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QUANTUM CORRELATIONS: A WINDOW INTO FUNDAMENTAL PHYSICS

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To my beloved family,
those who are gone,
and those to come...

DECLARATION

I hereby declare that the material presented in this thesis is a result of my work and that of my acknowledged collaborators, except where otherwise suitably referenced.

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ABSTRACT

The past century has seen many of nature's secrets unravelled by the immensely successful theories of particle physics and general relativity, frameworks in which the world is *described* as a collection of many quantum fields, lying on a background classical spacetime. High-energy signals, originating naturally from the cosmos, or artificially from particle accelerators, held many empirical clues in support of these descriptions. In recent years, the formidable advances in quantum control have brought to light a model-agnostic conception of physics, once thought to be merely philosophical, as an alternative path of fundamental investigations. This modern information theoretic framework, eschews any description of nature beyond the correlations between measurements predicted by quantum theory. In this thesis, three questions of fundamental physics are studied from the perspective of quantum information and quantum control.

PUBLICATIONS

This thesis features work and figures that have appeared previously in papers which were published throughout the course of my doctoral studies:

- [2] H Chevalier, AJ Paige, MS Kim. "*Witnessing the nonclassical nature of gravity in the presence of unknown interactions*". Physical Review A 102 (2), 022428 (2020).
- [3] H Chevalier, AJ Paige, H Kwon, MS Kim. "*Violating the Leggett-Garg inequalities with classical light*". Physical Review A 103 (4), 043707 (2021).
- [4] H Chevalier, H Kwon, KE Khosla, I Pikovski, MS Kim. "*Many-body probes for quantum features of spacetime*". AVS Quantum Science 4 (2), 021402 (2022)
- [5] S Aimet, H Chevalier, MS Kim. "*Gravity mediated entanglement between light beams as a table-top test of quantum gravity*". arXiv preprint arXiv:2210.12713 (2022).

Sec. 3.2 is based on publication [3]. Sec. 4.3 is based on publication [4]. Secs. 5.2 and 5.3 are based on publications [2] and [5] respectively.

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Knowledge is in the end based on acknowledgement.

— **Ludwig Wittgenstein** [6]

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FOREWORD

The saddest aspect of life right now is that science gathers knowledge faster than society gathers wisdom.

— **Isaac Asimov** [7]

In the four years of my doctoral training, I have sailed away from the familiar shores of introductory physics and ventured into an incredibly vast, sometimes tumultuous ocean of ideas, with the help of some of the most talented and experienced sailors of the mind. The tools I have gathered from quantum dynamics, quantum optics and quantum information theory, have made for an interesting exploration of table-top tests of fundamental physical hypotheses, such as realism, gravitational signatures hidden in quantum motion, or quantum signatures hidden in gravitational motion. This thesis summarizes my explorations and recounts a journey that has taken place in troubled times.

My PhD began in a context of rising populism and of post-truth trends, in a time where a global pandemic put half of the world's population into lockdown, in a period of general bewilderment pertaining to rapid human-induced climate change. In this landscape, I would like to say a few words about the microcosm of academia and our society, as I have come to perceive them.

The all-too-noble intellectual enterprise of academia, proudly withdrawn – we like to believe – from the lowly society of the spectacle, and thought to advance untroubled by commonplace vicissitudes, is above all a human and social one. Yet, the current state of academia also has a much less virtuous facet, one driven by a frantic race for citations, and higher h-indices.

In a society obsessed with retweets, likes and drama, the financially starved academic world has become an arena where researchers, aspiring free athletes turned gladiators, have been told that there is but one path to success: one where the raw numbers of citations and publications are worshiped as *the* ultimate value of science, and where the strongest prevail and the rest perish.

The very community that draws its future contributors from a pool of passionate and well-taught students, in promoting industrial-like article production as the sole purpose of a scientist, has disparaged teaching activities, pedagogical publications, and even peer-reviewing, for their alleged lack of innovation and *impact*. In a world where scientists are led to neglect outreach and teaching as second-rank tasks, for the sake of publishing a plethora of oft-cited yet seldom read papers, how can one be surprised by the widening schism between the scientific community and the rest of the society?

The rise of post-truth movements, of fundamental misconceptions, of mistrust in the intellectual elite, and ill-informed skepticism, is a sadly obvious outcome for a society that has undervalued teaching.

