau}_b \rangle \) extracted from the QMC simulations, we can compute LDE via the concurrence. For instance, the values of the canonical corrections in table 5.1 yield for the spin chain at zero temperature: \( E_C \approx 0.985 \). In this case the singlet is localized at the boundary sites (the probes) and thus the mechanism for LDE is optimal; since the singlet is already localized at the probes, before the canonical transformation, the renormalization of spins will not change much the density matrix given by the old expression of Eq. (4.51).

We represent the most important physical parameters for the entire family of lattices in Figure 5.3, namely \( J_{ab} \) (for the highest temperature considered in the simulations) and the critical temperature above which LDE vanishes. The black triangles represent effective coupling, \( J_{ab} \) at a distance \( l = 20 \), as a function of \( n_c, \) number of transverse chains, and \( k_B T = 2 \times 10^{-3} J \); blue and red dots: critical temperature above which LDE vanishes. The error bars from QMC cannot be seen as they are typically below 1%.

Figure 5.3.: Black triangles: effective coupling, \( J_{ab} \), at a distance \( l = 20 \), as a function of \( n_c, \) number of transverse chains, and \( k_B T = 2 \times 10^{-3} J \); blue and red dots: critical temperature above which LDE vanishes. The error bars from QMC cannot be seen as they are typically below 1%.
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Figure 5.4.: Left - Canonical correction $\Phi$ for the same family of spin lattices of Fig. 5.3. The inset shows that the $\eta$ correction is negligible compared to $\Phi$; the bars represent an estimate of the error due to QMC fluctuations. The $n_c = 2$ and $n_c = 4$ systems are not represented since the data does not provide reliable values for canonical corrections. Right - The singlet protection gap for finite probe coupling ($\alpha = 0.05$) in blue and red dots. The critical temperature is represented (small black dots) for comparison.

reduce the amount of genuine quantum correlations shared by the probes. This is borne out by the results of the QMC simulations, shown in Fig. 5.5 where $J_{ab}$ (and hence entanglement) is found to decrease at low temperatures, when the number of chains increase. Nevertheless, at higher temperatures, the opposite occurs, $J_{ab}$ increases with $n_c$; this reflects the increase of the probes protection gap, $J_{can}$, for it sets the temperature scale at which entanglement vanishes.

Having shown the QMC results for 20 spin lattices, we now compare them with Eq. (5.23) for several temperatures and compute the entanglement via the concurrence expression [Eq. (5.29)]: Fig. 5.5 shows a perfect fit to the data. For sake of clarity, we have presented the agreement just for 4 lattices although all them show the same degree of accuracy. The observed linear dependence of $J_{ab}$ with the temperature for $T \to 0$ is easily understood: a zero temperature (finite) entanglement below the maximum value of 1 requires $J_{ab}/T \to constant$. This constant can be derived from Eq. (5.23), yielding,

$$\beta J_{ab} \xrightarrow{T \to 0} \frac{1}{4} \ln \left[ \frac{4 - 3\Phi - \eta}{\Phi + \eta/3} \right].$$

Thus, the canonical corrections ($\Phi$ and $\eta$) determine the low-temperature physics of the probes. From this expression it is clear that the quasi-perfect LDE phenomenon reported in the previous chapter can only happen for $3\Phi + \eta \simeq 0$, when $\beta J_{ab}$ is very large and thus, according to Eq. (5.9), $\langle \tau_a \cdot \tau_b \rangle_{T=0} \simeq -3$ [see also Eq. (5.18)]. This is a very special scenario which happens in 1D antiferromagnets and also in dimerized chains (see [179] for an analytical treatment in the latter scenario). The present results reveal that quasi-perfect LDE is also possible in the 3-ladder chain $3\Phi + \eta \simeq 0.007$. As soon as we approach the 2D scenario, the $\Phi$ correction gets larger (see Fig. 5.4) and a fraction of the entanglement is lost.
Figure 5.5.: The points in the plot (Left) show $J_{ab}$ as function of the temperature from QMC simulations for $\alpha = 0.05$. The lines (Right) stand for the fit with the expression given in Eq. (5.23); with $n_c = 1$ (blue), $n_c = 10$ (red), $n_c = 15$ (blue) and $n_c = 20$ (black). All curves saturate for the highest temperatures [Eq. (5.31)] and therefore entanglement (Right) vanishes much before our method becomes inaccurate. The agreement between the QMC data is excellent resulting in an average deviation of $\sim 0.1 \pm 1\%$ depending on the lattice.

In all our simulations, the value of $\eta$ is negligible (a careful inspection shows that the fits we present are virtually indistinguishable from the fits with $\eta = 0$ up to $\alpha \simeq 0.1$). In 2D, the correction $\Phi$ will be appreciable (Fig. 5.4) and the singlet will be only partially localized at the probes. Indeed, $\Phi$ measures the "delocalization rate".

The $n_c = 3$ spin system has the best singlet localization rate towards the probes, $\Phi \simeq 0.007$, of all systems simulated (see Fig. 5.4), yielding $E_C \simeq 0.99$ — note that for an odd number of coupled chains, the case of $n_c = 3$ is peculiar: increasing the number of chains increases the protection gap and $\Phi$, with the exception of the $n_c = 1 \rightarrow n_c = 3$ transition, where the entanglement becomes less robust regarding temperature ($J_{can}$ decreases) and more efficient at $T = 0$ ($\Phi$ also decreases).

For the highest temperatures simulated, the effective coupling saturates (Fig. 5.5) to a constant value, $J_{can}(1 - \Phi)/4$, when $\eta$ is negligible (i.e. not far away from the perturbation limit), suffering a slightly change with temperature otherwise,

$$J_{ab}(T) \simeq \frac{J_{can}}{4} \left(1 - \Phi\right) - \frac{k_B T}{12} \eta + O\left(\frac{J_{can}^2 \Phi}{k_B T}\right).$$  \hfill (5.31)

Entanglement between the probes, and thus LDE, will survive up to $\beta J_{ab}(\beta) \simeq 0.27$ (Sec. 1.3.3). An estimate of the critical temperature is obtained by noting that $J_{ab}(T)$ has already saturated when the

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\(^4\)Curiously, this behaviour is not altered by varying the coupling, in the entire range we have simulated: $\alpha \in [0.05, 0.2]$. In fact, for large $\alpha$, namely $\alpha = 0.2$, the discrepancy between the $n_c = 1$ and $n_c = 3$ lattices is quite significant: $\Phi \simeq 0.238$ against $\Phi \simeq 0.079$, respectively.
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The square lattice is the system with best thermal robustness regarding LDE, despite its appreciable delocalization rate, $\Phi \approx 0.146$; a fact explained by the emergence of a large singlet-triplet gap, $J_{can}$, which is about 6 times the protection gap of the single spin chain. The regime of high temperatures, $T \gtrsim \Delta (\alpha = 0)$, is not described by Eq. (5.23) anymore, which requires zero thermal occupancy of excited states of the spin bath, a crucial assumption of our analytical modelling. However, according to our estimate [Eq. (5.32)], no LDE is to be expected in this scenario, and hence $J_{ab}(\beta)$ should decrease with the temperature, at some point, and eventually drop to zero, yielding probes totally uncorrelated.

Figures 5.3 and 5.4 deal with relatively small probe-bath coupling, but the results presented so far are more general. For instance, choosing a sufficiently large $\alpha$ to strongly suppress the zero temperature entanglement, via partial frustration among the neighborhood of the bulk spins connected with the probes, we again find an excellent agreement with Eq. (5.23). For intermediate probe-bath coupling, $\alpha = 0.1$ and $\alpha = 0.2$, the measured concurrence is fitted with an expression derived from Eq. (5.20), as shown in Fig. 5.6. These results show that in all our measured systems, the condition of a robust gap is verified. This is surprising, particularly in the case of large lattices, which has a gap much smaller than $\alpha J$; one would not expect, in this situation, the appearance of a well protected singlet. The emergence of the robust gap has to be attributed to the coupling of the probes: the lowest singlet and triplet are pulled down from the rest of the spectrum, allowing a complete description of entanglement only in terms of these two energy levels.

On the other hand, whereas the strong coupling to the spin bath reduces the zero temperature entanglement, it also allows a larger split between the singlet and triplet, leading to entangled probes at much higher temperatures. Typically, exchange interactions in antiferromagnets can be of the order of $0.1 \text{eV}$, resulting in an effective coupling of the order of $0.3 \text{meV}$ for the square lattice ($l = 20$) at temperature $\sim 12 \text{K}$ and $\alpha = 0.2$. This is to be compared with the value of $0.01 - 0.1 \text{meV}$ achievable in quantum dot spins [136, 180] although decoherence effects in spin lattices can lessen this difference.

Regarding the quantum-classical transition in these systems, we see that the critical temperature (above which the correlations shared by the probes are completely classical) can be increased by a factor of 20 from a weakly coupled spin chain ($\alpha = 0.05$) to an intermediate coupled ($\alpha = 0.2$) 2D
5.4. Concluding remarks

In the present chapter we have answered the most important questions left open previously, namely the effect of a larger probe-bath coupling and the performance of 2D lattices towards long-distance entanglement. We have studied a family of 20 spin systems serving as quantum baths, including a single spin chain and a square lattice, and considered the effect of weak and moderate probe-bath couplings. We found an increase of the thermal robustness of probe entanglement in 2D systems, due to the emergence of robust gaps. This was achieved by combining QMC simulations in large systems and an analytical model derived from the Schrieffer-Wolff canonical transformation formalism. We concluded that the canonical parameters give an adequate parametrization of correlations (and hence entanglement). They are:

1. the probes singlet-triplet gap, $J_{sc}$, In perturbation theory, this equals the effective coupling, $J_{\text{eff}}$— a single parameter, which in Chapter 4 led us to the conjecture of quasi-perfect LDE in 1D systems (where no symmetry breaking exists). However, to achieve a correct parametrization of the probe correlation, two new parameters must be considered, namely:

2. the "singlet delocalization rate", $\Phi$, which provides a crucial correction to LDE is the main factor leading to the real effective coupling, $J_{ab}(\beta)$. In particular, we have seen that $\Phi$ is very small in 1D validating the earlier conjecture on quasi-perfect LDE.

3. the canonical correction $\eta$ — a constant contribution to the probes correlator [see Eq. (5.20)],

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Figure 5.6.: Concurrence, an entanglement monotone for qubits, as function of temperature for different lattices and couplings. Lattices supporting more entanglement at strictly $T = 0$ have worse performance at higher temperatures.
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which does not play a role for small probe-bath coupling.

In the concluding remarks of the previous chapter, we anticipated that symmetry breaking, a phenomenon occurring for 2D systems in the thermodynamic limit, would decrease the amount of quantum correlations even in the finite size scenario, perhaps completely destroying LDE. Here, we have seen that, indeed, the $T = 0$ entanglement considerably decreases in the square lattice, but that, at the same time, a robust gap emerges, allowing moderate entanglement at higher temperatures than previously thought to be possible.

Although a numerical study had already been performed before in Ref. [124], here we measured directly the correlator $\langle \tau_a \cdot \tau_b \rangle$ by QMC; have not assumed a low-lying spectrum consisting of a singlet and triplet states, but rather confirmed it. Moreover, here we have gone beyond the 1D scenario by considering a 2D family of antiferromagnets. We demonstrated that entanglement mediated in 2D is more efficient, at realistic temperatures, and identified the opening of protected singlet-triplet states (well separated by the remaining spectrum, Fig. 5.2) as the main cause. Our analytical model provides reliable fits up to $\alpha = 0.2$, meaning that robust gaps, $\Delta(\alpha) > 0$, separate the low-lying energy sector from excited states, quite generally in $SU(2)$ spin lattices spin systems.

These results entail that, for two spin-1/2 probes interacting with large many body systems, the quantum-classical boundary is very sensitive to the particular model describing the underlying effective physics of such systems, and also to the dimensionality. We have seen a curious interplay between the capacity towards LDE at strictly zero temperature and finite (realistic) temperatures. 2D systems offer the possibility to reach quite large long-distance effective couplings, boosting entanglement, at temperature as high as $k_B T \sim \frac{1}{100} J$, where $J$ is the energy scale of the system’s exchange interaction.
6. Final Remarks

In this thesis we have applied Quantum Information tools to investigate the characteristics of the quantum-classical boundary in two distinct scenarios:

— a thermalized moveable mirror, in a cavity geometry, interacting via radiation-pressure with confined photons;

— a family of antiferromagnetic spin systems, with variable geometry, interacting with two-level systems.

Our motivation stemmed from promising developments in experimental physics, paving the way for the demonstration of genuine quantum effects beyond the microscopic domain.

While interference was observed in large molecules, it has been very difficult to overcome this barrier and even seek for similar phenomena in different contexts. The main obstacle is the existence of many channels of decoherence in systems endowed with large effective Hilbert spaces, for their internal degrees of freedom can be activated at any time by the environment, leading to dissipation and lost of coherence. A few notable exceptions do exist: in diamond defects, for instance, spins can exploit the large electronic gaps of these materials to maintain coherence for long times, or to get entangled with nuclear spins. Quite generally, however, the observed quantum effects fade away when the complexity increases.

The contribution of this thesis to the debate in the field was to develop methods based on the entanglement approach, to investigate the possibility of establishing quantum correlations at finite temperature in complex systems. The major conclusion emerging from these methods is that our bipartite systems, albeit very different energy scales, can attain entanglement at thermal equilibrium.

In the opto-mechanical scenario this arises due to the particularly robust radiation-pressure interaction and to the possibility of feeding continuously the cavity with many photons. In the two spins-1/2 interacting with large spin lattices, the possibility of high-quality entanglement, at moderate spin-lattice coupling, is due to the emergence of a protected singlet well separated from excited states.

The exact place where the quantum-to-classical transition takes place can be manipulated, within the limits imposed by Quantum Mechanics:

— by adding a coherent driving source, and considering non-zero source-cavity detuning, which
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results in stationary cavity-mirror entanglement at higher temperatures, in the opto-mechanical problem;

— by considering $SU(2)$ symmetric interactions and increasing the dimensionality of the bulk spin system, leading to entanglement at higher temperatures, in the problem of entanglement mediation by spin systems.

These studies are far from being exhaustive, and many questions are left open. Some possible lines of research have been mentioned throughout this monograph. Here we add two more regarding many-body systems: how does the "robust gap" picture changes by considering dimerization and frustration in the spin lattice? These mechanisms are common in magnetic compounds, and its effects on the generation of long-range correlations deserves further study. Also, we believe that the inspection of three-body correlations of bulk spins, via an entanglement approach, can give further insight on the properties of many-body systems, in the same manner that the study of entanglement entropy between regions in spin chains led to a better understanding of the efficiency of numerical methods. Up to our knowledge this is an unexplored field and may reveal nice surprises regarding the phases of matter.

Regarding entanglement between macroscopic systems, at the moment, physicists are approaching the first experimental demonstrations of quantum effects in macroscopic mechanical oscillators, and hence the results of the present thesis may be tested in the laboratory in the near future. It is thus important to consider feasible generalizations of our setup endeavoring to obtain larger amounts of entanglement. One possible route is to manipulate the cavity field statistics by changing the driving pump characteristics — there is plenty of room for entanglement in the cavity-mirror Hilbert space, as we have seen in this monograph.

In summary, we showed that entanglement can in principle exist between two quantum systems which interact directly, despite one of them being massive, and it can also be transferred from macroscopic systems to particles that otherwise would share classical correlations. These results suggest that macroscopic quantum behavior beyond the microscopic world is not restrict to collective phenomena, such as Bose-Einstein condensation, but can arise between two distinct systems, as long as a sufficient control of decoherence is achieved.
A. Appendices for chapter 2

A.1. The standard quantum limit

This appendix will be useful for the reader new to quantum measurements. It attempts to make a brief outline of single quantum measurements when applied to macroscopic systems. This section will be based on reviews and textbooks by Braginsky who greatly contributed to the field of high precision measurements [70, 81, 113].

The SQL can be defined as the ultimate precision an experimentalist has to achieve if he wishes to probe quantum effects of macroscopic objects. As pointed out many times by Braginsky, it is clear that a macroscopic body will behave the more quantum mechanically the more precise we measure it. On the other hand, the more precise a physical quantity, such as the position, is measured the more disturbed the system being measured gets. It is in the interplay between the maximum possible accuracy (in order to probe the quantum world) and the uncertainty principle that the SQL arises.