My short venture into the academic world was not one driven by extreme specialization and publications, but rather by the pleasure of learning and teaching a wide variety of concepts. Contrary to most PhD projects in which students are invited to delve as deep as possible into an incredibly narrow topic, the work presented in this thesis reflects a spirit of breadth that I have always longed for: a wonderful opportunity for which I thank my supervisor.

As an accidental symbol of breadth, it happens that the four publications on which this dissertation is based have been written in four different cities: Dubai, Paris, London and Berkeley.

As a further token of my yearning to broaden my horizons, I have elected to give a philosophical and historical cast to the introduction of this dissertation. Not to make this thesis unduly pedantic, this is rather to be taken as a tribute to my remarkably literate family: a meager compensation for not having been, by far, the best student in literature and history class.

Though I have grown to appreciate that historical, cultural, sociological and philosophical knowledge are of great importance, I have also observed that the scientific method, typically represented by the technological wonders and horrors its application has allowed, is too often falsely considered to be a mechanistic, lifeless and indoctrinating way of thinking, commonly opposed to the humanities.

Whereas most marvel at its practical outcomes, as a theorist I find scientific thinking's most precious gift to be that of structuring the mind. Formulating logical quantitative predictions from finite, biased and noisy data is an all but natural exercise for the ionic Bayesian calculators that are our human brains. Especially so in a chaotic, highly non-linear and complex world of intertwined influences acting on different scales of space and time.

Making rational decisions, and actually solving problems of various natures, requires a training of the mind in a simple and formal context, where the intricacies of logic and the subtle purity of reasoning lay bare, unobscured by vernacular polysemy. Such is the landscape of introductory mathematics and basic sciences like physics. In my view, this training may not only help sharpen the minds of scientists: it is also a crucial exercise for anyone who endeavors to formulate any hypothesis which bears some claim to reality.

But how would those outside of science know, if teaching has become so unrewarding that even some of the most passionate pedagogues may consider other careers?

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ACRONYMS

CC	Classical Communication
CP	Casimir-Polder
GR	General Relativity
MR	Macroscopic Realism
PR	Popescu-Rohrlich
BCH	Baker-Campbell-Hausdorff
DSR	Doubly Special Relativity
GME	Gravity Mediated Entanglement
GUP	Generalized Uncertainty Principle
NIM	Noninvansive Measurability
ONI	Ontic Noninvasiveness
PEA	Position Eigenstate Approximation
PPT	Positive Partial Transpose
RQM	Relational Quantum Mechanics
CHSH	Clauser-Horne-Shimony-Holt
CPTP	Completely Positive Trace-Preserving
LGIs	Leggett-Garg Inequalities
LOCC	Local Operations and Classical Communication
MRps	Macroscopic Realism *per se*
OpND	Operational Nondisturbance
POVM	Positive Operator Valued Measurement
DIGME	Doubly Interferometric Gravity Mediated Entanglement
OEMMR	Operational Eigenstate Mixture Macroscopic Realism
OESMR	Operational Eigenstate Support Macroscopic Realism
SESMR	Supra Eigenstate Support Macroscopic Realism
SQUID	Superconducting Quantum Interference Device

NOTATIONS

$\forall$	Universal quantifier
$\exists$	Existential quantifier
$\in$	Set membership
$:=$	Equal by definition
$\propto$	Proportional to
$\sim$	On the order of
$\approx$	Approximately equal to
$\lesssim$	Less or approximately equal to
$O(f)$	Asymptotic domination by function f
$[a, b]$	Closed real interval
$[\![n, m]\!]$	Integer interval $\{n, n+1, ..., m\}$
z^*	Complex conjugate of z
δ_{ij}	Kronecker symbol
$\delta(x)$	Dirac distribution
$đx$	Reduced differential operator $dx/2\pi$
$\lvert E \rvert$	Cardinality of set E
$\dim(E)$	Dimensionality of space E
M^T	Transpose of M
$\mathrm{supp}(f)$	Support of function f
$\partial_x f$	Partial derivative $\frac{\partial f}{\partial x}$
$\oplus$	Direct sum
$\otimes$	Tensor product
$\binom{n}{k}$	Binomial coefficient $\frac{n!}{k!(n-k)!}$
m	Meter
kg	Kilogram
s	Second
J	Joule
K	Kelvin
Hz	Hertz
H	Henry
$\hbar$	Reduced Planck constant, $\hbar \approx 1.05 \times 10^{-34}$ J s
c	Speed of light in vacuum, $c \approx 3 \times 10^8$ m s^{-1}
G	Gravitational constant, $G \approx 6.67 \times 10^{-11}$ m^3 kg^{-1} s^{-2}
k_B	Boltzmann constant, $k_B \approx 1.38 \times 10^{-23}$ J K^{-1}

Part I

EXORDIUM

1 PROLOGUE

What we observe is not nature itself but nature exposed to our method of questioning.

— **Werner Heisenberg** [8]

By way of an orthodox introduction, the overture of this thesis is an invitation to reflect on the history of fundamental scientific research, its inception, turning points, and developments. After a more specific summary of the history of quantum field theories and the advent of quantum information theory, the synopsis of this dissertation is presented.

1.1 FROM DEITIES TO INFORMATION: A STORY OF RECEDING ABSOLUTES

The history of scientific knowledge, from the earliest myths, medieval religious cosmogonies, to quantum theory and the measurement problem, is a multi-millennial tale of the tumultuous rapport between beliefs and disbelief, between faith and skepticism, between the establishment of absolutes and their dissolution through relationalism. In this opening section, we briefly look back on a long winding trail across spacetime and civilizations, marked by a series of paradigm shifts, originating in the Middle-Eastern regions, and leading us to the septentrional city of Copenhagen.

1.1.1 *The first awakenings to relativities*

Our story finds its earliest roots five millennia ago, in an era during which the entirety of scientific knowledge was sheltered within a handful of ancient Egyptian and Mesopotamian temples, where under the opaque veil of initiation rites, it remained secluded from the plebeian agitations [9]. Before they drifted into the darkness of forgotten history, these beacons of light few and far between had not gone unnoticed. From the opposite shore of the Mediterranean, a thousand kilometers northwards from the towering wonders of Giza, the ancient Greeks had caught a glimpse of the shimmering Egyptian lights: ancient mathematical, astronomical and medical knowledge that shaped their natural philosophy.

Six centuries before the common era, Thales (Θαλῆς) of Miletus set out on a journey to Egypt, to study among the priests of Memphis and Thebes [10]. Upon his return he founded the oldest Hellenistic

philosophical school, known as the Ionian school. Philosophers of the Ionian school sought to relinquish mythology and supernatural hypotheses, in favour of rational explanations of the origins of the world and of physical phenomena, based on experiments and observation. Thales and his disciples, the *physikoi* (φυσιχοι), had revolutionized the way the world was thought of: gone were the anthropomorphic gods and heroes who wielded the power to shake the Earth. The *physikoi* believed instead that the Earth floated on water, and that earthquakes occurred as Earth was rocked by waves. In essence, the *physikoi* had replaced beliefs in imaginary entities whose intentions would govern observable physical phenomena, with beliefs in physical models which could intuitively account for the emergence of those phenomena. Although this paradigm shift is seldom mentioned in scientific curricula, I believe it is by no means less important than the more popular ones that have followed.

In the story leading up to our current scientific understanding of the world, the next paradigm shift has been long in coming. Two centuries after Thales founded the Ionian school and transformed our relationship to phenomenology, the Greek intellectual life became increasingly centered around its capital city state [11]. Athens grew to become a fertile ground for the advancement of science and philosophy, and saw within its aristocracy the birth of Plato (Πλάτων), who went on to become the founder of the academy (Ἀκαδημία). Among his many contributions to human knowledge, Plato had been the proponent of an ontological stance, called dualism, which broadly postulates a separation between the body and the soul, between the sensible world and the intelligible world. In particular, Plato believed that true substances were not physical, but eternal forms of which bodies are imperfect copies. Platonic dualism trickled its way through the conceptions of one of his pupils, who, although not a believer of platonic forms, turned out to become perhaps the most influential thinker in the history of physics: Aristotle (Ἀριστοτέλης), founder of the lyceum (Λύκειον).