Following [70] let us derive the SQL for an harmonic oscillator (representing, for instance, a single-mode of a mechanical oscillator with natural frequency $\omega$ and mass $m$). The Hamiltonian of the harmonic oscillator with generalized coordinates $Q$ and $P$, satisfying $[Q, P] = i\hbar$, reads:

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2Q^2.$$  \hfill (A.1)

The Heisenberg equations of motion produce the following evolution for the generalized position:

$$Q(t) = q_1 \cos(\omega t) + q_2 \sin(\omega t),$$  \hfill (A.2)

where $q_1 = Q(0)$ and $q_2 = P(0)/(m\omega)$ are the initial values of the mode’s quadratures. The Heisenberg uncertainty relation, $\Delta P(0)\Delta Q(0) \geq \hbar/2$ [with $\Delta O$ meaning the usual root-mean-square deviation of the mean value of operator $O$, i.e. $\Delta O = \sqrt{\langle (O - \langle O \rangle)^2 \rangle}$] entails a similar relation for the quadratures, namely $\Delta q_1 \Delta q_2 \geq \hbar/(2m\omega)$. In this scenario, the SQL is defined as the best precision an experimentalist may achieve if he/she wishes to monitor $Q(t)$ with a precision which is time-independent. Indeed, according to Eq. (A.2) this implies that the experiment must be designed as to measure both mode quadratures, $q_1$ and $q_2$, with equal precisions: $\Delta q_1 = \Delta q_2$. The SQL therefore
reads,

$$\Delta Q_{\text{SQL}} = \Delta q_1 = \Delta q_2 = \sqrt{\frac{\hbar}{2m\omega}},$$

(A.3)

and equals the ZPF. The SQL is then the best possible time-independent accuracy we can reach in monitoring the position of the mechanical oscillator. When the oscillator is in a heat bath, the SQL depends crucially on the measurement time (in general will depend on the specific measurement apparatus) and again, due to quantum fluctuations, cannot be made arbitrarily small for two canonical conjugate variables. It is possible, however, to overcome the standard quantum limit in some cases by performing a QND measurement. Historically, the first example of such a measurement is based precisely on the same opto-mechanical system of Chapters 2 and 3, i.e. by measuring the radiation pressure we can measure the energy of the resonator with boundless sensitivity. The position of a particle cannot be measured in a QND way; in fact only integrals of motion, such as the number of photons in the radiation pressure interaction [Eq. (2.14)] admit such high sensitivity (the reader is referred to [81, 113] for more details on QND measurements).

The SQL for the oscillator’s energy can be obtained in a similar way by recalling that the energy is related to the amplitude $A = \sqrt{q_1^2 + q_2^2}$ of the oscillations by

$$E = \frac{1}{2}m\omega^2A^2 + \frac{1}{2}\hbar\omega = \hbar\omega(n + 1/2),$$

(A.4)

where $n$ stands for the number of quanta in the oscillator. From a continuous measurement of $Q(t)$, the amplitude can be obtained with the same precision than the quadratures: $\Delta A = \Delta q_{1(2)}$, which results in an accuracy for the energy of $\Delta E \simeq m\omega^2\Delta A A$, yielding the following SQL

$$\Delta E_{\text{SQL}} = \hbar\omega_m\sqrt{n},$$

(A.5)

The latter expression is only valid for large number of quanta as $\Delta A \ll A$ (necessary for the validity of the expression given above for $\Delta E$) implies $n \gg 1$. In order to observe the mechanical oscillator up to such accuracy, we have to overcome all the classical sources of noise and especially temperature. This imposes hard constraints on the experiment as one needs to guarantee,

$$k_B T \lesssim \frac{\hbar\omega_m}{2},$$

(A.6)

in order to actually observe the macroscopic object behaving quantum mechanically. In fact, the rigid constraint (A.6) applies only when the measuring time, $\tau$, is much larger than a typical mechanical oscillator’s relaxation time, $\tau_{\text{relax}}$ (in a dissipative environment this is the inverse of the damping constant). For $\tau \ll \tau_{\text{relax}}$, it can be shown that the relevant criterion is instead,

$$k_B T \lesssim \frac{\tau_{\text{relax}}}{\tau} \frac{\hbar\omega_m}{2}.$$  

(A.7)

The latter can be easily satisfied at Helium liquid temperatures both in mechanical oscillators and
A.2. Coherent states of bosons

Bosonic coherent states are very familiar in Quantum Optics as they describe the statistical properties of coherent sources such as the LASER light and preserve their coherent character when interacting with linear optical elements. Also, they are very useful in other branches of physics for their mathematical properties. In this short appendix, we review the properties of coherent states in the basis of the derivations of Chap. 2. The bosonic coherent state, $|\alpha\rangle$, is defined as the eigenstate of the annihilation operator, $a |\alpha\rangle = \alpha |\alpha\rangle$. (A.8)

Inserting an expansion in the Fock basis, $|n\rangle$ (with $n \in \mathbb{N}_0$), in both sides of the above equation, we get a recurrence relation whose solution is,

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n \in \mathbb{N}_0} \frac{\alpha^n}{\sqrt{n!}} |n\rangle.$$  

(A.9)

Using the Campbell-Baker-Hausdorff formula one readily concludes that the displacement operator [Eq. (1.68)] is the suitable operator form of the latter equation, that is,

$$|\alpha\rangle = D(\alpha) |0\rangle = e^{\alpha a^\dagger - \alpha^* a} |0\rangle.$$  

(A.10)

The box below summarizes the main properties of the displacement operator and the coherent-states. All of them can be easily proved from the definition (A.8), equations (A.9) and (A.10).
A. Appendices for chapter 2

1. In the Heisenberg picture the operators are displaced as to preserve \( (A.8) \),

\[
D^\dagger(\alpha) a D(\alpha) = a + \alpha. \tag{A.11}
\]

2. The consecutive action of displacement operators displaces the vacuum,

\[
D(\alpha) D(\beta) = e^{i \Im(\alpha\beta^*)} D(\alpha + \beta). \tag{A.12}
\]

3. Although the coherent states are not orthogonal,

\[
\langle \alpha \rvert \beta \rangle = e^{-|\alpha|^2 + |\beta|^2 / 2 + \alpha \beta^*} \tag{A.13}
\]

4. they form an overcomplete basis of the Hilbert space,

\[
\int_C \frac{d^2 \alpha}{\pi} \langle \alpha \rvert \langle \alpha \rvert = \sum_{n \in \mathbb{N}_0} \langle n \rvert n \rvert = I. \tag{A.14}
\]

The latter feature turns out to be very useful in calculating partial states \[Eq. (1.14)\] and it has been widely used in the derivations of Chap. 2. Let us derive the partial state of a confined EM field, \( \rho_{\text{cav}}(t) \), for the opto-mechanical problem analyzed in this monograph \[Eqs. (2.38) and (2.39)\] by means of bosonic coherent states.

We wish to compute \( \rho_{\text{cav}}(t) = \rho_{nm}(t) \langle n \rvert m \rangle \) for the initial state \( (2.17) \). From Eq. (2.18) and defining \( \Phi_{nm} := \Phi_{nm00} \) we obtain,

\[
\rho_{nm}(t) = \Phi_{nm} \text{Tr}_m \left[ \int_C \frac{d^2 z}{\pi} \frac{e^{-|z|^2 / 2 - |z + \eta(t)kn|^{2} / 2}}{z + \eta(t)km} \right]. \tag{A.15}
\]

Now we insert the resolution of identity as given previously \[A.14\] and compute the corresponding coherent state overlaps \[A.13\].

\[
\rho_{nm}(t) = \Phi_{nm} \int \frac{d^2 w}{\pi} \int \frac{d^2 z}{\pi} e^{-|w|^2 / 2 - |z + \eta(t)kn|^2 / 2} \tag{A.16}
\]

\[
* e^{-|z + \eta(t)km|^2 / 2 + w^* (z + \eta(t)kn) + (z^* + \eta(t)^* km) w} \tag{A.17}
\]

The integrals in the above equation can be solved by an useful identity\[^1\]

\[
\int_C \frac{d^2 z}{\pi} e^{-A|z|^2 + Bz + Cz^*} = \frac{1}{A} e^{\pi B / A} \tag{A.18}
\]

valid for \( B, C \in \mathbb{C} \) and \( \text{Re} A > 0 \). After integration in the all complex plane defined by \( w \) and \( z \), we

\[^1\text{This identity is straightforwardly derived by expanding the exponential in the integrand in Taylor Series around } B = 0 \text{ and } C = 0, \text{ integrate each of the terms of the expansion and make the resummation at the end.}\]
recover the result of Chap. 2 [Eq. (2.38)],
\[ \rho_{nm}(t) = e^{-|k\eta(t)|^2(n-m)^2(2+n)/4}. \] (A.19)

It is curious to observe that although the formal treatment of Chap. 2 did not include the issue of decoherence, the cavity field perceives the mirror as an effective thermal bath. This can be seen in the strong suppression of the off-diagonal elements when \(|m-n| \gg 1\). The same happens with the coherence between different positions (with separation \(\Delta x\)) of a particle interacting with a bath. The off-diagonal elements of the density matrix are rapidly suppressed with a rate proportional to \(\Delta x^2\) \[61\]. Naturally, this analogy with the universal phenomenon of decoherence cannot be pushed too far. Recall that (A.19) was derived by unitary evolution of the compound system; the entropy flows back and forward from the mirror to the cavity field without any dilution with an active environment.

### A.3. Unitary evolution of the opto-mechanical density matrix

In Chapter 2 we consider the interaction of a moveable mirror (with mass \(m\) and natural frequency \(\omega_m\)), placed at one end of a Fabry-Perot cavity, and a single-mode of the intra-cavity EM field (with frequency \(\omega_c\)). In the adiabatic limit, \(\omega_c \gg \omega_m\), this interaction is well-described by the radiation-pressure Hamiltonian [Eq. (2.14)]. Our idealized physical situation considers a completely thermalized mirror, with thermal occupation \(\bar{n}\), which is put in contact with a cavity prepared in a well-defined coherent state of the EM field, with complex amplitude \(\alpha\),
\[ \rho(t_0) = \frac{1}{\bar{n}} \int_{\mathbb{C}} \frac{d^2 z}{\pi} e^{-|z|^2/\bar{n}} |\alpha\rangle \langle \alpha| \otimes |z\rangle \langle z|, \] (A.20)

which is taken to evolve unitarily according to the evolution operator \(U(t)\) [Eq. (2.15)]:
\[ \rho(t) = e^{-i\omega_m b^\dagger b t} D_m(\eta(t)k a^\dagger a) e^{-i\omega_m b^\dagger b t} \rho(t_0) e^{i\omega_m b^\dagger b t} D_m^\dagger(\eta(t)k a^\dagger a) e^{-i\omega_m b^\dagger b t}. \] (A.21)

The effect of the free evolution of the mirror, \(U_b(t) = \exp(-i\omega_m b^\dagger b t)\), in the coherent states \(|z\rangle\) is to rotate the amplitude \(z\) in the phase space:
\[ U_b(t)|z\rangle = |e^{-i\omega_m t} z\rangle, \] (A.22)

This has no effect when performing the integration in \(z\) to get the thermal state of the mirror [Eq. (A.20)]:
\[
\begin{align*}
&= \int_{\mathbb{C}} \frac{d^2 z}{\pi} e^{-|z|^2/\bar{n}} e^{-i\omega_m b^\dagger b t} |z\rangle \langle z| e^{i\omega_m b^\dagger b t} \\
&= \int_{\mathbb{C}} \frac{d z d^* \omega}{\pi} e^{-|z|^2/\bar{n}} e^{-i\omega t} |z\rangle \langle z| e^{-i\omega t} \\
&= \int_{\mathbb{C}} \frac{d \omega d \omega^*}{\pi} e^{-|\omega|^2/\bar{n}} |\omega\rangle \langle \omega|. 
\end{align*}
\]
A. Appendices for chapter 2

Hence, without loss of rigour, we can write:

\[ \rho(t) = e^{-i\alpha a^+ a t} e^{i k^2 (a^+ a)^2 \Lambda(t)} D_m(\eta(t) k a^+ a) \rho(t_0) D_m^\dagger(\eta(t) k a^+ a) e^{-i k^2 (a^+ a)^2 \Lambda(t)} e^{i\alpha a^+ a t} \]  

(A.23)

\[ \rho(t) = \frac{1}{\tilde{n}} \sum_{n,m} \Theta_{nm} \int_C \frac{d^2 z}{\pi} e^{-|z|^2/\tilde{n}} U(t) |n\rangle \otimes |z\rangle \langle z| U^\dagger(t). \]  

(A.24)

The last line follows from expanding the coherent state of the cavity field in the Fock basis [Eq. (A.9)] and

\[ \Theta_{nm} = \frac{\alpha^n (\alpha^*)^m}{\sqrt{n! m!}} e^{-|\alpha|^2}. \]  

(A.25)

It is useful to write explicitly the action of \( U(t) \) on a generic separable state of the form \( |n\rangle \otimes |z\rangle \), with \( n \in \mathbb{N} \) and \( z \in \mathbb{C} \), before proceeding with the calculation [compare with Eq. (2.19)]:

\[ \left( e^{-i\alpha a^+ a t} e^{i k^2 (a^+ a)^2 \Lambda(t)} D_m(\eta(t) k a^+ a) \right) |n\rangle \otimes |z\rangle = e^{-i\phi_n(t)} |n\rangle \otimes |z + k \eta(t)\rangle, \]  

(A.26)

where \( \phi_n(t) := -i\alpha_n + i k^2 n^2 \Lambda(t) \). Indeed, the integrand in Eq. (A.24) can be written in a more convenient form;

\[ \rho(t) = \frac{1}{\tilde{n}} \sum_{n,m} \Theta_{nm} \int_C \frac{d^2 z}{\pi} e^{-|z|^2/\tilde{n}} e^{-i(\phi_n(t) - \phi_m(t))} |n\rangle \langle m| \otimes |z + k \eta(t)\rangle \langle z + k \eta(t)|. \]  

(A.27)

The next step is to express the coherent states (on the righ-hand side of the latter equation) in the Fock basis [Eq. (A.9)]:

\[ \rho(t) = \frac{1}{\tilde{n}} \sum_{n,m} \Phi_{nm\mu \nu}(t) \int_C \frac{d^2 z}{\pi} e^{-K_{nm}(z)} F_n(z)^\mu F_m^*(z)^\nu |n\rangle \langle m| \otimes |\mu\rangle \langle \nu|. \]  

(A.28)

We have defined \( \Phi_{nm\mu \nu}(t) := \Theta_{nm} e^{-i(\phi_n(t) - \phi_m(t))} / \sqrt{\mu \nu!} \) as to meet the notation of Chapter 2, the definitions of \( K_{nm}(z) \) and \( F_n(z) \) read:

\[ F_n(z) := z + k \eta(t) \]  

(A.29)

\[ K_{nm}(z) := |F_n(z)|^2 / 2 + |F_m(z)|^2 / 2 + |z|^2 / \tilde{n}. \]  

(A.30)

The density matrix elements \( \rho_{nm\mu \nu}(t) \) will now be worked out more explicitly. Let

\[ \sigma_{nm\mu \nu}(t) = \left( \tilde{n} / \Phi_{nm\mu \nu}(t) \right) \rho_{nm\mu \nu}(t), \]  

(A.31)

hence, from Eq. (A.28), we have

\[ \sigma_{nm\mu \nu}(t) = \int_C \frac{d^2 z}{\pi} e^{-K_{nm}(z)} F_n(z)^\mu F_m^*(z)^\nu \]  

(A.32)
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The exponential in the integrand reads

\[ e^{-K_{nm}(z)} = \exp \left[ -k^2 |\eta(t)|^2 \frac{n^2 + m^2}{2} - z \frac{k}{2} \eta(-t) (n + m) - z^* \frac{k}{2} \eta(t) (n + m) - \frac{|z|^2}{x} \right]. \]  (A.33)

In the last line we have used the fact that \( \eta(t) = \eta(-t) \) [see Eq. (2.15) and comments therein] and defined \( x := \bar{n}/(\bar{n} + 1) \). In order to perform the integration in the variables \( z \) and \( z^* \) we add two terms to \( K_{nm}(z) \) (which we set to zero at the end of calculation):

\[ K_{nm}(z) \rightarrow J_{nm}(z, a, b) := K_{nm}(z) + a (z + kn\eta(t)) + b (z^* + km\eta(-t)). \]  (A.34)

The density matrix elements can be written by taking the correct number of derivatives with respect to \( a \) and \( b \) (the same method used to evaluate path integrals):

\[ \sigma_{nm\mu\nu}(t) = \left[ \int_{C} \frac{d^2z}{\pi} \partial_{a}^\mu \partial_{b}^\nu \exp \left(-J_{nm}(z, a, b)\right) \right]_{(a=0, b=0)}. \]  (A.35)

We now evaluate explicitly the integral by exchanging the partial derivatives and the integral sign. First we evaluate the following function,

\[ I(a, b) := \int_{C} \frac{d^2z}{\pi} \exp \left(-J_{nm}(z, a, b)\right) \]  (A.36)

\[ = \int_{C} \frac{d^2z}{\pi} \exp \left(-|z|^2/x + zG_1(a, -t) + z^*G_1(b, t)\right) e^{R(a, b)}, \]  (A.37)

with \( G_1(X, t) = X - \eta(t) (n + m) / 2 \) and

\[ R(a, b) := -k^2 |\eta(t)|^2 \frac{n^2 + m^2}{2} + akn\eta(t) + bkm\eta(-t). \]  (A.38)

With the integral written in the above form [Eq. (A.37)] we can apply directly formula (A.18) to obtain:

\[ I(a, b) = x \exp \left[G_1(a, -t)G_1(b, t)/x\right] e^{R(a, b)}. \]  (A.39)

Finally, the equation given in Chapter 2 [namely, Eq. (2.24)] follows immediately from equations (A.31), (A.35) and (A.39):

\[ \rho_{nm\mu\nu}(t) = \frac{\Phi_{nm\mu\nu}(t)}{\bar{n} + 1} \left\{ \partial_{a}^\mu \partial_{b}^\nu \exp \left[G_1(a, -t)G_1(b, t)/x + R(a, b)\right] \right\}_{(a=0, b=0)}. \]  (A.40)

The above expression is an explicit formula for the complete density matrix of the system for all times and it is expected to be a good description of the opto-mechanical system in the conditions described in Chapter 2, namely in the adiabatic regime and for perfect reflecting Fabry-Perot end mirrors.