Aristotelian physics divides the universe into corruptible spheres made up of four elements, where humans lived; and unchanging celestial spheres made of a special weightless element called aether. Although Thales and the *physikoi* had ventured into a new way of thinking about phenomenology, the world-view of ontology that was held by most European scholars throughout the middle-ages and up to the seventeenth century, was due to Aristotle. The underlying platonic duality of Aristotelian physics, along with its conception of the universe in terms of purpose rather than cause and effect, was not unbefitting in the eyes of a society which became structured around the institutionalisation of monotheistic absolutist religious doctrines. The fifteenth and sixteenth centuries saw the first stirrings of the revolution to come, when Copernicus through the observation of planetary

motion arrived at a conclusion last reached by Aristarchus (Ἀρίσταρχος) of Samos eighteen centuries earlier: heliocentrism. Half a century later, Kepler formulated laws of motion for celestial bodies which are still of use to this day. In the wake of these findings, which shattered the absoluteness of spatial position inscribed in Aristotelian physics, a relational approach to the physics of motion became conceivable. This constituted what is now called Galilean relativity. It was not long before Huygens, Newton and Leibniz formulated the mathematical concepts crucial to the expression of relationships between observed phenomena involving the relative motion of massive bodies.

1.1.2 *The Einsteinian relativities*

In our fast paced narrative, we have followed the first known steps of mankind towards a rational understanding of nature with the Ionian school, and seen the persistence of Aristotelian physics through the rise and fall of early empires, then brought to an abrupt end with Galilean relativity and the advent of Newtonian physics.

This brings us to the eighteenth century, an epoch by which it had become well accepted that motion was relative, and where the mathematical formalization of physical models had gained importance, with notable contributions to the understanding of vibrating motion and the behavior of gas owed to mathematicians like Taylor, D. Bernoulli and Euler. Advances in more and more abstract mathematical models of physics continued towards the end of the eighteenth into the nineteenth century, notably with the Langrangian and Hamiltonian formulations of mechanics, which had established the notion of energy as more fundamental than that of force. The study of chemical reactions also saw the formulation of founding principles such as the conservation of mass.

The nineteenth century was a time of countless substantial advances in the understanding of nature through new ontological models, such as fields in Maxwellian electromagnetism, the kinetic theory of gases fundamental to thermodynamics, as well as groundbreaking mathematical representations provided by the birth of Fourier analysis. Despite the myriad of discoveries, the foundations of physics had not evolved much since the Newtonian revolution in essence. Physics was simply understood to be the study of the causal, deterministic (although sometimes chaotic) relationship between naturally occurring events. By the end of the nineteenth century, the success of classical physics culminating in the engineering marvels that had driven industrial development, left little room for skeptical upheaval. Human work was progressively replaced by machines, the exponential energy production fueled by fossilized pre-historic life stoked productivity and would constitute the stepping stones of social rights.

The once so vast and arcane world had grown smaller and more transparent. It was as though nature's completely deterministic and calculable inner workings had been fully exposed by Newtonian gravitation, Maxwell's theory of electromagnetism, and the principles of thermodynamics. History turned out to have been graceful to the romantics, who found beauty far from the noxious smell of smoke and soot of the newly industrialized society, and sought meaning beyond the cold, rational, mechanistic description of nature that marked their time. Indeed, the failed detection of luminiferous ether in the Michelson-Morley experiment [12], and the ultra-violet catastrophe, would soon catapult mankind into foreign lands.

The result of the Michelson-Morley experiment from 1887 required a new understanding of the propagation of light. It took the genius mind of Einstein to devise a solution in 1905, provided by the theory of special relativity [13]. In some sense, the inception of special relativity marked the very first instance in which thinkers had taken the Ionian school of thought to its pinnacle: in the face of reliable empirical observations, one's belief in metaphysical preconceptions, however deeply rooted they may be, must yield to reason. What constitutes a challenge in understanding special relativity, is not so much its mathematical formulation, but rather that it dissolves the absoluteness of lengths, durations and simultaneity. While Galilean relativity and heliocentricity were important paradigm shifts, they were ones where human scale intuition had to take primacy over unverified beliefs. Einsteinian relativity took this a step further: one now had to relinquish physical intuition and accept principles which could only be arrived at through the mathematical analysis of empirical data, that itself could only be collected through the use of measurement devices which largely surpassed our bodily senses.

After another ten years, Einstein published the theory of general relativity [14], which described mutual interactions between physical systems and the background on which they evolve, called spacetime. To this day, general relativity remains undisputed, and stands as the best model of gravitation ever conceived. General relativity, at its inception, provided explanations for the perihelion precession of Mercury otherwise inexplicable with Newtonian gravity alone. This new theory of gravitation also predicted the existence of objects that Einstein himself thought to be unphysical, such as black holes and gravitational waves. These objects have been directly observed a century later [15, 16].