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A. Appendices for chapter 2

A.4. Entropy, mutual information and entropic inequalities

In this appendix we introduce the mutual information and the Araki-Lieb inequality which is in the basis of the entropic inequality used by the authors in Chapter 2. We first summarize the main properties of the von Neumann entropy [Eq. (1.9)];

\[ H_{\rho} = \frac{1}{d} \ln d, \]  

\[ S(\rho) = S(U\rho U^{\dagger}), \]  

\[ S(\sum \lambda_i \rho_i) \geq \sum \lambda_i S(\rho_i), \]  

\[ S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B). \]

With the exception of the concavity [Eq. (A.44)] (please refer to [2] for a derivation) all the other properties follow trivially from the definition. Let us, for instance, prove the additivity of entropy (A.45). We first note that the trace of a matrix is invariant under change of basis, and conveniently choose the basis where \( \rho_A \) and \( \rho_B \) are diagonal and denote their eigenvalues by \( a_1\ldots a_d \) and \( b_1\ldots b_d \), respectively. Let \( U := U_A \otimes U_B \) be the unitary matrix bringing \( \rho_A \otimes \rho_B \) to its diagonal form. Thus,

\[ U \rho_A \otimes \rho_B U^{\dagger} = \bigoplus_{i=1}^{d} a_i \otimes \bigoplus_{i=1}^{d} b_i, \]
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and hence,

\[ S(\rho_A \otimes \rho_B) = \sum_{i,j=1}^{d} a_i b_j \ln(a_i b_j) = \sum_{i,j=1}^{d} a_i b_j (\ln a_i + \ln b_j) \]

\[ = \sum_{i} (a_i \ln a_i + b_i \ln b_i) \]

\[ = S(\rho_A) + S(\rho_B). \]

From the above expression we conclude that, analogously to classical statistical mechanics, the following inequalities hold,

\[ S(\rho_A \otimes \rho_B) \geq S(\rho_A) \quad (A.46) \]

\[ S(\rho_A \otimes \rho_B) \geq S(\rho_B) \quad (A.47) \]

This is in agreement with the classical picture of the whole at least as entropic as its parts. However, we know from our earlier discussion on EPR correlations [Sec. 1.2] that the quantum world can easily violate the above inequalities, when the state is non separable [see for instance Eq. (1.15)], being the compound state well-defined but not its parts. Araki and Lieb showed that a "triangle inequality" holds for bipartite quantum states [182],

\[ |S(\rho_A) - S(\rho_B)| \leq S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B). \]

(A.48)

The first inequality encompasses all classes of bipartite states and differs significantly from the classical analogue based on the Shannon entropy [Eq. (1.7)],

\[ H(X,Y) \geq \max \{H(X),H(Y)\}. \]

(A.49)

We can take advantage of the above discrepancy between the entropic content shared by two random classical variables and that of quantum states in order to derive an entropic witness of "quantumness" for bipartite states. For that end, we use the mutual information which quantifies the total amount of correlations in a given state,

\[ I(\rho_{AB}) := S(\rho_A) + S(\rho_B) - S(\rho_{AB}). \]

(A.50)

In general the above quantity does not discriminate between purely classical and genuine quantum correlations, but still has some desirable properties; i) it is zero for separable states of the form \( \rho_A \otimes \rho_B \); ii) it is maximal for maximally entangled pure states (e.g. the singlet [Eq. (1.13)]); iii) it meets a natural upper bound within the framework of classical random variables (or canonical variables in statistical mechanics). The latter turns out to be a very useful result when one is not able to compute the exact entanglement of a mixed bipartite state. In order to expose more clearly this
A. Appendices for chapter 2

idea, we define the normalized mutual information as,

\[ \mathcal{J}(\rho_{AB}) := \frac{I(\rho_{AB})}{S(\rho_A) + S(\rho_B)}. \]  \hspace{1cm} (A.51)

It should be clear that this definition holds only when \( S(\rho_A) + S(\rho_B) > 0 \). This of course excludes separable pure states but, nevertheless, it holds for the most relevant cases, \textit{i.e.} when the partial states have some entropy (see Sections 1.2 and 1.3). From inequality (A.49) we derive the upper bound for classical random variables,

\[ \mathcal{J}_c \leq \frac{1}{2}. \]  \hspace{1cm} (A.52)

The above result has a clear and important interpretation: the correlations shared by classical random variables cannot be as strong (when properly normalized by the entropy of the subsystems) as their quantum counterpart. Thus, violation of the upper bound (A.52) is an indicator of quantumness. On the other hand, however, it is not guaranteed that a large normalized mutual information expresses a large amount of entanglement. For instance, for every pure state of two two-level systems the normalized mutual information is always maximal even if the parties share little entanglement, that is, for \( \theta \in [0, \pi/2] \) we have,

\[ \mathcal{J}(\cos \theta |\uparrow, \uparrow\rangle + \sin \theta |\downarrow, \downarrow\rangle) = 1, \]

although entanglement vanishes when \( \cos \theta \to 0 \) or \( \sin \theta \to 0 \).
B. Appendices for chapter 3

B.1. An outline of optical cavities

In this appendix we derive the mode spectrum of a generic Fabry-Perot optical resonator and afterwards discuss the relevant physical parameters driving the operation of an optical cavity. A Fabry-Perot cavity (also known as Fabry-Perot interferometer) is made of two parallel highly reflecting flat mirrors [see Fig. (B.1)] and is widely used for controlling and measuring the state of light. Its mode spectrum is characterized by looking at the transmittance for different wavelengths. Let us consider a Fabry-Perot cavity made of equals mirrors placed in vacuum (with real transmission and reflection coefficients $t$ and $r$, respectively, obeying $r^2 + t^2 = 1$). A classical EM wave with amplitude $\mathcal{E}_i$ and wave number $k$ will be partially transmitted into the cavity through mirror 1 (e.g. the one at left). We make the useful definitions; $\mathcal{E}_r$ and $\mathcal{E}_t$ are the outer-cavity amplitudes leaving the resonator through mirror 1 and 2, respectively. Also, we define the intra-cavity field leaving mirror 1 and mirror 2 by $\mathcal{E}_1$ and $\mathcal{E}_2$, respectively. Then we can write, $\mathcal{E}_1 = t\mathcal{E}_i - r\mathcal{E}_2$, where the minus sign must be included in order to guarantee conservation of energy flux in mirror 1:

$$|\mathcal{E}_1|^2 + |\mathcal{E}_r|^2 = |\mathcal{E}_i|^2 + |\mathcal{E}_2|^2,$$

(B.1)

The relation between the fields read,

$$\mathcal{E}_1 = t\mathcal{E}_i e^{ikL},$$

(B.2)

$$\mathcal{E}_2 = -r\mathcal{E}_1 e^{2ikL},$$

(B.3)

where the origin of the phases have conveniently be chosen at mirror 1. The transmittance is defined as,

$$T := \left| \frac{\mathcal{E}_t}{\mathcal{E}_i} \right|^2.$$

(B.4)

Using the equations above it is straightforward to derive,

$$T = \frac{1}{1 + \frac{4R}{1 - R^2} \sin^2 (kL)},$$

(B.5)

The transmittance is maximum for $kL = n\pi$ (with $n \in \mathbb{N}_0$) even if the mirror’s reflectance $R := r^2$ is
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Figure B.1.: The transmissivity mode spectrum of a Fabry-Perot cavity (i.e., a linear optical cavity with flat end-mirrors) of size $L$ and reflectivity $R < 1$ has characteristic lineshapes, frequency separations and other properties controlling their operation. The most important features of an optical cavity are the free-spectral range ($\Delta \omega = \frac{2\pi c}{L}$) and the FWHM ($\delta \omega$). The peaks get sharper as one approaches the limit of a perfect reflective mirror $R = 0$. The interplay between the resonant enhancement, the free-spectral range, and the FWHM will determine the finesse and the quality factor of the cavity.

arbitrarily close to one. This defines the resonant frequencies of the cavity

$$\omega_n = \frac{\pi c}{L} n.$$  \hspace{1cm} (B.6)

The function $\frac{4R}{(1 - R)^2}$ in Eq. (B.5) measures the resolution of the peaks in the spectrum. It is therefore the most important physical parameter driving the operation of an optical cavity and defines the so-called optical finesse, $\mathcal{F} := \frac{\pi \sqrt{R}}{(1 - R)}$, which equals the ratio between the frequency intervals and the full-width at half-maximum (FWHM) [Fig. (B.1)]. Hence, a Fabry-Perot cavity is fully characterized by,

1. the free-spectral range, $\Delta \omega_c$. This is a simply function of the cavity size, $\Delta \omega_c = \frac{\pi c}{L}$, and measures the distance between two resonant frequencies;

2. the FWHM, $\delta \omega_c$. This depends on the reflectivity of both mirrors and it measures how many modes are actually contributing to the real mode spectrum of the cavity (see Fig. B.1).

The relevant physical quantities describing how adequate is a cavity for a given experiment will depend on the interplay between the free-spectral range and the FWHM (Fig. B.1). They are,

1. the $Q$-factor. This is defined in the same manner as in electronics; the ratio between the frequency at which the field oscillates and the rate at which it dissipates its energy. It is an important measure as it tell us about the life-time of resonant photons $\tau = \frac{Q}{\omega_c}$, and thus the reliability of a cavity as a stable amplifier of the radiation-pressure mechanism. It can be expressed as,

$$Q = \frac{\omega_c}{\delta \omega_c},$$  \hspace{1cm} (B.7)
B.2. The input-output theory

and depends on the frequency of the photons;

2. the optical-finesse, $\mathcal{F}$. It measures the resolution of the peaks separation in the mode spectrum,

$$\mathcal{F} = \frac{\Delta \omega_c}{\delta \omega_c}.$$  \hspace{1cm} (B.8)

For a Fabry-Perot microcavity, the free-spectral range is similar to the cavity mode frequency and thus the optical finesse and the $Q$-factor are essentially the same. The finesse can be determined by the ring-down time of the cavity, $\tau$. The latter can be measured using an avalanche photodiode counting the individual photons leaking out the cavity as function of time \cite{95},

$$\mathcal{F} = \frac{\pi c}{L \tau}.$$  \hspace{1cm} (B.9)

B.2. The input-output theory

This appendix is concerned with the theory of Gardiner and Collett and aims to give a derivation of the input-output relations for optical cavities \cite{107, 108}. We consider an optical cavity with fixed length $L$, and a single-mode (with frequency $\omega_c$) interacting with an input field. The full Hamiltonian of the system reads,

$$H = \hbar \omega_c a^\dagger a + H_{\text{bath}} + H_{\text{int}}.$$  \hspace{1cm} (B.10)

The term $H_{\text{bath}}$ is the Hamiltonian of the external fields and $H_{\text{int}}$ describes the interaction of these fields with the mode of interest, $a$. The standard assumptions of Quantum Optics are made, namely,

1. the interaction between the bath and the cavity is chosen to be linear in the bath operators;

2. an approximated form of $H_{\text{int}}$ is considered (the rotating-wave approximation);

3. the bath is made of many independent harmonic oscillators,

$$H_{\text{bath}} = \int_0^\infty d \omega \hbar \omega b^\dagger(\omega) b(\omega),$$  \hspace{1cm} (B.11)

and the coupling constant (in $H_{\text{int}}$) is made frequency-independent (the so-called Markovian approximation).

With these premises a Langevin equation describing the dissipative dynamics of the cavity mode can be derived as follows. We start by writing the interaction term in the rotating-wave approximation\footnote{The motivation behind the rotating-wave approximation is the following; terms like $a^\dagger b^\dagger$ (corresponding to emission with excitation) and $ab$ (corresponding to absorption with de-excitation) oscillate at very high frequencies — in the Heisenberg picture $(ab)(t) \sim \exp [i(\omega_c + \omega)t]$ — and thus its contribution to the dynamics is negligible.}

$$H_{\text{int}} = i\hbar \int_0^\infty d \omega \kappa(\omega) \left( a b^\dagger(\omega) - a^\dagger b(\omega) \right),$$  \hspace{1cm} (B.12)
B. Appendices for chapter 3

where $\kappa(\omega)$ is the coupling between the modes. The only contribution to time averages of the operators will come from frequencies near $\omega_c$, and thus we extend the integration limit in Eq. (B.12) which is consistent with the rotating-wave approximation. The dynamics of $a$ and $b(\omega)$ will follow the Heisenberg equation of motion, $i\hbar \dot{a} = [a|b\rangle, H]$, yielding,

$$\dot{a} = -i\omega_a a - \int_{-\infty}^{\infty} d\omega \kappa(\omega) b(\omega), \quad (B.13)$$
$$b(\omega) = -i\omega b(\omega) + \kappa(\omega)a. \quad (B.14)$$

The integration of the above equations is straightforward. Defining the initial and final times by subscripts $i$ and $f$, respectively, and the under the Markovian assumption, $\kappa^2(\omega) = \gamma/2\pi$, we have,

$$b(\omega) = e^{-i\omega(t-t_i)} b_i(\omega) + \sqrt{\frac{\gamma}{2\pi}} \int_{t_i}^{f} d\tau e^{-i\omega(t-\tau)} a(\tau), \quad (B.15)$$

when integrating Eq. (B.14) for $t > t_i$. The initial time, $t_i$, should be interpreted as a remote time in the past when no wave packet has reached the cavity; while the first term is just the free evolution of the bath modes, the second represents the waves radiated by the cavity. A similar equation holds for $t > t_f$, namely,

$$b(\omega) = e^{-i\omega(t-t_f)} b_f(\omega) - \sqrt{\frac{\gamma}{2\pi}} \int_{t}^{f_f} d\tau e^{-i\omega(t-\tau)} a(\tau), \quad (B.16)$$

The cavity mode will evolve according to,

$$\dot{a} = -i\omega_a a - \sqrt{\frac{\gamma}{2\pi}} \int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t_i)} b_i(\omega) - \frac{\gamma}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{t_i}^{f} d\tau e^{-i\omega(t-\tau)} a(\tau). \quad (B.17)$$

The parameter $\gamma$ clearly plays the role of the damping frequency of the cavity due to partial reflectivity of the mirror. Now we make the crucial step of the derivation by defining the input-output field

\[ a_{in}(t) \quad \rightarrow \quad a(t) \quad \rightarrow \quad a_{out}(t) \]

Figure B.2.: The input field, $a_{in}$, couples to a cavity with partial reflecting mirrors ($R < 1$). The relation between this field, the cavity field and the field leaking from the cavity, $a_{out}$, is given by Eq. (B.23).
B.2. The input-output theory

operators,

$$a_{\text{in}}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t_i)} b_i(\omega),$$  \hspace{1cm} (B.18)

$$a_{\text{out}}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t_f)} b_f(\omega).$$  \hspace{1cm} (B.19)

In an open-system like a lossy cavity the input, output and intra-cavity fields are not essentially different one from each others, but the formal separation in the above equations is justified for high-quality cavities where an effective model of spontaneous emission processes (where a bath boson is created at the expense of a cavity boson) describes well the physics. These operators satisfy the canonical commutation relations,

$$[a_{\text{in}}(t), a_{\text{in}}^\dagger(t')] = [a_{\text{out}}(t), a_{\text{out}}^\dagger(t')] = \delta(t-t').$$  \hspace{1cm} (B.20)

The Langevin equation containing the dynamics of the cavity mode reads,

$$\dot{a} = -i\omega_c a - \frac{\gamma}{2} a - \sqrt{\gamma} a_{\text{in}}(t).$$  \hspace{1cm} (B.21)

We can easily compute any averages containing the cavity operator, $a$, if the statistical properties to the input field, $a_{\text{in}}$, are known. For this fact, the latter equation is central for the discussion of Chap. 3. There we focus on a cavity which is continuously fed by a pumping laser and therefore an adequate operator equation relating the flux of energy entering and exiting the cavity is compulsory. A similar equation to (B.21) can be obtained that depends on $a_{\text{out}}$,

$$\dot{a} = -i\omega_c a + \frac{\gamma}{2} a - \sqrt{\gamma} a_{\text{out}}(t).$$  \hspace{1cm} (B.22)

The latter is not as useful as Eq. (B.21) as it depends on unknown boundary conditions ($b_f$), but together with the Langevin equation [Eq. (B.21)] it provides an important input-output relation in Quantum Optics,

$$a_{\text{out}}(t) = a_{\text{in}}(t) + \sqrt{\gamma} a(t).$$  \hspace{1cm} (B.23)

Assuming the bath to be initially in a thermal state with temperature $T$, in the rotating-wave approximation, the statistical properties of the input-field assume a simple form [83]:

$$\langle a_{\text{in}}(t) \rangle = 0,$$  \hspace{1cm} (B.24)

$$\langle a_{\text{in}}^\dagger(t) a_{\text{in}}(t') \rangle \approx \bar{n}(\omega_c) \delta(t-t'),$$  \hspace{1cm} (B.25)

$$\langle a_{\text{in}}(t) a_{\text{in}}^\dagger(t') \rangle \approx (\bar{n}(\omega_c) + 1) \delta(t-t'),$$  \hspace{1cm} (B.26)

where $\bar{n}(\omega_c)$ represents the Bose occupation number at temperature $T$ and frequency $\omega_c$. These relations allow us to compute the thermal averages of cavity operators evolving according to the Langevin equation [Eq. (B.21)] (or the Langevin equation of Sec. 3.2 in which the cavity field also
interacts with a moveable mirror). To this end, one can for instance take the Fourier transform of 
Eq. (B.21) to get:
\[
(\mathcal{F}a)[\omega] = \frac{-\sqrt{\gamma}}{i(\omega_0 - \omega) + \gamma/2} (\mathcal{F}a_{in})[\omega] = -\sqrt{\gamma} \chi_c[\omega] (\mathcal{F}a_{in})[\omega],
\]
where \(\chi_c[\omega]\) is the susceptibility of the cavity. This together with the time statistics for \(a_{in}\) allow us to extract easily any time-dependent average of cavity operators.