1.1.3 *The quantum relativities*

While the advent of Einsteinian relativity sent tremors throughout the physical and philosophical communities, for its counter-intuitive dissolution of the absoluteness of durations and lengths, a sword of

Damocles still hung over the heads of all who held on to an ontological vision of physics, including Einstein himself. In the beginning of the twentieth century, in efforts to solve the ultraviolet catastrophe, a new theory of physics called quantum theory, fathered by Planck, Einstein, Heisenberg, Schrödinger and many others [17–20], came in as a deluge that would soon unroot whatever was left of absoluteness and deterministic conceptions of nature.

In this new theory, the fundamental object representing a physical system was no longer a collection of point-like masses but a mystical wavefunction often denoted ψ, a field of complex numbers extending everywhere in spacetime, which does not predict deterministic measurement outcomes, but instead provides probability distributions of such measurement outcomes, according to the Born rule [21]. Although quantum theory rapidly became an object of fascination for its bizarre features, such as the uncertainty principle, the wave-corpuscle duality and its non-deterministic nature, its quiet equations that filled new manuscripts held greater changes within. It became apparent within a few years that something unworldly hid beneath the formalism, and in 1935 a critical challenge to quantum theory was put forward by Einstein, Podolsky and Rosen, in a publication now known as the EPR paradox [22].

The EPR paper claimed that quantum theory was incomplete, as it allowed in certain cases for an action on a given particle to have an instantaneous effect on the quantum state of a second particle, regardless of their separation. Because this was at odds with special relativity, the conclusion of the EPR paper was that quantum states could not be ontic states, but merely epistemic ones[1]. In Einstein's view, physics consisted in studying nature for what it was, and any indeterminism would arise from the lack of knowledge about an underlying description, called hidden variable theory, which actually captured the ontic states. What had happened in 1935 spoke volumes about the extreme profoundness of the paradigm shift humanity had arrived on the brink of: the first lucid encounter with quantum entanglement resulted in the straight negation of the theory's completeness, by some of its very pioneers!

The publication of the EPR paper further shook the foundations of physics, and widened an existing chasm between Einstein and Bohr [23], but remained an issue deemed too philosophical for most. Although the immense power of quantum theory in its applications to atomic, molecular and nuclear physics constituted the building blocks of technologies that would come to shape the information era almost a century later, its practical efficiency would marginalize fundamental research over decades to come.

It is in 1964 only that the EPR debate was finally stripped of its cryptic philosophical apparel by Bell, who devised what is now con-

1 That is, states of knowledge of an agent, rather than objective states of reality.

sidered to be the first ever experimental metaphysics protocol [24]. Bell had demonstrated that the existence of ontological local hidden variables, more fundamental than the quantum state, necessarily implied a set of inequalities which now bear his name. These inequalities relating different measurement correlations performed on a bipartite system, were predicted to be violated by quantum theory. In 1969 the inequalities were reformulated to cater for experimental tests [25] and the first experimental violations of Bell type inequalities were reported in 1972 [26], followed by a refined test in the following years [27]. These early experiments were recently rewarded with a Nobel prize. In 2015 a series of loophole free tests were carried out [28–30], and have all conclusively violated Bell's inequalities, in accordance with the predictions of quantum theory.

The violation of Bell's inequalities bore profound philosophical consequences, as they invalidated all objective local theories of physics: one cannot account for their violation without abandoning either locality or realism. A minority of physicists accepted forms of non-locality for the sake of preserving the reality of the quantum state, a position called ψ-ontic. Among the popular ψ-ontic interpretations there is the Bohmian pilot wave theory [31], the many worlds interpretation [32], spontaneous collapse models [33], and modal interpretations [34]. On the other hand, a majority of the physical community had gone the alternate route of ψ-epistemic-complete interpretations, commonly referred to as Copenhagen-type interpretations, such as quantum Bayesianism [35], quantum pragmatism [36], quantum empiricism [37] and the relational interpretation [38]. An excellent review of arguments in the ψ-ontic/ψ-epistemic-complete debate can be found in Ref. [39].

Let us pause and reflect on this state of affairs. The failure of local-realism signifies that measurements do not merely reveal pre-existing physical values contained within the object. To put it loosely, in ψ-ontic interpretations, a measurement of the physical property of an object reveals a pre-existing value, but this value was not contained within the object, it depended on a non-local entity, such as a pilot-wave or the context of the object. In Copenhagen-type interpretations, physical properties of quantum systems effectively do not exist, or are undefined, before the measurement. Physical values are thus bound to the interaction between the agent and the system, and have no existence before or without the measurement. In the language of the relational interpretation[2], one arrives at the conclusion that there are only relative facts, some of which may be effectively stabilized by a decoherence process [40].

As far as the elimination of absolutes goes, quantum theory may be viewed as a culminating point, where after the successive disap-

2 I should disclose that at the time of writing, this is my preferred interpretation of quantum theory. Informal thoughts can be found in Appendix A.

pearance of ancient deities, of the Aristotelian celestial spheres, of the absolute position of Earth, and of the absoluteness of lengths, durations and simultaneity, the very intuitive absoluteness of measurement values, outside of the specific relationship between a subject and its object that the measurement constitutes, must be surrendered. In that regard, quantum theory has constituted by far the most mind-bending paradigm shift humanity has faced.

Contrary to previous revolutions, the advent quantum theory has not just changed our conception of the world, it has transformed our conception of how one should conceive of the world. Whereas physics was previously thought to be the study of nature, a direct representation of reality, we have come to realize that it is but the study of our knowledge of nature as it presents itself through the lens of measurement devices. Regardless of one's interpretation of quantum theory, at its most fundamental level, physics no longer deals with well delimited ontological systems, but rather with the dynamics of information, of correlations, between sequences of interaction events.

1.2 A WORLD OF QUANTUM FIELDS AND INFORMATION

Much of our current understanding of the universe stems from the standard model of particle physics. Fundamental research has long been driven by the study of quantum field theories, and in this section, we give a short historic overview of this incredibly fruitful approach, before we review the shorter, but no less exciting history of quantum information theory, as another method to approach fundamental physics.

1.2.1 *Some knowledge from quantum fields*

Most of the historical breakthroughs that have brought us to our current understanding of fundamental physics over the past century have been owed to the immense success of quantum field theories. The first steps of quantum field theory can be traced back to the early 1920s, a time by which Heisenberg's quantum mechanics had matured enough to describe simple systems, such as harmonic oscillators. It did not take a great leap of faith to imagine why electromagnetism could be quantized, as the free electromagnetic field was well known to be formally equivalent to arrays of such oscillators.

The possibility of a quantized free electromagnetic field was first imagined two decades prior, by Einstein [18], and further motivated by the works of Ehrenfest [41] and Debye [42] who had shown that blackbody radiation could be accounted for, by having the electromagnetic field take on a discrete set of energies. Further hints came from Einstein's statistical treatment of fluctuations in the blackbody radiation [43], derived from Planck's law, a result which remained out

of reach from standard quantum mechanics or classical electromagnetism. The physical community stood ready for the advent of a quantized field theory, and it was not long before it saw daylight in the works of Jordan [44], in 1926. In the two years that followed, with the combined mathematical brilliance of Heisenberg, Schrödinger and Dirac, the once obscure and multifaceted theory of quantum mechanics had become an imposing monument of sophistication. Dirac's formulation of quantum mechanics, the one most avant-garde and general, exposed a boundless landscape of applications. Three distinct programs of field quantization were launched.

While Jordan had successfully quantized the free electromagnetic field, the quantization of an interacting field was first achieved by Dirac [45]. Because of its Hamiltonian formulation however, Dirac's attempt was incompatible with the Lorentz invariance imposed by Einstein's special relativity. Dirac's following and most distant endeavor was to unify his quantum field theory with relativity, a theory that would later be called quantum electrodynamics. Such a program, he thought, could not be accomplished in a single blow.

In early 1927, Heisenberg and Pauli had begun an enterprise of their own, more ambitious even than that of Dirac, of which quantum electrodynamics would be a particular case. Despite the involvement of Jordan, Klein and Oppenheimer, the unforeseen and formidable difficulties they had encountered forced them to tread more lightly, in Dirac's steps. The path Heisenberg and Pauli had traced led them all the way to the edge of a conceptual abyss: renormalization of the infinites; this marked the end of their collaboration in 1930.