### B.3. The quantum Brownian motion

**Quantum Langevin equations (brief outline)**

The original derivation of the quantum Langevin equation has more than 20 years and is due to Benguria and Kac [184, 185]. Here we outline a more recent derivation by Giovannetti and Vitali [102], and briefly discuss the differences between classical and quantum Brownian motion. For a complete survey into this subject and related topics (the master equation and phase-space methods) the reader may consult the excellent book on quantum noise by Gardiner [183].

We consider a particle with Hamiltonian \(H_0\) interacting with a reservoir made of \(N\) independent harmonic oscillators with frequencies \(\omega_j\) and couplings \(k_j\) (with \(j = 1, \ldots, N\)), whose rescaled canonical coordinates read \(Q_j\) and \(P_j\). The interaction is chosen such that the bath is sensitive to displacements of the position of the particle, \(q\). After an appropriate canonical transformation, the total Hamiltonian of the system reads [183]
\[
H = H_0 + \frac{1}{2} \sum_{j=1}^{N} \left( P_j - k_j q \right)^2 + \omega_j^2 Q_j^2.
\]

The reservoir annihilation (and creation) operators are defined in the usual way,
\[
a_j = \frac{1}{\sqrt{2\hbar\omega_j}} (\omega_j Q_j + iP_j).
\]

The Heisenberg equations of motion for the particle operators are obtained from (B.28), and their integration from the initial time \(t_0\) resemble the derivation presented in Sec. (B.2), but the final expression is somewhat cumbersome and will not be displayed in full generality. Here we present the solution for a bath spectrum approximated by a continuum \((N \to \infty)\). The continuous limit is taken according to,
\[
\sum_{j=1}^{N} k_j^2 (\ldots) \to \int_{0}^{\infty} k^2(\omega) \frac{dn}{d\omega}(\ldots) \equiv \frac{2\eta}{\pi} \int_{0}^{\infty} d\omega (\ldots),
\]
where \(n'(\omega)\) is the oscillator density and \(\eta\) is the friction coefficient. The ideal situation occurs when \(k^2(\omega)n'(\omega) = \text{constant} \) — the so-called Markovian approximation (recall that in classical dynamics
B.3. The quantum Brownian motion

This approximation leads to a stochastic Langevin equation with an extra random force term without memory. This prescription introduces the mechanical damping for the particle via $\eta$ and assumes a very large cut-off compared to typical frequencies $\Omega_{\text{cutoff}} \to \infty$ reflecting the extremely fast dynamics of a large reservoir. The interested reader is referred to [102] for a detailed and rigorous calculation.

The quantum Langevin equations resemble their classical version:

$$\dot{q}(t) = \frac{p(t)}{m}, \quad \dot{p}(t) = \frac{i}{\hbar} [H_0, p] - \frac{p}{m} + \xi(t).$$

But now the noise, $\xi$, is a Hermitian operator obeying the following commutation relation,

$$[\xi(t), \xi(t')] = 2i\eta \hbar \frac{d}{dt} \delta(t-t').$$

Although a Markov assumption has been made [Eqs. (B.31) and (B.32)] the differential equations do not entail a Markovian process. This fact, unfamiliar to classical statistical mechanics, emerges for the physics also depends on the state vector and this introduces a non-zero correlation time in a genuine quantum stochastic process. The auto-correlation function of the quantum random force reads [183],

$$\langle \xi(t) \xi(t') \rangle = \hbar \eta \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \left[ \coth \left( \frac{\hbar \omega}{2 k_B T} \right) + 1 \right].$$

Clearly a genuine quantum Brownian motion is not a Markovian process in general. It is well-known that the quantum harmonic oscillator finds anomalies at very small temperature and/or strong damping; e.g. power-decay of expectation values of correlation functions and strong squeezing of the position and momentum uncertainties, a clear signature of quantumness [186]. At which extent we should expect non-Markovian physics will depend on the balance of the thermal correlation time, $\tau_T = \hbar / (2\pi k_B T)$, and the time-scale of a given physical process. The classical limit is obtained setting $\hbar \to 0$ in the auto-correlation function$^1$

$$\langle \xi(t) \xi(t') \rangle \bigg|_{\hbar \to 0} = 2\eta k_B T \delta(t-t'),$$

which is the familiar result of the classical Brownian motion. It is pedagogical to review the case of zero temperature of a free particle, since it entails the ultimate quantum Brownian motion as no thermal noise plays and only the vacuum fluctuations drive the system. The Hamiltonian of the particle reads $H_0 = p^2 / 2m$, and the position equation of motion [Eq. (B.31)] can be immediately solved,

$$q(t) = q(0) + \frac{p(0)}{\eta} \left( 1 - e^{-\eta t/m} \right) + \frac{1}{m} \int_0^t d\tau \int_0^\tau ds e^{-\eta(\tau-s)/m} \xi(\tau).$$

$^1$In fact this limit must be interpreted with some care, since for any finite $\hbar$ the integrand in Eq. (B.34) diverges. The origin of the problem is in the "first Markovian approximation", namely $k^2(\omega)\phi''(\omega) = \text{constant}$. In a realistic scenario this function is not constant but falls off at very high frequencies. The result [Eq. (B.35)] is thus the wide bandwidth limit of the classical limit.
The mean square displacement, $\langle [q(t_2) - q(t_1)]^2 \rangle$, can be calculated from the above expression and Eq. (B.34) (with $\omega \coth(\hbar \omega/2k_B T) \rightarrow |\omega|$) by making two assumptions: i) $t_1$ and $t_2$ are very large so that transient terms vanish and ii) a frequency cutoff is introduced in the divergent terms in the integrand [183]. Here, we just state the result,

$$\langle [q(t_2) - q(t_1)]^2 \rangle \rightarrow \frac{2\hbar}{\eta \pi} \ln \left( \frac{\eta |t_2 - t_1|}{m} \right).$$

(B.37)

The result (B.37) is remarkable; the ZPF of the bath oscillators induce a genuine quantum Brownian motion which takes place much slower than its thermal classical version,

$$\langle [q(t_2) - q(t_1)]^2 \rangle \approx \frac{2k_B T}{\eta} |t_2 - t_1|.$$  

(B.38)

The interested reader is referred to the excellent book on quantum noise by Gardiner and Zoller for more insight into the distinctive features of quantum Brownian processes [183].

The opto-mechanical regime for Brownian motion

What is the physical regime an experimentalist will face in a opto-mechanical experiment with a massive mechanical oscillator? In order to answer this question we recall the definition of the quality-factor, $Q$, of a mechanical oscillator. The quality factor is defined analogously as for a resonator cavity [Eq. (B.7)], i.e. as the ratio between the natural frequency of the oscillator and the rate at which it dissipates its energy,

$$Q := \frac{m \omega_m}{\eta} = \frac{\omega_m}{\gamma_m}.$$  

(B.39)

It should be clear that the mechanical oscillator (e.g. a free-standing mirror, a mirror attached to a cantilever, etc.) must dissipate its energy to the bath very slowly compared to its own dynamics, if one wishes to observe bona fide quantum phenomena. Indeed, the experimentalist must use high-quality mirrors, $Q \gg 1$. Also, one must deal with the limit of high-temperatures, for we have $k_B T \gg \hbar \omega_m$ even at cryogenic temperatures. The latter condition poses a serious problem in reaching the realm of quantum effects. In fact, the large number of phononic excitations is responsible for making the famous Penrose proposal [62, 66] impossible to realize even with state-of-the-art cooling methods — see the discussion of [73, 75].

Notwithstanding, we found a way to circumscribe the effect of high-temperature in opto-mechanical systems and recover quantum effects beyond the low temperature regime. This is accomplish by preparing the cavity field with a sufficiently large number of coherent photons as conjectured in Sec. 2.2.3 and confirmed, for a realistic scenario of a driven open system, in Sec. 3.2 by showing that the effective opto-mechanical coupling [Eq. (3.22)] is proportional to the square root of the number of intra-cavity photons. As a consequence, entanglement may be observed at temperatures much higher than than the mirror’s ground state (Sec. 3.3). This clearly makes the life much easier to the experimentalist aiming to observe genuine quantum effects on macroscopic oscillators.
In what follows, and to make a more clear connection between Sec. 3.2 and the Brownian motion, we re-define the position and momentum operators to be dimensionless [Eq. (3.2)]. As a consequence the auto-correlation function of the noise operator acquires dimensions of frequency and its high-temperature limit reads [187][184],

\[
\langle \xi(t)\xi(t') \rangle = \frac{\gamma_m}{\beta \hbar} \left(2\bar{n} + 1\right) \delta(t - t'),
\]

(B.40)

where \(\bar{n}\) is the Bose occupation number of phonons for the mechanical frequency \(\omega_m\) at temperature \(T\). This expression coincides with the classical limit [recall that for \(\beta \bar{n} \ll 1\) we have \(\bar{n} \approx k_B T / \hbar \omega_m\) and the above expression reduces to Eq. (B.35) with \(m \to 1 / \hbar \omega_m\)] of the quantum Brownian motion and holds for weak mirror-environment coupling (i.e. \(Q \gg 1\)). Experimentally, the quality-factor can be as high as \(10^4\) for low free-standing mirrors (with \(m \simeq 400\) ng) [83] and may be improved with state-of-the-art microfabrication techniques; in fact, very recently, the Vienna group has demonstrated a micromechanical resonator with \(Q \approx 30000\) and \(m \simeq 43\) ng operating at \(T = 5\) K [87]. This makes the Markovian assumption very accurate in realistic scenarios.

B.4. Equation of motion for the covariance matrix

Here we derive the equation of motion for the covariance matrix associated with the dynamical system:

\[
X(t) = A(t)X(t) + Y(t).
\]

(B.41)

An example of a time-dependent first order inhomogeneous equations is found in Chapter 3. For the sake of generality, in this appendix, we will think of \(X(t)\) as being a generic \(d\)-dimensional vector with components \((X_1(t),...,X_d(t))\), where each \(X_i(t)\) is the Heisenberg representation for the quantum operator \(X_i\); the \(d \times d\) matrix \(A\) will depend on time, in general, and \(Y(t)\) is a generic vector of operators \(Y(t) = (Y_1(t),...,Y_d(t))\). The formal solution of (B.41) reads;

\[
X(t) = M(t)X(0) + \int_0^t dsM(s)Y(t - s),
\]

(B.42)

where \(M(t)\) denotes the principal matrix solution of the homogeneous system \(\dot{M}(t) = A(t)M(t)\) with \(M(0) = 1_d\). Recall that for the opto-mechanical linearized equations of motion \(A\) does not depend on time and hence \(M(t) = \exp(At)\) [Eq. (3.26)]; in this case, \(M(t) = \exp(At)\). The covariance matrix associated with the operators \(\{X_i(t)\}\) is defined in the usual way,

\[
V_{ij}(t) = \frac{1}{2} \langle \{X_i(t),X_j(t)\} \rangle,
\]

(B.43)
where \( \{A, B\} = [A, B] \) is the anti-commutator. To find the equation of motion for \( V(t) \) we take the derivative of the latter equation:

\[
\dot{V}_{ij}(t) = \frac{1}{2}\left\langle \{\dot{X}_i(t), X_j(t)\} + \{X_i(t), \dot{X}_j(t)\} \right\rangle 
= \frac{1}{2} \sum_{k=1}^{d} \left\{ \{A_{ik}(t)X_k(t) + Y_i(t), X_j(t)\} + \{X_i, A_{jk}(t)X_k(t) + Y_j(t)\} \right\}.
\] (B.45)

The last equality was obtained inserting the left-hand side of Eq. (B.41) in \( \dot{X}_{i(j)}(t) \). We now drop the explicit time dependence and adopt the summation convention for repeated indexes as to ease the notation. Indeed, we can recast the above formulas into the form

\[
\dot{V}_{ij} = \langle A_{ik} \frac{1}{2} \{X_k, X_j\} \rangle + \langle A_{jk} \frac{1}{2} \{X_i, X_k\} \rangle + \frac{1}{2} \{\{Y_i, X_j\} + \{X_i, Y_j\}\}. 
\] (B.46)

It is useful to define the symmetric matrix,

\[
W_{ij} := \frac{1}{2} \left\langle \{Y_i, X_j\} + \{X_i, Y_j\} \right\rangle. 
\] (B.47)

We then get the general form for the equation of motion of the covariance matrix:

\[
\dot{V}(t) = A.V(t) + V(t).A^T + W. 
\] (B.48)

In order to solve for the above dynamical system, we have to resort to some particular case. Indeed, we focus on those cases equivalent to the case studied in this monograph (Sec. 3.2) and solve for the stationary solution, i.e. we consider the only non-vanishing averages containing "noise operators" \( Y_i \) to be \( \langle Y_iY_j \rangle \), and

\[
\langle Y_i(t) \rangle = 0. 
\] (B.49)

This should not be thought as restrictive in the context of quantum open systems as single averages of noise operators vanish in quite general grounds. We now introduce the formal solution of \( X_i(t) \) in \( W \) to get:

\[
W_{ij}(t) = \frac{1}{2} \left\langle \{Y_i(t), M_{jk}(t)X_k(0) + \int_0^t dsM_{jk}(s)Y_k(t-s)\} + \\
\{M_{ik}(t)X_k(0) + \int_0^t dsM_{ik}(s)Y_k(t-s), Y_j(t)\} \right\rangle 
= \frac{1}{2} \int_0^t dsM_{ik}(s) \{Y_i(t), Y_k(t-s)\} + \int_0^t dsM_{ik}(s) \{Y_i(t-s), Y_j(t)\}. 
\] (B.50)

The existence of a stable solution depends on the nature of the principal matrix solution \( M(t) \); in order to keep going we assume \( A \) to be time-independent and \( A < 0 \) so that \( M(t) = \exp(A t) \to 1_d \) when \( t \to \infty \). In practice we do not actually need to solve for the eigenvalues of \( A \); applying the
Routh-Hurwitz criterion is sufficient \[111\]. In the asymptotic regime, and for a stable system, we have, \( \dot{V}(\infty) = 0 \), and hence,
\[
A.V(\infty) + V(\infty).A^T = -W(\infty),
\]
(B.52)

Further progress is obtained by simplifying Eq. (B.51) by considering Markovian delta-correlated noise; to this end we introduce the matrix of stationary noise correlation functions:
\[
\Phi_{ij}(s - s') = \frac{1}{2} \langle \{ Y_i(s), Y_j(s') \} \rangle,
\]
(B.53)
\[
\Phi_{ij} := D_{ij} \delta(s - s').
\]
(B.54)

This entails the following simplification,
\[
W_{ij}(t) = \text{Markovian} \left\langle \int_0^t ds M_{jk}(s) D_{ik} \delta(s) + \int_0^t ds M_{ik}(s) D_{kj}(s) \right\rangle.
\]
(B.55)

The asymptotic limit \( t \to \infty \) yields\(^3\) \( W_{ij}(\infty) = D_{ij} \). We thus arrive at the following equation for the steady-state correlation matrix:
\[
A.V(\infty) + V(\infty).A^T = -D(\infty),
\]
(B.56)

which is a linear algebraic equation for \( V \) and can be straightforwardly solved.

\(^3\)The justification to extend the integral to \(-\infty\) (with factor 1/2 to compensate) stems from \( \Phi_{ij}(s, s') \) being an even function of the time difference \( s - s' \), that is, \( \Phi_{ij}(s, s') = \Phi_{ij}(s' - s) \).
B. Appendices for chapter
C. Appendices for chapter 4

C.1. Degenerate perturbation theory

In the problems of Chapters 4 and 5 we have an enlargement of the Hilbert space of a many-body system with Hamiltonian $H_0$ due to the introduction of extra quantum systems (i.e., probes). In general grounds, the system-probes interaction is described by Eq. (4.8), namely

$$V = \sum_{\alpha=1}^{n} \left( \gamma_a^\alpha O_n^\alpha \otimes A^\alpha \otimes 1_b + \gamma_b^\alpha O_n^\alpha \otimes 1_a \otimes B^\alpha \right),$$

where $A$ and $B$ are generic operators of two probes, $a$ and $b$, respectively, and $O$ denote system’s operators. The Hamiltonian of the full system reads,

$$H = H_0 + V.$$  

The many-body system Hamiltonian has the following spectrum,

$$H_0 |\psi_k\rangle = E_k |\psi_k\rangle.$$  

When the couplings vanish, $\gamma_a^{(b)} = 0$, the full system becomes degenerate as any quantum configuration of the probes contributes with the same energy. In this case,

$$H(\gamma = 0) |\Psi_k\rangle = E_k |\Psi_k\rangle,$$

where $|\Psi_k\rangle$ has degeneracy that equals the Hilbert dimension of the probes and hence the projectors onto the eigenstates obey,

$$\mathcal{P}_k = |\psi_k\rangle \langle \psi_k| \otimes 1_a \otimes 1_b.$$  

In general this degeneracy is lifted when the coupling to the probes is turned on, $|\gamma| > 0$. If this coupling is not too strong then degenerate perturbation theory will account for the necessary correction to the energy (and eigenstates) of the system. Since we are only interested in the physics of the probes, such as their correlations, we may get a general description of the problem by integrating out the degrees of freedom of the many-body system. This corresponds to projecting the Hamiltonian into the probes’s subspace.
C. Appendices for chapter 4

Here we derive equations (4.10) and (4.11) via the formalism of degenerate perturbation theory; a more general method — the Schrieffer-Wolff canonical transformation — will be introduced later (Appendix D.1). The procedure leading to the integration of the many-body degrees of freedom reads,

\[ H = H_0 + V \rightarrow H^{(ab)} := \mathcal{P}_0 \left( H_0 + W^{(1)} + W^{(2)} + \ldots \right) \mathcal{P}_0, \quad (C.6) \]

where \( H_0 + W^{(1)} + W^{(2)} + \ldots \) stands for an adequate perturbation series of \( H \) and \( H^{(ab)} \) the corresponding effective Hamiltonian of the probes. Please remark that \( \mathcal{P}_0 \) commutes with any operator with support in the Hilbert space of the probes; indeed, Eq. (C.6) corresponds to a ground state average. In what follows, for the sake of generality, we specify neither the nature of the probes nor the type of coupling to the many-body system.