Between 1928 and 1930, in a country that was slowly plagued by Mussolinian ideas, Fermi, who paid more heed to mathematical practicality than formal desiderata like Lorentz invariance, had reformulated Dirac's quantum field theory [46]. Curiously enough, Fermi's nonchalance for foundations had in fact provided an elegant circumvention of the critical obstacle that had extinguished Heisenberg and Pauli's ambitions [47]. Though renormalization issues would linger for decades to come, the formal foundations of modern quantum electrodynamics were born.

The fundamental ideas of quantum field theory were deeply consequential, as they had given rise to a new and formal definition of the concept of particle. Fundamental particles, which formed all the atoms of the inanimate, and weaved the dream-like molecules of the living, were no longer corpuscles or waves, but excitations of the normal modes of a quantum field. The hunt for new particles had begun.

In 1930 as Ghandi led the first acts of civil disobedience against the British Crown, Cockcroft and Walton had built the first particle accelerator in Cambridge, and performed the first artificial nuclear disintegration in history [48]. Two years later, the neutron and the proton were discovered. In 1935, as Hitlerian Germany re-armed in violation

of the treaty of Versailles, the mysterious interaction between protons and neutrons within atomic nuclei found its first explanations in the works of Yukawa [49], which marked the birth of the pion. After the second world war, in 1947, physicists such as Feynman developed new procedures to represent interactions [50], and the first instance of pion was found in cosmic rays [51]. In the year that followed, the first artificial pion was produced within a particle accelerator in Berkeley [52]. In 1952, the 1.3 GeV Brookhaven cosmotron began operation, and a shower of new particles ensued.

By 1960 the once familiar botanical garden of known particles had grown into an impermeable jungle. Gell-Mann and Zweig, in their endeavour to find some order in the chaotic wilderness of particles, developed the quark model in 1964 [53]. Quarks combine to form hadrons, such as protons and neutrons. While initially perceived as mere mathematical persiflage, the quark model found empirical support at only four years of age, in the Stanford linear accelerator [54].

While the invention of quarks had led to the establishment of quantum chromodynamics – the quantum theory of the atomic nucleus – it did not speak of the other fundamental forces, such as electromagnetism and the weak force. It took several brilliant minds around the planet another decade to form a unified picture, culminating in the unification of the electroweak theory with quantum chromodynamics, an edifice called the standard model of particle physics [55]. The standard model represents all observable phenomena, at the exception of gravity, with seventeen fundamental particles. Matter is made of fermions, which break down into of six types of quarks, and six types of leptons, while forces are carried by bosons, four gauge bosons, and a single scalar boson called the Higgs particle. The quest for fundamental particles predicted by the standard model reached its grand finale in Geneva in 2012, where the detection of the final missing piece, the Higgs boson, was confirmed in the Large Hadron Collider [56].

Today, quantum field theory is widely regarded as the best theory available to describe nature[3], for its spectacular predictive power, as illustrated by the detection of the Higgs boson almost half a century after its prediction by the standard model. With empirical measurements of the dipole moment of the electron in agreement with its predictions up to eleven significant figures, quantum electrodynamics stands out as the most accurately tested physical theory in the history of mankind [57].

Given their glorious history and far reaching consequences, particularly in their applications to high energy particle physics, it is not surprising that quantum field theoretic approaches, despite their well-deserved reputation for difficulty, have become the mainstream

3 At the exception of gravitation, which to this day is best described by a classical field theory given by Einstein's theory of general relativity.

path of study of fundamental physics. As any theory however, they cannot be all-encompassing. And curiously enough, the earliest of the known forces to have been studied by mankind, gravity, turns out to be the one that seems to elude all techniques of quantization that had worked for other forces. Despite the ingenious complexity of quantum field theories and the steady humming of the ever more power-hungry particle accelerators, it remains unknown whether or not gravity can, or should be quantized.

1.2.2 *Some wisdom from quantum information*

Compared to particle physics, the quantum information theoretic approach to fundamental physics, is one much younger, much less ontologically committed, and much more attentive to the enigmatic features of quantum theory for what they are.