Generic Formalism

We rewrite Eq. (C.2) as \( H(\alpha) = H_0 + \alpha V \) where \( \alpha \) is a dimensionless parameter which we suppose sufficiently small so that near \( \alpha = 0 \) the energy eigenstates are differentiable functions of \( \alpha \). It is convenient to write the projector onto the degenerate ground state as:

\[ \mathcal{P}_0 = \sum_{n=1}^{d} |\Psi_{0,n}\rangle \langle \Psi_{0,n}|, \]

where \( \{|\Psi_{0,n}\rangle\} \), with dimension \( d \), spans the degenerate ground state wave functions. An approximation to the ground state energy, \( E_{0,n} \), can be obtained through a Taylor expansion of \( E_{0,n}(\alpha) \), namely,

\[ E_{0,n}(\alpha) = E^{(0)}_n + \alpha E^{(1)}_n + \alpha^2 E^{(2)}_n + \ldots, \quad (C.7) \]

where we have defined \( E^{(0)}_n := E_{0,n}(0) \), \( E^{(1)}_n = \dot{E}_{0,n}(0) \) and \( E^{(2)}_n = \ddot{E}_{0,n}(0)/2 \) (overdot denotes \( \partial_\alpha \)).

By taking derivatives to the Schrödinger equation we get:

\[ (H - E_{0,n}) |\Psi_{0,n}\rangle = 0: \begin{cases} \left( H - E^{(1)}_n \right) |\Psi_{0,n}\rangle + \left( H - E^{(0)}_n \right) |\Psi_{0,n}\rangle = 0 \\ \left( H - E^{(0)}_n \right) |\Psi_{0,n}\rangle - 2 E^{(2)}_n |\Psi_{0,n}\rangle + 2 \left( H - E^{(1)}_n \right) |\Psi_{0,n}\rangle = 0 \end{cases}, \quad (C.8) \]

where all kets and operators are evaluated at \( \alpha = 0 \). We simplify the notation by making the following identifications: \( H(0) = H_0 \) and \( \dot{H} = V \) to get the following set of equations,

\[ \left( H_0 - E^{(0)}_n \right) |\Psi_{0,n}\rangle = 0, \quad (C.9) \]

\[ \left( V - E^{(1)}_n \right) |\Psi_{0,n}\rangle + \left( H_0 - E^{(0)}_n \right)|\Psi_{0,n}\rangle = 0, \quad (C.10) \]

\[ -2 E^{(2)}_n |\Psi_{0,n}\rangle + 2 \left( V - E^{(1)}_n \right) |\Psi_{0,n}\rangle + \left( H_0 - E^{(0)}_n \right) |\Psi_{0,n}\rangle = 0. \quad (C.11) \]

The first-order shift to the ground state energy is obtained acting with the projector onto the subspace...
of states with energy \(E_{0,n}\) when \(\alpha = 0\), i.e. with \(P_0\), on Eq. (C.10),

\[
E^{(1)}_n = \langle \Psi_{0,n} | V | \Psi_{0,n} \rangle, \quad \text{(C.12)}
\]

\[
P_0 V | \Psi_{0,n} \rangle = E^{(1)}_n | \Psi_{0,n} \rangle. \quad \text{(C.13)}
\]

The latter equation tells us that in the limit \(\alpha \rightarrow 0\) the eigenstate \(| \Psi_{0,n}(\alpha) \rangle\) of \(H(\alpha)\) is also an eigenstate of \(P_0 V\). This equation can be written in matrix form by introducing the resolution of the identity and making the inner product with an unperturbed state

\[
\sum_q \langle \psi_p | V | \psi_q \rangle \langle \psi_q | \Psi_{0,n} \rangle = E^{(1)}_n \langle \psi_p | \Psi_{0,n} \rangle, \quad \text{(C.14)}
\]

where \(| \psi_q \rangle \) is the unperturbed energy eigenbasis spanning the degenerate subspace with energy \(E^{(0)}_n\). The first-order contribution in Eq. (C.6) therefore reads

\[
W^{(1)} = V. \quad \text{(C.15)}
\]

The derivation of \(W^{(2)}\) can be carried out as follows; define the projector onto the states with unperturbed energy \(E^{(0)}_n\) that at the same time are eigenvectors of \(P_0 V\) with eigenvalue \(E^{(1)}_n\), i.e.

\[
P'_n | \Psi_{0,n} \rangle = | \Psi_{0,n} \rangle, \quad \text{(C.17)}
\]

\[
P'_n \left( V - E^{(1)}_n \right) P_0 = 0. \quad \text{(C.18)}
\]

We act with \(P'_n\) on Eq. (C.11): \(P'_n \left( V - E^{(1)}_n \right) | \Psi_{0,n} \rangle = E^{(2)}_n | \Psi_{0,n} \rangle\), and use relation (C.18) to get

\[
P'_n \left( V - E^{(1)}_n \right) (1 - P_0) | \Psi_{0,n} \rangle = E^{(2)}_n | \Psi_{0,n} \rangle. \quad \text{(C.19)}
\]

All we have to do now is to recast \(| \Psi_{0,n} \rangle\) into a suitable form; this can be done acting with \((1 - P_0)\) on (C.10), yielding

\[
(1 - P_0) | \Psi_{0,n} \rangle = \frac{1}{E^{(0)}_n - H_0} (1 - P_0) V | \Psi_{0,n} \rangle. \quad \text{(C.20)}
\]

Eq. (C.19) now reads:

\[
P'_n V \frac{1}{E^{(0)}_n - H_0} (1 - P_0) V | \Psi_{0,n} \rangle = E^{(2)}_n | \Psi_{0,n} \rangle. \quad \text{(C.21)}
\]

\(^1\)From Eq. (C.12) and the definition of \(P'_n\) we can write \(P_0 V\) as,

\[
P_0 V = E^{(1)}_n P'_n + \sum \xi Q^\xi, \quad \text{(C.16)}
\]

where \(\{ \xi \}\) stand for the eigenvalues of \(P_0 V\) other than \(E^{(1)}_n\) and \(Q^\xi\) the projectors onto the respective eigenvectors. Applying \(P'_n\) to the right of Eq. (C.16) and using the fact that the vectors forming each \(Q^\xi\) must be orthogonal to \(| \Psi_{0,n} \rangle\), one gets Eq. (C.18).
In problem of the probes interacting with a spin bath, one has $E^0_n = E_0$, with $E_0$ standing for the spin bath GS energy assumed non-degenerate [Eq. (C.5)]. Hence, we drop the subscript $n$ from now on. Finally, by noticing that $1 - \mathcal{P}_0 = \sum_{k>0} \mathcal{P}_k$, and applying the same procedure leading to Eq. (C.14), we get

$$ \sum_q \sum_{k>0} \left[ \frac{\langle \psi_p | V | \psi_k \rangle \langle \psi_k | V | \psi_q \rangle}{E(0) - E_k} \right] \langle \psi_q | \Psi_0 \rangle = E(2) \langle \psi_p | \Psi_0 \rangle, $$

(C.22)

from which the expression for the second-order term in Eq. (C.6) can be read out:

$$ W^{(2)} = - \sum_{k>0} V \frac{\mathcal{P}_k}{E_k - E(0)} V. $$

(C.23)

According to Eq. (C.6) the effective Hamiltonian is obtained by adding up the zero and first-order contributions to the latter equation and computing their ground state average

$$ H^{(ab)} = \left( E_0 + \langle V \rangle_0 - \sum_{k>0} \frac{1}{E_k - E(0)} \langle V \mathcal{P}_k V \rangle_0 + \cdots \right) \mathcal{P}_0, $$

(C.24)

where we have introduced the operator $\tilde{V} = V - \langle V \rangle_0$ and use the fact that $\langle \mathcal{P}_k \rangle_0 = \langle V \mathcal{P}_k \rangle_0 = 0$ when $k \neq 0$.

**Local coupling to the many-body system**

The treatment above is totally general and applies for any kind of perturbation $V$ as long as the many-body system is gapped. Now we specialize to the case where the probes interact locally with the many-body bulk. To this end we follow a similar procedure used to express cross sections of scattering by many-body systems in terms of its correlation functions [149]. Indeed, we start by expressing the denominator in the second-order term of Eq. (C.24) as:

$$ H^{(ab)}_{NL} = - \int_{-\infty}^{+\infty} dE \frac{1}{E} \sum_{k>0} \langle \psi_0 | \tilde{V} \mathcal{P}_k \tilde{V} | \psi_0 \rangle \delta(E - E_k - E_0), $$

(C.25)

and use the integral representation of the Dirac delta function,

$$ \delta(E) = (2\pi)^{-1} \int_{-\infty}^{+\infty} dt e^{iEt}, $$

(C.26)

to make the following manipulation,

$$ \langle \psi_0 | \tilde{V} \mathcal{P}_k \tilde{V} | \psi_0 \rangle \delta(E - E_k - E_0) \rightarrow \langle \psi_0 | e^{iEt} \tilde{V} e^{-iEt} \mathcal{P}_k \tilde{V} | \psi_0 \rangle $$

(C.27)

which conveniently introduces the evolution of the operators in the Heisenberg representation for the many-body system:

$$ e^{iEt} \tilde{V} e^{-iEt} = \tilde{V}(t) $$

(C.28)

Finally, because $\langle \tilde{V} \rangle_0 = 0$ by definition we can include the term $k = 0$ in the sum over $k$ to our
C.2. The response function and time correlation functions

In this appendix we derive the relation between the adiabatic susceptibility at zero frequency and time-dependent correlation functions [Eq. (4.15)]. In order to do so we use the spectral and Lehman representations. We assume time translation invariance and introduce the following notation,

\[ S_{AB}(t_1, t_2) = \langle A(t_1) B(t_2) \rangle = \langle A(t_1 - t_2) B(0) \rangle := S_{AB}(t_1 - t_2), \quad (C.30) \]

and \( O(t) = e^{iHt} O e^{-iHt} \) is the Heisenberg representation for operator \( O \). With this notation it is sufficient to show that the following relation holds

\[ \tilde{\chi}_{AB}(0) = i \int_{-\infty}^{\infty} dt \left( S_{AB}(t) + S_{BA}(t) \right) \text{sign}(t) e^{-\beta |t|}, \quad (C.31) \]

where \( \tilde{\chi}_{AB}(0) \) is the adiabatic susceptibility (or response function) at zero frequency; then, Eq. (4.15) immediately follows as it can be seen by direct inspection. To this purpose, we introduce (for later convenience) the *spectral function* \( \phi_{AB} \):

\[ \phi_{AB}(t) = S_{AB}(t) \mp S_{BA}(-t), \quad (C.32) \]

where the \( \mp \) applies when the operators \( A(B) \) are boson(fermion)-like operators. Following the tradition, we define the following Green functions

\[ G_{AB}^R(t) := -i \langle [A(t), B(0)]_\mp \rangle \theta(t) \quad \text{(retarded)} \quad (C.33) \]
\[ G_{AB}^A(t) := i \langle [A(t), B(0)]_\mp \rangle \theta(-t) \quad \text{(advanced)} \quad (C.34) \]

and recall that the response function \( \chi_{AB}(t) \) — the central object of linear response theory — is basically given by the retarded Green function,

\[ \chi_{AB}(t) = -G_{AB}^R(t). \quad (C.35) \]

The Lehman representation of correlation functions is obtained inserting the resolution of identity \( 1 = \sum_n |n\rangle \langle n| \), where \( \{ |n\rangle \} \) is a complete set of energy eigenstates:

\[ S_{AB}(t) = \frac{1}{2\beta} \sum_{n,m} e^{-\beta E_n} \langle n|A|m\rangle \langle m|B|n\rangle e^{i(E_n - E_m)t}, \quad (C.36) \]
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whose Fourier transform \( \tilde{S}_{AB}(\omega) \) reads

\[
\tilde{S}_{AB}(\omega) = \frac{2\pi}{i} \sum_{n,m} e^{-\beta E_n} \langle n|A|m\rangle \langle m|B|n\rangle \delta(\omega - E_m + E_n), \tag{C.37}
\]

obeying the detailed balance condition:

\[
\tilde{S}_{AB}(\omega) = e^{\beta\omega} S_{BA}(\omega). \tag{C.38}
\]

The latter can be easily proven by noticing that because of the delta function we can make the substitution: \( E_n \to E_m - \omega \), in Eq. (C.37). Using the detailed balance condition and the definition of spectral function we arrive at the important relations,

\[
\tilde{\phi}_{AB}(\omega) = \tilde{S}_{AB}(\omega) \left( 1 \mp e^{-\beta\omega} \right) \tag{C.39}
\]

\[
\tilde{\phi}_{BA}(\omega) = \tilde{S}_{BA}(\omega) \left( e^{-\beta\omega} \mp 1 \right). \tag{C.40}
\]

We are interested in the limit of zero temperature;

\[
\tilde{\phi}_{AB}(\omega) = \begin{cases} 
\tilde{S}_{AB}(\omega) & , \omega > 0 \\
0 & , \omega < 0.
\end{cases} \quad T = 0 \tag{C.41}
\]

The second line comes from Eq. (C.37) as \( \beta \to \infty \) implies a single contribution to the sum, namely \( n = 0 \), and thus \( \tilde{S}_{AB}(\omega) \to 0 \) for \( \omega < 0 \), since all states have \( E_m > E_0 \). Let us introduce the spectral representation of the retarded Green function (analogous formulas holds for the advanced Green function); from the definitions \( \text{(C.32)-(C.33)} \) we have

\[
iG_R^{AB}(t) = \phi_{AB}(t) \theta(t), \tag{C.42}
\]

from which we expect analytical behavior in the upper half of the complex plane as long as \( \phi_{AB}(t) \) does not grow as an exponential when \( t \to \infty \),

\[
i\tilde{G}^R_{AB}(z) = \int_0^\infty dt \phi_{AB}(t) e^{itz}, \quad \text{Im} z > 0. \tag{C.43}
\]

We now introduce the Fourier representation of the spectral function to write the Laplace transform as,

\[
i\tilde{G}^R_{AB}(z) = \int_{-\infty}^{\infty} d\omega \frac{\phi_{AB}(\omega)}{2\pi i} \frac{1}{z - \omega}, \quad \text{Im} z > 0. \tag{C.44}
\]

We know take advantage of the special form of \( \phi_{AB}(\omega) \) at zero temperature [Eq. (C.41)] to write the Fourier transform [obtained via analytical continuation to the real axis \( z \to \omega + i0^+ \)] of the Laplace
C.3. Analytic continuation of Green’s functions

It is possible to relate time ordered Green functions (with real or imaginary time) to the retarded Green’s function for bosons $G_{AB}^R(t)$ by making a proper analytic continuation into the whole complex transform:

$$iG_{AB}^R(\omega) = \int_0^\infty \frac{dx}{2\pi i} \frac{\tilde{\phi}_{AB}(x)}{\omega - x + 0^+},$$  \hspace{1cm} (C.45)

$$= PV \int_0^\infty \frac{dx}{2\pi i} \frac{\tilde{\phi}_{AB}(x)}{\omega - x} - \frac{1}{2} \tilde{\phi}_{AB}(\omega),$$  \hspace{1cm} (C.46)

where PV denotes the Cauchy principal value. The detailed balance condition at $T = 0$ yields

$$iG_{AB}^R(\omega) = PV \int_0^\infty \frac{dx}{2\pi i} \left( \frac{\tilde{S}_{AB}(x)}{\omega - x} + \frac{\tilde{S}_{BA}(x)}{\omega + x} - \frac{1}{2} (S_{AB}(\omega) + S_{BA}(\omega)) \right).$$  \hspace{1cm} (C.47)

If the system has an unique ground state and a gap then it is clear from the Lehman representation of the correlations [Eq. (C.37)] that in the limit $T \to 0$ the only term surviving for $\omega = 0$ is

$$\tilde{S}_{AB}(0) = \tilde{S}_{BA}(0) = 2\pi \langle A \rangle_0 \langle B \rangle_0 \delta(\omega).$$  \hspace{1cm} (C.48)

The zero frequency response for boson-like operators, $\tilde{\chi}_{AB}(0) = -\tilde{G}_{AB}^R(0)$, is therefore given by,

$$\tilde{\chi}_{AB}(0) = PV \int_0^\infty dx 2\pi \left( \frac{\tilde{S}_{AB}(x)}{x} + \frac{\tilde{S}_{BA}(x)}{x} \right), \hspace{1cm} T = 0.$$  \hspace{1cm} (C.49)

In order to obtain relation (C.31) we must relate the integral above to an integral in the time domain,

$$\int_0^\infty dt S_{AB}(t)e^{i(\omega t + 0^+)} = -\int_{-\infty}^0 dx \frac{\tilde{S}_{AB}(x)}{2\pi i \omega - x + 0^+},$$  \hspace{1cm} (C.50)

$$\int_{-\infty}^0 dt S_{AB}(t)e^{i(\omega t - 0^+)} = \int_{-\infty}^\infty dx \frac{\tilde{S}_{AB}(x)}{2\pi i \omega - x - 0^+},$$  \hspace{1cm} (C.51)

where $0^+$ assures convergence. We now perform the following manipulation,

$$\int_{-\infty}^\infty dx \frac{\tilde{S}_{AB}(x)}{2\pi i \omega - x + i0^+} = PV \int_{-\infty}^\infty dx \frac{\tilde{S}_{AB}(x)}{2\pi i \omega - x} + \frac{\tilde{S}_{AB}(\omega)}{2}.\hspace{1cm} (C.52)$$

Finally we add up contributions (C.50) and (C.51) in the light of the latter relation to get,

$$\int_{-\infty}^\infty dt \text{sign}(t)S_{AB}(t)e^{-0^+|t|} = PV \int_{-\infty}^\infty dx \frac{\tilde{S}_{AB}(x)}{\pi i x} \hspace{1cm} \omega = 0,$$  \hspace{1cm} (C.53)

from which we prove the desired result [Eq. (C.31)] and thus Eq. (4.15).
plane. These relations can be useful when some method is available that is easier to compute one of them. For instance, functional integral methods allow to obtain time-ordered correlation functions in a consistent way, although, at the end, we are always interested in physical quantities such as the adiabatic susceptibility and these correspond to retarded Green’s functions [Eq. (C.35)] not to ordered functions. Analytic continuation is a powerful method that makes the bridge between these two kinds of Green’s functions. They can take place in the frequency domain (commonly seen in Condensed Matter) or in the time domain (this will be used to compute the retarded Green’s function on a cylinder in Appendix C.3). This appendix outlines both methods.

Denoting real time by $t$, imaginary time (or temperature variable) by $\sigma$ and the time ordering operator by $T$, these Green’s functions read:

$$ G_{AB}^{R}(t) := -i\langle [A(t), B(0)] \rangle \theta(t) \quad \text{(retarded Green function)} \quad (C.54) $$

$$ G_{AB}^{T}(t) := \langle T_{t} [A(t)B(0)] \rangle \quad \text{(time-ordered Green function)} \quad (C.55) $$

$$ G_{AB}(\tau) := \langle T_{\sigma} [A(\sigma)B(0)] \rangle \quad \text{(Matsubara Green function)} \quad (C.56) $$

where the action of the time ordering operator is to take the operators defined at later time to the left:

$$ T_{t}[A(t)B(0)] := \theta(t)A(t)B(0) + \theta(-t)B(0)A(t), \quad (C.57) $$

$$ T_{\sigma}[A(\sigma)B(0)] := \theta(\sigma)A(\sigma)B(0) + \theta(-\sigma)B(0)A(\sigma), \quad (C.58) $$

and all the operators are written in the Heisenberg representation, namely, $A(t) = e^{iHt}Ae^{-iHt}$ and $A(\sigma) = e^{i\sigma H}Ae^{-i\sigma H}$.

Analytic continuation (frequency domain)

We wish to relate the Matsubara Green’s function to the retarded Green’s function in the frequency domain. To this end we express $G_{AB}(\tau)$ in the Lehman representation [see in Eq. (C.36)]:

$$ \langle A(\sigma)B(0) \rangle = \frac{1}{2\beta} \sum_{n,m} e^{-\beta E_{n}} \langle m|A|n \rangle \langle n|B|m \rangle e^{\sigma(E_{m} - E_{n})}, \quad (C.59) $$

$$ \langle B(0)A(\sigma) \rangle = \frac{1}{2\beta} \sum_{n,m} e^{-\beta E_{n}} \langle n|B|m \rangle \langle m|A|n \rangle e^{\sigma(E_{m} - E_{n})}. \quad (C.60) $$

These expressions imply that the Matsubara Green’s function (or temperature Green’s function) is periodic as:

$$ G_{AB}(\sigma) = G_{AB}(\sigma - \beta), \quad (C.61) $$

for $\sigma \in [0, \beta]$. Therefore one should be able to expand $G_{AB}(\sigma)$ in Fourier series in the interval $0 \leq \sigma \leq \beta$:

$$ G_{AB}(\sigma) = \sum_{\mu} e^{2\pi i \mu \sigma / \beta} \tilde{G}_{AB}(\mu), \quad (C.62) $$

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C.3. Analytic continuation of Green’s functions

where \( \mu = 0, \pm 1, \pm 2, \ldots \). The Fourier coefficients read

\[
\tilde{G}_{AB}(\mu) = \frac{1}{\beta} \int_0^\infty d\sigma e^{-2\pi \mu \sigma / \beta} G_{AB}(\sigma)
\]

\[
= \frac{1}{\beta} \int_0^\infty d\sigma e^{-2\pi \mu \sigma / \beta} A(\sigma)B(0)
\]

\[
= \frac{1}{\beta \bar{\mu}} \int_0^\infty d\sigma e^{-2\pi \mu \sigma / \beta} \sum_{n,m} e^{-\beta E_n} \langle m|A|n\rangle \langle n|B|m \rangle e^{\sigma(E_m-E_n)}
\]

\[
= \frac{1}{\beta \bar{\mu}} \sum_{n,m} \langle m|A|n\rangle \langle n|B|m \rangle \frac{e^{-\beta E_n} - e^{-\beta E_m}}{E_m - E_n - i\bar{\mu}},
\]

where we have defined \( \bar{\mu} = 2\pi \mu / \beta \). Comparing the latter equation with the Fourier transform \( \tilde{S}_{AB}(\omega) \) of the correlation function \( \langle A(t)B(0) \rangle \) [Eq. (C.37)] we immediately conclude,

\[
\tilde{G}_{AB}(\bar{\mu}) = \frac{1}{\beta} \int_{-\infty}^{\infty} dx \tilde{S}_{AB}(x) \frac{e^{-\beta \bar{\mu} x}}{i\bar{\mu} + x},
\]

\[
= \frac{1}{\beta \bar{\mu}} \int_{-\infty}^{\infty} dx \tilde{\phi}_{AB}(x)
\]

\[
= \frac{1}{\beta \bar{\mu}} \sum_{n,m} \langle m|A|n\rangle \langle n|B|m \rangle \frac{e^{-\beta E_n} - e^{-\beta E_m}}{E_m - E_n - i\bar{\mu}}.
\]

The last equality was obtained via the definition of spectral function [Eq. (C.32)] and can be simplified using the detailed balance condition [Eq. (C.39)]:

\[
\tilde{G}_{AB}(\bar{\mu}) = \frac{1}{\beta} \int_{-\infty}^{\infty} dx \tilde{S}_{AB}(x) \frac{1 - e^{-\beta x}}{2\pi i \bar{\mu} + x},
\]

showing that the Fourier coefficients can be computed from a single correlation function. Comparing (C.65) with the Fourier transform of the retarded Green’s function [Eq. (C.45)] we get the desired relation:

\[
\tilde{G}_{AB}^R(\omega) = -\beta G_{AB}(\bar{\mu} \rightarrow i\omega - 0^+).
\]

The formal procedure \( \bar{\mu} \rightarrow i\omega - 0^+ \) amounts to an analytic continuation for \( \tilde{G}_{AB}(\bar{\mu}) \) is defined only at a discrete set of points in the complex plane, namely, \( \bar{\mu} = 0, \pm 2\pi / \beta, \pm 4\pi / \beta, \ldots \).

**Analytic continuation (time domain)**

In the time domain the relation between the time-ordered (C.55) and retarded (C.54) Green’s functions can be obtained with little algebra:

\[
G_{AB}^R(t) = i \left[ G_{AB}^T(t) - (G_{B^A^T}^T(-t))^\dagger \right] \theta(t).
\]

It is useful to consider the particular case of Hermitian operators (i.e. \( A^\dagger = A \) and \( B^\dagger = B \)). In this case we get a simpler expression,

\[
G_{AB}^R(t) = -2\text{Im} \left[ G_{AB}^T(t) \right] \theta(t).
\]
Since one usually works with imaginary time \((e.g.)\) when computing correlations from finite temperature path integral methods, it is convenient to express \(G_{AB}^R(t)\) as function of the Matsubara’s Green function. This is done via Wick rotation according to \(\sigma \rightarrow it + 0^+ \text{sign}(t)\),

\[
G_{AB}^R(t) = -2\text{Im} \left[ G_{AB} \left( \sigma \rightarrow it + 0^+ \text{sign}(t) \right) \right] \theta(t). \tag{C.70}
\]

### C.4. Time-ordered Green’s function from conformal mapping

The method of relating the physics of different geometries from conformal invariance was originally developed by Cardy [154, 188]. Here we apply this method to our problem, namely that of computing the time-ordered Green’s function \(G_{AB}^T(t)\) for the finite AF spin chain with \(SU(2)\) symmetric Heisenberg interactions. First we extract the asymptotic Matsubara function of the AF Heisenberg ring from the correlations of the infinite chain and, at the end, perform an analytic continuation to real time in order to get \(G_{AB}^T(t)\).

The crucial point is to find a proper analytic mapping between the critical theory (which is defined in the whole plane: \(1 + 1\) space-time) and the theory defined in the ring (which including time corresponds to a strip with boundary conditions along the spatial direction). The analytic mapping performing such mapping is

\[
w = \frac{L}{2\pi} \ln z = \sigma + ir, \tag{C.71}
\]

where we have taken the primary branch of the log-function and \(z\) is a complex coordinate in the plane \(z = \nu_F \tau + ix\). The imaginary part of \(\ln z\) lies in the interval \([-\pi, \pi]\) whereas its real part can take any value, thus achieving the desired mapping (see Fig. 1).

![Figure C.1](image)

Figure C.1.: The conformal transformation \(w(z) = \sigma + ir\) maps every point \((\nu_F \tau, x)\) in the plane into the strip geometry \((\sigma \in [-\infty, \infty], r \in [-L/2, L/2])\) with periodic boundary conditions along the \(r\) direction. The plane is effectively compactified acquiring the topology of a cylinder.

Afterwards, all one has to do is to apply the transformation law for conformal invariant systems.
Indeed, we begin by writing the Matsubara Green’s function of the 1D antiferromagnet [see \[153,155\] for a derivation and also Eq. (4.26)] in an appropriate form,

$$\langle M(z)M(0) \rangle_\infty \sim \frac{\mathcal{A}}{|x - ivF\tau|} = \frac{\mathcal{A}}{\sqrt{(z\bar{z})}}$$  \hspace{1cm} (C.72)

We have used the notation $G(x, \tau) = \langle \hat{T} \tau M(x, \tau)M(0,0) \rangle = \langle M(z)M(0) \rangle$, where $M(x, \tau) = e^{\tau H}M(x)e^{-\tau H}$ denotes the staggered magnetization in the Heisenberg representation with imaginary time. The theory is critical with conformal weight $\mu = 1/2$ [Eq. (4.22)] and therefore conformal invariance implies the following transformation law [Eq. (4.24)]:

$$\langle M(w)M(0) \rangle_{\text{strip}} = \left| \frac{\partial w}{\partial z}(z) \frac{\partial w}{\partial z}(0) \right|^{-1/2} \langle M(w)M(0) \rangle_\infty,$$  \hspace{1cm} (C.73)

with $\langle M(w)M(0) \rangle_{\text{strip}}$ being the Matsubara Green’s function defined in the strip geometry corresponding to a finite chain with periodic boundary conditions. Denoting the time variable by $u$ and the space variable by $r$, a simple calculation yields Eq. (4.27), namely,

$$\langle M(w)M(0) \rangle_{\text{strip}} = \frac{2\pi}{\sqrt{2L}} \frac{\mathcal{A}}{\sqrt{\cosh(\frac{2\pi \sigma}{L}) - \cos(\frac{2\pi r}{L})}}.$$  \hspace{1cm} (C.74)

Some comments are in order; the latter expression is periodic in the spatial coordinate ($r$) in accordance with the choice we made in the space-time labelling [Eq. (C.71)]. The analytic form of the non-universal amplitude $\mathcal{A}$ arising from the bosonization of the Hamiltonian is unknown, but Eq. (C.74) has all the information we need to prove quasi-perfect LDE (Sec. 4.3.1). We also remark that the finite temperature correlator of the infinite chain can be obtained via conformal invariance if instead of make a compactification of the spatial variable [Eq. (C.71)] we do it in time. This amounts to make the analytic continuation $L \rightarrow i\beta$, since now it is the temperature that takes values within a

---

Figure C.2.: The principal branch cut of the logarithm function: $\mathbb{C} \setminus \{x + iy | x \leq 0 \land y = 0 \}$. 

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finite range, one gets:

$$
\langle M(w)M(0) \rangle_\beta = \frac{2\pi}{\sqrt{2\beta}} \sqrt{\frac{\mathcal{A}}{\cosh \left( \frac{2\pi r}{\beta} \right) - \cos \left( \frac{2\pi \sigma}{\beta} \right)}}.
$$

recovering the familiar result of statistical mechanics of a exponentially decaying correlation function

$$
\sim e^{-\pi r/\beta}
$$

with correlation length inversely proportional to the temperature $\xi = \beta/\pi$ in the limit $r \gg \beta$.

We now compute $G^R(x,t)$ from Matsubara’s Green’s function [Eq. (C.74)] via the procedure discussed in the previous Appendix [see Eqs. (C.69)-(C.70)]. First, we need the time-ordered Green’s function,

$$
G_T(x,t) = \langle \hat{T} M(x,t)M(0,0) \rangle.
$$

To this end, we Wick rotate the imaginary time variable $\sigma \rightarrow it + 0^+ \text{sign}(t)$. In accordance, we must perform the replacement

$$
\cosh \left( \frac{2\pi \sigma}{L} \right) \rightarrow \cosh \left[ \frac{2\pi}{L} (it + 0^+ \text{sign}(t)) \right]
$$

(C.76)

and take the imaginary part. It is convenient to recast $G^R(x,t)$ into the form

$$
G^R(x,t) = \sqrt{2\pi} (\mathcal{A}/L)e^{-1/2\ln K(t)},
$$

(C.78)

where we have considered the branch cut of the square-root-function to be the principal branch cut of the log-function, i.e. $\mathbb{C} \setminus \{x+iy \mid x \leq 0 \land y = 0\}$ (see Fig. C.2). With these definitions,

$$
K(t) = \cos \left( \frac{2\pi t}{L} \right) - i0^+ \text{sign}(t) \sin \left( \frac{2\pi t}{L} \right) - \cos \left( \frac{2\pi r}{L} \right).
$$

(C.79)

Hence, $G^T(x,t)$ has a imaginary part if and only if $\cos (2\pi t/L) < \cos (2\pi r/L)$:

$$
\ln K(t) = \ln \left[ \cos \left( \frac{2\pi t}{L} \right) - \cos \left( \frac{2\pi r}{L} \right) \right] +
$$

$$
+ i\pi \text{sign} \left[ \sin \left( \frac{2\pi t}{L} \right) \right] \theta \left[ \cos \left( \frac{2\pi t}{L} \right) - \cos \left( \frac{2\pi r}{L} \right) \right].
$$

(C.80)

From the latter expression and Eq. (C.69) we finally get the retarded Green’s function:

$$
G^R(x,t) = -\frac{2\pi}{\sqrt{2L}} \theta \left[ \frac{\cos \left( \frac{2\pi t}{L} \right) - \cos \left( \frac{2\pi r}{L} \right) \theta(t)}{\cos \left( \frac{2\pi t}{L} \right) - \cos \left( \frac{2\pi r}{L} \right)} \right] \text{sign} \left[ \sin \left( \frac{2\pi t}{L} \right) \right].
$$

(C.81)
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D.1. The Schrieffer-Wolff canonical transformation

In Appendix C.1 the effective Hamiltonian between two probes interacting with a larger system was derived via degenerate perturbation theory. Here we will derive the same result via a more powerful method, namely the Schrieffer-Wolff canonical transformation [189]. This method will allow us to take into consideration the effect of the probes renormalization and open the door to compute their partial state in perturbation theory (Appendix D.2).

We start by recalling the Hamiltonian of the full system:

\[ H = H_0 + V, \]  
\[ (D.1) \]

where \( H_0 \) is the many-body Hamiltonian and \( V \) describes an interaction. In Chapters 4 and 5 the interaction corresponds to two probes, \( a \) and \( b \), coupling locally to the many-body bulk, but we make \( V \) unspecified for the moment for the sake of generality. We represent the ground-state wavefunction of the many-body system (the spin bath) by \( |\psi_0\rangle \) and conveniently write \( (D.1) \) in the form,

\[ \bar{H}_0 = \sum_i P_i H P_i \]  
\[ (D.3) \]

\[ \bar{V} = \sum_{i \neq j} P_i H P_j \]  
\[ (D.4) \]

\[ \bar{V} = V - \langle \psi_0 | V | \psi_0 \rangle. \]

Following the standard condensed-matter approach, we assume that the spectrum of \( H_0 \) consists of disjoint sectors labeled by the index \( i \) in each of which the spectrum can be either continuous or semicontinuous, i.e. \( |E_{i\mu} - E_{i\nu}| \ll |E_{i\alpha} - E_{i\beta}| \). We denote by \( P_i = \sum_\mu |\psi_{i,\mu}\rangle \langle \psi_{i,\mu}| \) the projector operator into the eigenstates of \( H_0 \) with energy \( E_i \) and suppose that \( \bar{V} \) has no matrix elements between eigenstates in the same sector (this is always the case in the systems of spins we study in this monograph 1).

\[ \langle \psi_i | \bar{V} | \psi_i \rangle = 0. \]

With these definitions in mind we can write,

\[ \begin{align*}
\bar{H}_0 &= \sum_i P_i H P_i \\
\bar{V} &= \sum_{i \neq j} P_i H P_j
\end{align*} \]

\[ (D.3) \]

\[ (D.4) \]

\[ 1 \text{ To see this is sufficient to take the rotational invariant form of } V \text{ [Eq. (5.1)] and take the average in sector } i \text{. This yields, } \alpha J \langle \psi_i | S_a \cdot \tau_a + S_b \cdot \tau_b | \psi_i \rangle. \text{ On the other hand, each of these averages must vanish due to the probe’s full degeneracy at } \alpha = 0, \text{ that is } \langle \psi_i | r^{a/b}_m | \psi_i \rangle = 0 \text{ [see Eqs. (C.4)-(C.5) and comments therein].} \]
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The canonical transformation $S$ will change Eq. (D.2) according to,

$$e^{-i\epsilon S} He^{i\epsilon S} = \tilde{H}_0 + \epsilon (\tilde{V} - i [\tilde{S}, \tilde{H}_0]) + O(\epsilon^2), \quad (D.5)$$

where $\epsilon$ is formal expansion parameter that we set equal to one at the end of the calculation. We fix the generator to be $\tilde{S} = \tilde{S}$, such that,

$$\tilde{V} + i [\tilde{H}_0, \tilde{S}] = 0. \quad (D.6)$$

In the spirit of degenerate perturbation theory (Appendix C.1), we apply projectors operators to the left and right of the latter equation. Using relation (D.4) we find,

$$P_i (\tilde{V} + i [\tilde{H}_0, \tilde{S}]) P_j \equiv P_i P_j (1 - \delta_{ij}) = 0 \iff P_i (\tilde{S} \tilde{P}_j - \tilde{P}_j \tilde{S} P_j) = 0 \iff P_i P_j = -i (\tilde{P}_i \tilde{S} P_j \tilde{P}_j - \tilde{P}_j \tilde{P}_i \tilde{S} P_j) \quad (D.7)$$

where in the last step we assumed $i \neq j$. Making the substitution $P_j \tilde{P}_j \rightarrow E_j P_j$, with $E_i \mu \approx \langle E_i \mu \rangle$ or $E_i$ approximated by the average energy of sector $E_i$, i.e. $E_i \mu \approx \langle E_i \mu \rangle \equiv E_i$, we finally get,

$$i P_i \tilde{S} P_j \approx \frac{\tilde{P} \tilde{V} P_j}{E_i - E_j} (1 - \delta_{ij}). \quad (D.10)$$

On the other hand, from the definition of the generator $\tilde{S}$ [Eq. (D.6)] we easily choose $P_i \tilde{S} P_i = 0$ and thus the equation above give us all the non-zero matrix elements of $\tilde{S}$. Indeed, we return to the transformed Hamiltonian [Eq. (D.5)] under the generator $\tilde{S}$,

$$H \rightarrow e^{-i\tilde{S}} He^{i\tilde{S}} = \tilde{H}_0 + \frac{1}{2} \tilde{S} [\tilde{H}_0 + \tilde{V}] + O(\alpha^3 \Delta^{-2})$$

where $\nu$ denotes an energy scale of $\tilde{V}$ and $\Delta$ a gap scale of the unperturbed Hamiltonian $H_0$. We define the effective Hamiltonian,

$$H_S := \tilde{H}_0 - \frac{1}{2} \tilde{S} \tilde{V} \quad (D.11)$$

which, by the virtue of Eq. (D.10), equals the effective Hamiltonian derived earlier [Eq. (C.24)], when projected onto the many-body lowest energy sector by the action of $P_0$.

We are finally in position to specialize to the case of two probes, $a$ and $b$, that locally couple to a spin bath. The projection procedure [Eq. (C.6)] integrates out the redundant degrees of freedom, and yields an effective low-dimensional Hamiltonian describing the physics of the probes as function of $\alpha$ and all the relevant parameters of the condensed-matter bulk. The probe-bath interaction has the
following form

\[ V = J\alpha (\mathbf{\tau}_a \cdot \mathbf{S}_A + \mathbf{\tau}_b \cdot \mathbf{S}_B), \quad (D.14) \]

where \( \alpha J \) is the coupling strength between the probe qubits and the lattice, and \( J \) a characteristic energy scale of the lattice. Eq. (D.14) describes an isotropic interaction between the probes [with Pauli operators, \( \mathbf{\tau}_a(b) \)] and the bath spins, \( \mathbf{S}_A(B) \), at specific lattice sites \( A(B) \). Denoting the probe \( a(b) \) space state by \( |\chi^{a(b)}_\alpha\rangle \) with \( \alpha = \{\uparrow, \downarrow\} \), the projection onto the many-body system ground state reads,

\[
H^{(ab)}_{\text{eff}} = \langle \psi_0 | H_{S} | \psi_0 \rangle = (J^2 \alpha^2 \tilde{\chi}_{ab}^{zz}(0) + O(\alpha^3 \Delta^{-2})) \mathbf{\tau}_a \cdot \mathbf{\tau}_b, \quad (D.18)
\]

where we have set to zero all the constants as they not change the eigenstates.

D.2. The probe operators renormalization

In the previous appendix we derived the effective Hamiltonian of two probes interacting with a gapped many-body system via the Schrieffer-Wolff canonical transformation formalism. We obtained the same result of degenerate perturbation theory, namely Eq. (D.18). In order to get the low energy of the probes, we projected the effective Hamiltonian, \( H_S \), onto the spin bath ground state

\[
H_{\text{eff}} := \langle \psi_0 | H_{S} | \psi_0 \rangle = (J^2 \alpha^2 \tilde{\chi}_{ab}^{zz}(0) + O(\alpha^3 \Delta^{-2})) \mathbf{\tau}_a \cdot \mathbf{\tau}_b, \quad (D.19)
\]

At first sight one concludes that, as long as \( \tilde{\chi}_{ab}^{zz}(0) > 0 \), the probes form a perfect singlet for sufficiently small \( \alpha \). Indeed, the average value of \( \mathbf{\tau}_a \cdot \mathbf{\tau}_b \) in the ground state \( |\psi_{\text{eff}}\rangle \) of the effective Hamiltonian, \( |\psi_{\text{eff}}\rangle \), reads

\[
\langle \psi_{\text{eff}} | \mathbf{\tau}_a \cdot \mathbf{\tau}_b | \psi_{\text{eff}} \rangle = -3 = \min_{\phi \in \mathbb{C}^2 \otimes \mathbb{C}^2} \langle \phi | \mathbf{\tau}_a \cdot \mathbf{\tau}_b | \phi \rangle. \quad (D.20)
\]
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However, the value of $-3$ must be an approximation to the real average of $\tau_a \cdot \tau_b$:

$$\langle \Psi_0 | \tau_a \cdot \tau_b | \Psi_0 \rangle \geq -3.$$  \hspace{1cm} (D.21)

The origin of the apparent incompatibility between Eqs. (D.20) and (D.21) can be comprehended by noting that wave functions also change according to the canonical transformation $\hat{S}$:

$$H \rightarrow e^{-i\hat{S}}He^{i\hat{S}} = H_S$$  \hspace{1cm} (D.22)

$$|\Psi_0 \rangle \rightarrow e^{-i\hat{S}}|\Psi_0 \rangle = |\Psi_0^{(S)} \rangle$$  \hspace{1cm} (D.23)

The above formulae show how operators and wave-functions change according to $\hat{S}$. Let us inspect how the averages of a generic operator $A$ look like in both pictures,

$$\langle \Psi_0 | A | \Psi_0 \rangle = \langle \Psi_0^{(S)} | e^{-i\hat{S}}Ae^{i\hat{S}} | \Psi_0^{(S)} \rangle$$  \hspace{1cm} (D.24)

Given the perturbative nature of the transformation, we can make following operator expansion

$$e^{-i\hat{S}}Ae^{i\hat{S}} = A - [i\hat{S}, A] + O(J^2 \alpha^2 \Delta^{-2})$$  \hspace{1cm} (D.25)

and so,

$$\langle \Psi_0 | A | \Psi_0 \rangle = \langle \Psi_0^{(S)} | A | \Psi_0^{(S)} \rangle - \langle \Psi_0^{(S)} | [i\hat{S}, A] | \Psi_0^{(S)} \rangle + O(J^2 \alpha^2 \Delta^{-2}).$$  \hspace{1cm} (D.26)

The second term is already a $J\alpha/\Delta$ correction, so, we would conclude that, to lowest order in the perturbation, one has

$$\langle \Psi_0 | \tau_a \cdot \tau_b | \Psi_0 \rangle = \langle \Psi_0^{(S)} | \tau_a \cdot \tau_b | \Psi_0^{(S)} \rangle + O(J\alpha/\Delta).$$  \hspace{1cm} (D.27)

In fact, in this particular case, one can show that the first correction is zero. Since the state $|\Psi_0^{(S)} \rangle$ is a $\tau_a$, $\tau_b$ singlet, it is an eigenstate of $\tau_a \cdot \tau_b$ with eigenvalue $-3$. In that case, the average $\langle \Psi_0^{(S)} | [i\hat{S}, A] | \Psi_0^{(S)} \rangle$ is trivially zero. Therefore,

$$\langle \Psi_0 | \tau_a \cdot \tau_b | \Psi_0 \rangle = -3 + O(J^2 \alpha^2 / \Delta^2).$$  \hspace{1cm} (D.28)

The value of the negativity will deviate from the value of maximum entanglement (singlet state) with $O(J^2 \alpha^2 / \Delta^2)$ corrections. This as an important consequence: when computing averages in the canonical basis we have to properly renormalize the operators, since, as we have just seen,

$$\langle \Psi_0 | \tau_a \cdot \tau_b | \Psi_0 \rangle \neq \langle \Psi_0^{(S)} | \tau_a \cdot \tau_b | \Psi_0^{(S)} \rangle.$$  \hspace{1cm} (D.29)
The correct value of the probes correlation, $\langle \Psi_0^S | \tau_a \cdot \tau_b | \Psi_0^S \rangle$, must take into account the way $\tau_a \cdot \tau_b$ changes due to the canonical transformation:

$$\langle \tau_a \cdot \tau_b \rangle = \langle \Psi_0^S | e^{-i \hat{S}_a \cdot \tau_b} e^{i \hat{S}_a \cdot \tau_b} | \Psi_0^S \rangle = \langle \Psi_0^S | \tau^R_a \cdot \tau^R_b | \Psi_0^S \rangle,$$

(D.30)

where the superscript $R$ means that the operator is properly renormalized by the action of $\hat{S}$. These observations make it clear that the quantitative physics of the probes is not captured by the effective Hamiltonian alone.

An important conclusion of this observation is that the effective Hamiltonian cannot be employed directly to derive the partial state of the probes. We now compute the correct partial state of the probes and see how it relates with $H_{\text{eff}}$ and especially with its energy scale $J_{\text{eff}}$ [see Eq. (4.19) for definition]. The full rotational symmetry entails that the probe density matrix can be written as a function of a single invariant,

$$\hat{\rho}_{ab} = \frac{1}{3} e^{-\beta J_{ab}(\beta)} + e^{3 \beta J_{ab}(\beta)} \exp(-\beta J_{ab}(\beta) \tau_a \cdot \tau_b),$$

(D.31)

This tells us very little for the moment since the temperature dependence of $J_{ab}(\beta)$ is unknown. On the other hand, by definition,

$$\langle \tau_a \cdot \tau_b \rangle = \text{Tr}_{\rho} \left[ e^{-\beta H_{\text{eff}}} \tau_a \cdot \tau_b e^{\beta H_{\text{eff}}} \right]$$

(D.32)

and, using the canonical transformation $\hat{S}$,

$$\langle \tau_a \cdot \tau_b \rangle = \frac{\text{Tr} \left[ e^{-\beta H_{\text{eff}}} \tau_a \cdot \tau_b e^{\beta H_{\text{eff}}} \right]}{\text{Tr} \left[ e^{-\beta H_{\text{eff}}} \right]}$$

(D.33)

The transformed Hamiltonian is $H_{\text{eff}} = H_p + H_{\text{eff}}$, the corresponding eigenbasis is made of product states [Eqs. (5.4)-(5.5)]. Under the assumption that $k_B T \ll \Delta(\alpha)$ (i.e. that the temperature is much smaller than the gap to excited states of the bath), we can limit the trace to the states of the form $| \psi_0 \rangle \otimes | \chi \rangle$, where $| \chi \rangle$ is any probe state, and $| \psi_0 \rangle$ is the non-degenerate ground state of the spin bath. This leads to

$$\langle \tau_a \cdot \tau_b \rangle = \frac{\text{Tr}_p \left[ e^{-\beta H_p} \langle \psi_0 | e^{-i \hat{S}_a \cdot \tau_b} e^{i \hat{S}_a \cdot \tau_b} | \psi_0 \rangle \right]}{\text{Tr}_p \left[ e^{-\beta H_p} \right]}$$

(D.34)

where $\text{Tr}_p(\ldots)$ is a trace over probe states only. Since the operator $\tau_a \cdot \tau_b$ is diagonal in bath space,
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this can obviously be written as

\[
\langle \tau_a \cdot \tau_b \rangle = \frac{\text{Tr} \left[ e^{-\beta H_p} \sum_m \langle \psi_0 | e^{-i\hat{S}} | \psi_m \rangle \tau_a \cdot \tau_b \langle \psi_m | e^{i\hat{S}} | \psi_0 \rangle \right]}{\text{Tr} \left[ e^{-\beta H_p} \right]} \tag{D.36}
\]

\[
\frac{\text{Tr} \left[ e^{-\beta H_p} \sum_m A_m \tau_a \cdot \tau_b A_m^\dagger \right]}{\text{Tr} \left[ e^{-\beta H_p} \right]} \tag{D.37}
\]

where \( A_m \equiv \langle \phi_0 | e^{-i\hat{S}} \phi_m \rangle \) is an operator defined in probe space. By symmetry, the operator

\[
\sum_m A_m \tau_a \cdot \tau_b A_m^\dagger = \langle \psi_0 | e^{-i\hat{S}} \tau_a \cdot \tau_b e^{i\hat{S}} | \psi_0 \rangle \tag{D.38}
\]

must be a scalar in probe space, and, therefore, of the form

\[
\sum_m A_m \tau_a \cdot \tau_b A_m^\dagger = \eta + (1 - \Phi) \tau_a \cdot \tau_b \tag{D.39}
\]

where \( \eta \) and \( \Phi \) are, by construction, temperature independent renormalization constants. Since

\[
\text{Tr} \left[ \tau_a \cdot \tau_b \right] = 0, \quad \text{and} \quad \tau_a \cdot \tau_b \right)^2 = 3 - 2 \tau_a \cdot \tau_b \tag{D.40}
\]

we obtain

\[
\frac{\text{Tr} \left[ \sum_m A_m \tau_a \cdot \tau_b A_m^\dagger \right]}{\text{Tr} \left[ e^{-\beta H_p} \right]} = 4 \eta \tag{D.41}
\]

\[
\frac{\text{Tr} \left[ \sum_m \tau_a \cdot \tau_b A_m \tau_a \cdot \tau_b A_m^\dagger \right]}{\text{Tr} \left[ e^{-\beta H_p} \right]} = 12(1 - \Phi) \tag{D.42}
\]

With these definitions it is clear that

\[
\langle \tau_a \cdot \tau_b \rangle = \eta + (1 - \Phi) \langle \tau_a \cdot \tau_b \rangle_{\text{can}} \tag{D.43}
\]

where,

\[
\langle \tau_a \cdot \tau_b \rangle_{\text{can}} := \frac{\text{Tr} \left[ e^{-\beta H_p} \tau_a \cdot \tau_b \right]}{\text{Tr} \left[ e^{-\beta H_p} \right]} = \frac{e^{-\beta J_{\text{can}}}}{1 + 1/3} \tag{D.44}
\]

This looks exactly like the expression above, except that now \( J_{\text{can}} \), unlike \( J_{ab} \), is temperature independent. So we achieve a parametrization of \( \langle \tau_a \cdot \tau_b \rangle \) in terms of 3 temperature independent parameters \( J_{\text{can}}, \Phi \) and \( \eta \). This result although being simple has important consequences; for instance, we see that symmetry implies that \( J_{\text{can}} \) is in fact the gap separating the probes singlet and the probes triplet up to any order\(^2\) for neither a particular form for \( \hat{S} \) was adopted, nor an approximation was made in deriving the latter expression. We thus can write,

\[
J_{\text{can}} = \Delta_{ab}(\alpha) := E_{\text{triplet}}(\alpha) - E_{\text{singlet}}(\alpha). \tag{D.45}
\]

\(^2\)Under the assumption of a low energy sector mapped to a probe singlet, \( |\chi^s\rangle \), and probe triplet, \( |\chi^t\rangle \), via the canonical
Using equations [D.32], [D.43] and [D.44], we can express $J_{ab}(\beta)$ explicitly in these temperature independent parameters:

$$J_{ab}(\beta) = \frac{1}{4\beta} \ln \left[ \frac{3(\Phi - \eta) + (4 - 3\Phi - \eta) \exp(\beta J_{\text{can}})}{4 - \Phi + \eta + (\Phi + \eta)/3 \exp(\beta J_{\text{can}})} \right].$$  \hspace{1cm} (D.46)

In the following appendix we derive the expression for $\Phi$, and show that it is of second order in the small parameter $J_\alpha/\Delta$, in resemblance to $J_{\text{can}}$ [the expression of $J_{\text{can}}$ in second order perturbation theory can be read from Eqs. (D.18) and (D.45)]:

$$\Phi = O\left(\frac{\alpha^2 J^2}{\Delta^2}\right),$$  \hspace{1cm} (D.47)

and that $\eta$ is at most of fourth order.

D.3. The canonical parameters in perturbation theory

According to the discussion of the previous appendix, the correct probe-probe correlation (and hence their partial state) must be computed by expressing the renormalized spins $\tau^a(\mathbf{R}_b)$ [see Eq. (D.30) for definition] in the original basis of the spins, $\{ | \uparrow_a, \uparrow_b \rangle, | \uparrow_a, \downarrow_b \rangle, | \downarrow_a, \uparrow_b \rangle, | \downarrow_a, \downarrow_b \rangle \}$. Here, we compute the canonical corrections, $\Phi$ and $\eta$, to the probe canonical correlation [Eq. (D.44)] in perturbation theory. The derivation of the effective canonical coupling $J_{\text{can}}$ was performed in Appendix D.1:

$$J_{\text{can}} = 4(J\alpha)^2 \chi_{ab}(0) + O\left(\frac{\alpha^3 J^3}{\Delta^3}\right).$$

We assume the following conditions to hold:

transformation, the gap is given by:

$$\Delta_{ab} := \langle \Psi_{0,m}|H|\Psi_{0,m}\rangle - \langle \Psi_{0,h}|H|\Psi_{0,h}\rangle$$

$$= \langle \chi^*_{m}|(\psi_0)(H_p + H'_b)|\psi_0\rangle |\chi'^*_{m}\rangle - \langle \chi^*_{m}|(\psi_0)(H_p)|\psi_0\rangle |\chi'^*_{m}\rangle$$

$$= \langle \chi^*_{m}|H_p|\chi^*_{m}\rangle - \langle \chi^*_{m}|H_p|\chi^*_{m}\rangle := J_{\text{can}}.$$  \hspace{1cm} (D.44)

The definition in the last equality is the same found in $(\tau_a \cdot \tau_b)_{\text{can}}$, namely Eq. (D.44). This is consistent as the $SU(2)$ symmetry forces $H_p$ to have the form,

$$H_p = \text{constant} + \gamma \tau_a \cdot \tau_b,$$

yielding a gap of $\Delta_{ab} = 4\gamma$. In our notation we have chosen to express the probe Hamiltonian in terms of the gap, directly, $J_{\text{can}} := 4\gamma$. 

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1. the temperature is small enough as not to generate real excitations of the spin bath,

\[ k_B T \ll \Delta \equiv \Delta_{ab}(\alpha = 0). \quad (D.48) \]

2. the probes couple weakly to the spin bath via an isotropic interaction with strength \( \alpha J \), such that

\[ (J\alpha)^2 \ll J\Delta, \quad (D.49) \]

where \( J \) is a typical energy scale for the bath (e.g. an exchange interaction).

These conditions allow us to write:

\[
\langle \tau_a \cdot \tau_b \rangle_\beta = \text{Tr} \left[ \rho_{ab} \tau_a \cdot \tau_b \right] = \text{Tr} \left[ e^{-\beta \hat{H}_S} e^{i [\hat{S}, \tau_a \cdot \tau_b]} e^{-i [\hat{S}, \tau_a \cdot \tau_b]} \right] = \text{Tr} \left[ \frac{e^{-\beta \hat{H}_S}}{Z_{ab}} \left( \tau_a \cdot \tau_b - i \left[ \hat{S}, \tau_a \cdot \tau_b \right] - \frac{1}{2} \left[ \hat{S}, \left[ \hat{S}, \tau_a \cdot \tau_b \right] \right] + O(J^3\alpha^3\Delta^{-2}) \right) \right]_{\text{1st order}} \quad (D.52)
\]

with \( Z_{ab} := \text{Tr}[e^{-\beta \hat{H}_S}] \). From the latter result, we can express the \( \hat{S} \) renormalized spins as function of the original spins:

\[
\tau_a \cdot \tau_b \rightarrow \tau^R_a \cdot \tau^R_b = \tau_a \cdot \tau_b + \xi_{ab} \quad (D.53)
\]

with,

\[
\xi_{ab} = -\frac{1}{2} \left[ \hat{S}, \left[ \hat{S}, \tau_a \cdot \tau_b \right] \right] + O(J^3\alpha^3\Delta^{-2}), \quad (D.54)
\]

entailing that the GS of the probes will never be a perfect singlet if \( \langle \xi_{ab} \rangle_\beta \) is non-negligible. The trace in Eq. (D.52) can be executed in two steps: 1. tracing out the bath by considering just the overlap with the ground-state, which is justified by condition (D.48) and 2. performing a thermal average in the \( 2 \otimes 2 \) Hilbert space of the probes.

The first order term does not contribute as the generator \( \hat{S} \) has null matrix elements between the ground state, \( i.e. \)

\[
\langle \psi_0 | \left[ \hat{S}, \tau_a \cdot \tau_b \right] | \psi_0 \rangle = \left[ \langle \psi_0 | \hat{S} | \psi_0 \rangle, \tau_a \cdot \tau_b \right] = 0. \quad (D.55)
\]

Then we are left with a zero-order term,

\[
C_0 = \text{Tr} \left[ \frac{e^{-\beta \hat{H}_S}}{Z_{ab}} \tau_a \cdot \tau_b \right],
\]
D.3. The canonical parameters in perturbation theory

yielding the canonical correlation, \( \langle \tau_a \cdot \tau_b \rangle_{\text{can}} \), and with a second-order correction \( C_2 \).

\[ C_2 = -\frac{1}{2Z_{ab}} \text{Tr} \left\{ e^{-\beta H_S} \left[ \hat{S}, \left[ \hat{S}, \tau_a \cdot \tau_b \right] \right] \right\}. \quad \text{(D.56)} \]

We must have some care in order to evaluate the above thermal average. Let us reproduce the main steps,

\[ C_2 = -\frac{1}{2Z_{ab}} \text{Tr} \left\{ e^{-\beta H_S} \left( \hat{S} \hat{S} \tau_a \cdot \tau_b - 2\hat{S} \tau_a \cdot \tau_b \hat{S} + \tau_a \cdot \tau_b \hat{S} \right) \right\} \quad \text{(D.57)} \]

\[ = -\frac{1}{2Z_{ab}} \text{Tr} \left\{ e^{-\beta H_S} \left( \hat{S} \hat{S} \tau_a \cdot \tau_b - \hat{S} \tau_a \cdot \tau_b \hat{S} \right) \right\} \quad \text{(D.58)} \]

\[ \simeq -\frac{1}{2Z_{ab}} \sum_{k \geq 0} \text{Tr}_{a,b} \left\{ \langle \psi_0 | e^{-\beta H_S} | \psi_k \rangle \langle \psi_k | (\hat{S} \hat{S} \tau_a \cdot \tau_b - \hat{S} \tau_a \cdot \tau_b \hat{S}) | \psi_0 \rangle \right\}. \quad \text{(D.59)} \]

The effective Hamiltonian has no matrix elements between eigenstates belonging to different sectors (up to the order we are working at), which simplifies the above summation as only the GS contributes [compare with Eqs. (D.34)-(D.35)]:

\[ \langle \psi_0 | e^{-\beta H_S} | \psi_k \rangle = e^{-\beta H_F} \langle \psi_0 | e^{-\beta H_F} | \psi_k \rangle \delta_{0k}. \quad \text{(D.60)} \]

We further get,

\[ C_2 = -\frac{1}{2Z_{ab}} \text{Tr}_{a,b} \left\{ \langle \psi_0 | e^{-\beta H_S} | \psi_0 \rangle \langle \psi_0 | (\hat{S} \hat{S} \tau_a \cdot \tau_b - \hat{S} \tau_a \cdot \tau_b \hat{S}) | \psi_0 \rangle \right\} \quad \text{(D.61)} \]

\[ = -\frac{1}{2Z_{ab}} \text{Tr}_{a,b} \left\{ e^{-\beta H_F} \langle \psi_0 | (\hat{S} \hat{S} \tau_a \cdot \tau_b - \hat{S} \tau_a \cdot \tau_b \hat{S}) | \psi_0 \rangle \right\} \quad \text{(D.62)} \]

\[ := -\frac{1}{2Z_{ab}} (A_1 - A_2). \quad \text{(D.63)} \]

The averages of the quadratic terms \( \sim \hat{S} \hat{S} \) must be done separately as \( \hat{S} \) does not commute with the probe’s operators in general,

\[ A_1 = \sum_{k \geq 0} \text{Tr}_{a,b} \left\{ e^{-\beta H_F} \langle \psi_0 | \hat{S} | \psi_k \rangle \langle \psi_k | \hat{S} | \psi_0 \rangle \tau_a \cdot \tau_b \right\} \quad \text{(D.64)} \]

\[ = \sum_{k \geq 0} \text{Tr}_{a,b} \left\{ e^{-\beta H_F} S_{ab}(0,k) S_{ab}(k,0) \tau_a \cdot \tau_b \right\} \quad \text{(D.65)} \]

\[ A_2 = \sum_{k \geq 0} \text{Tr}_{a,b} \left\{ e^{-\beta H_F} S_{ab}(0,k) S_{ab}(k,0) \tau_a \cdot \tau_b \right\} \quad \text{(D.66)} \]

\[ = \sum_{k \geq 0} \text{Tr}_{a,b} \left\{ e^{-\beta H_F} S_{ab}(0,k) S_{ab}(k,0) \tau_a \cdot \tau_b \right\}. \quad \text{(D.67)} \]
where we have conveniently introduced the operator:

\[ S_{ab}(m,n) := \langle \psi_m | \hat{S} | \psi_n \rangle \]  
(D.68)

\[ = \langle \psi_m | \mathcal{P}_m \hat{S} \mathcal{P}_n | \psi_n \rangle \]  
(D.69)

\[ = J \alpha \frac{\langle \psi_m | (\mathbf{t}_a \cdot \mathbf{S}_A + \mathbf{t}_b \cdot \mathbf{S}_B) | \psi_n \rangle}{i(E_m - E_n)} \]  
(D.70)

\[ := \frac{J \alpha}{i\Delta_{mn}} (\mathbf{t}_a \cdot \langle \psi_m | \mathbf{S}_A | \psi_n \rangle + \mathbf{t}_b \cdot \langle \psi_m | \mathbf{S}_B | \psi_n \rangle). \]  
(D.71)

The matrix elements of the operator \( \mathcal{P}_m \hat{S} \mathcal{P}_n \) in second order perturbation theory were derived in Appendix D.1 via the Schrieffer-Wolff formalism [see Eq. (D.10)]. Inserting the last equality in the corrections \( A_1 \) and \( A_2 \), we find, after some algebra,

\[ A_1 - A_2 = 4 \sum_{k>0} \frac{\| \psi_0 \| |(\mathbf{S}_A - \mathbf{S}_B^\dagger)| \psi_k \|^2}{\Delta_{k0}^2}. \]  
(D.72)

We finally get the desired result

\[ \langle \mathbf{t}_a \cdot \mathbf{t}_b \rangle = \langle \mathbf{t}_a \cdot \mathbf{t}_b \rangle_{\text{can}} (1 - \Phi) + \eta. \]  
(D.73)

\[ \Phi := 4(J \alpha)^2 \sum_{k>0} \frac{\| \psi_0 \| |(\mathbf{S}_A - \mathbf{S}_B^\dagger)| \psi_k \|^2}{\Delta_{k0}^2}, \]  
(D.74)

with \( \langle \mathbf{t}_a \cdot \mathbf{t}_b \rangle_{\text{can}} \) given previously in Eqs. (D.43)-(D.44), and where \( \eta = 0 \) up to second-order perturbation theory since no constant term has emerged from our expansion. In fact this term is at most of fourth order, \( O[(J \alpha/\Delta)^4] \). Let us show this result more carefully.

We take the definition of \( \eta \) [Eq. (D.41)] and Eq. (D.38) to get:

\[ 4 \eta = \frac{1}{2} \text{Tr}_p (\psi_0 | [i \hat{S}, [i \hat{S}, \mathbf{t}_a \cdot \mathbf{t}_b]] | \psi_0) \]

\[ = -\frac{1}{2} \text{Tr}_p \left[ \langle \psi_0 | (\hat{S}^2 | \psi_0) \mathbf{t}_a \cdot \mathbf{t}_b + \mathbf{t}_a \cdot \mathbf{t}_b (\psi_0 | \hat{S}^2 | \psi_0) \right] \]

\[ -2 \sum_m \langle \psi_0 | \hat{S} | \psi_m \rangle \mathbf{t}_a \cdot \mathbf{t}_b (\psi_m | \hat{S} | \psi_0) \]

\[ = -\frac{1}{2} \text{Tr}_p \left[ \langle \psi_0 | \hat{S} | \psi_m \rangle \langle \psi_m | \hat{S} | \psi_0 \rangle \mathbf{t}_a \cdot \mathbf{t}_b ight. \]

\[ + \mathbf{t}_a \cdot \mathbf{t}_b (\psi_0 | \hat{S} | \psi_m \rangle \langle \psi_m | \hat{S} | \psi_0 \rangle) \]

\[ -2 \sum_m \langle \psi_0 | \hat{S} | \psi_m \rangle \mathbf{t}_a \cdot \mathbf{t}_b (\psi_m | \hat{S} | \psi_0) \]

denoting \( S_m = \langle \phi_0 | \hat{S} | \phi_m \rangle \) (a probe operator) we recognize

\[ 4 \eta = -\frac{1}{2} \sum_m \text{Tr}_p \left[ S_m S_m^\dagger \mathbf{t}_a \cdot \mathbf{t}_b + \mathbf{t}_a \cdot \mathbf{t}_b S_m S_m^\dagger - 2 S_m \mathbf{t}_a \cdot \mathbf{t}_p S_m^\dagger \right] \]  
(D.75)
Using the cyclic invariance of the trace, this reduces to

\[
4\eta = -\sum_m \text{Tr}_p \left[ s_m s_m^\dagger \tau_a \tau_b - s_m \tau_a \tau_b s_m^\dagger \right] \tag{D.76}
\]

To proceed, we must specify the operator \( s_m \),

\[
s_m = \frac{i\alpha}{\Delta m} \langle \psi_0 | [\tau_a \cdot s_A + \tau_b \cdot s_B] | \psi_m \rangle \tag{D.77}
\]

\[
= i\alpha (\tau_a \cdot u_{ma} + \tau_b \cdot u_{mb}) \tag{D.78}
\]

with \( u_{ma(b)} \) (a c-number in probe space) is defined as

\[
u_{ma(b)} = \frac{1}{\Delta m} \langle \psi_0 | s_A(s_B) | \psi_m \rangle \tag{D.79}
\]

We arrive at

\[
4\eta = -\alpha^2 \sum_m \text{Tr}_p \left[ (\tau_a \cdot u_{ma} + \tau_b \cdot u_{mb}) (\tau_a \cdot u_{ma}^* + \tau_b \cdot u_{mb}^*) \tau_a \cdot \tau_b \\
- (\tau_a \cdot u_{ma} + \tau_b \cdot u_{mb}) \tau_a \cdot \tau_b (\tau_a \cdot u_{ma}^* + \tau_b \cdot u_{mb}^*) \right] \tag{D.80}
\]

At this point we can again use the cyclic invariance of the trace on the \( \tau \) operators, and obtain

\[
4\eta = -\alpha^2 \sum_m \text{Tr}_p \left[ (\tau_a \cdot \tau_a^l - \tau_b \cdot \tau_b^l) u_{ma}^l (u_{ma}^\dagger)^l \\
+ (\tau_a \cdot \tau_a^l - \tau_b \cdot \tau_b^l) u_{mb}^l (u_{mb}^\dagger)^l \right] \tau_a \cdot \tau_b = 0 \tag{D.81}
\]

The cross terms in \( \tau_a \) and \( \tau_b \) are zero because the corresponding operators commute; in this form, the trace over probe space kills this expression because there is always an alone \( \tau_a^l \) or \( \tau_b^l \) operator in all terms.
D. Appendices for chapter 5
List of publications by the author

- *Emergence of robust gaps in 2D antiferromagnets via additional spin-1/2 probes*, AIRES FERREIRA, J. Viana Lopes, and J. M. B. Lopes dos Santos, submitted to PRL (2009).

- *Production of bright entangled photons from optical moving boundaries*, A. Guerreiro, AIRES FERREIRA, and J. T. Mendonça. arXiv: 0906.0522, to be submitted (2009).

- *Analytical results in long distance entanglement mediated by gapped spin chains*, AIRES FERREIRA, and J. M. B. Lopes dos Santos, Phys. Rev. A 77, 034301 (2008).

- *Optomechanical entanglement between a movable mirror and a cavity field*, D. Vitali, S. Gigan, AIRES FERREIRA, H. R. Bohm, P. Tombesi, A. Guerreiro, V. Vedral, A. Zeilinger, and M. Aspelmeyer, Phys. Rev. Lett. 98, 030405 (2007).

- *Macroscopic thermal entanglement due to radiation pressure*, AIRES FERREIRA, A. Guerreiro, and V. Vedral, Phys. Rev. Lett. 96, 060407 (2006).
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