It is one in which quantum weirdness, such as entanglement, is not so much seen as the Achilles heel to our understanding of the universe, but rather the Achilles lance waiting to pierce through the fabric that ensheathes nature's deepest secrets. Although this more abstract formalism does not provide clear mental pictures of reality humans are so fond of, the suspension of ontological beliefs it stemmed from came with much less burdensome expressions, and gave a global vantage point from which the raw structure of quantum theory would be viewed unobstructed.

Carrying out investigations in a model-agnostic framework naturally opened the way to the formulation of statements that transcended any ontology: quantum information theoretic laws should outlive the standard model. One of the earliest contributions of such model-agnostic approaches to our fundamental understanding of nature is Bell's theorem. Since then, advances in quantum information have been eye-opening in their own way.

As a prime example of the power of such modern frameworks, the possibility of quantum teleportation was already inscribed in the early formulations of quantum mechanics, owed to Dirac and Von-Neumann, in the late 1920s. This mysterious phenomenon was however so deeply buried under a formalism exclusively devoted to the description of matter and forces, that it had eluded physicists for over half a century, before it was uncovered in the light of a more virginal formulation of quantum theory [58]. In the even more abstract diagrammatic representation of quantum information theory [59], the process of quantum teleportation has become essentially trivial.

Despite their youth, the information theoretic approaches bore gifts to the investigation of fundamental physics that reached further than their ability to unmask some ensconced features of quantum theory such as teleportation: they provided a path to answer questions that are entirely beyond the scope of particle physics. Bell's theorem, once

again, fell in this category, as it did not simply rule out classes of interpretations of quantum mechanics, but spoke of any attempt to describe observed correlations in any sort of objective local theory.

A much more recent and no less astounding discovery which was also found through the information-theoretic formalism of the Bell-CHSH theorem, originated in the works of Popescu and Rohrlich, in 1994. In a seminal paper [60], Popescu and Rohrlich had ventured to propose a hypothetical post-quantum non-local correlation that attained the maximal winning probability for the Bell-CHSH game $\mathbb{P}_{PR} = 1$, while optimal classical and quantum strategies had respective win rates of $\mathbb{P}_C = 0.75$ and $\mathbb{P}_Q = (2+\sqrt{2})/2 \approx 0.85$. Interestingly, the Popescu-Rohrlich (PR) post-quantum correlation still respected the no-signalling condition[4], and as such had no reason to be ruled-out as unphysical. Could it be that a natural correlation stronger than entanglement had yet to be discovered?

The beginning of an answer to this puzzle first appeared in 2000 in the postgraduate works of Van Dam [61]. He had proven that in any universe which admitted a PR process, all distributed computations, no matter how costly, could be carried-out with the communication of just a single bit. In other words, the existence of PR correlations would trivialize communication complexity. This result, known as Van Dam's theorem, had essentially ruled out the PR correlations under the plausible assumption that we should live in a universe with a non-trivial communication complexity. This naturally led physicists to wonder what could be said of correlations weaker than PR, but stronger than quantum entanglement.

The year 2009 saw the birth of the concept of information causality, a hypothesis by which "*the information gain that Bob can reach about a previously unknown to him data set of Alice, by using all his local resources and* m *classical bits communicated by Alice, is at most* m *bits*" [62]. This can be viewed as a natural generalization of the no-signalling hypothesis ($m = 0$). In the same article, it was demonstrated that there could be no winning probability greater than what was attainable with the entangled states of quantum theory, that would not violate information causality. Such a result brought concrete justification to the success of quantum mechanics: quantum theory was not merely an accidental discovery that stemmed from the observation of black-body radiation, which could one day be superseded by yet another futuristic discovery featuring correlations stronger even than entanglement. Quantum entanglement, as it appears, turned out to be the strongest possible natural correlation of any universe satisfying the admittedly weak requirement of information causality.

4 Non-signalling theories are those in which no information can be transmitted faster than causality, a critical condition to satisfy in order to be consistent with special relativity.

In the same spirit as thermodynamical laws, quantum information theory which formulates what is or is not possible from an operational perspective, has become an ever growing area of interest, not only to philosophers or computer scientists, but to physicists themselves.

1.3 THESIS OUTLINE

Greek tragedies had a characteristic set of conventions: they usually opened with a prologue (πρόλογος) in which the drama and the background of the story were introduced: the reader is now reaching the end of the prologue.

This was traditionally followed with the parodos (πάροδος) where the characters were introduced. In this thesis, the parodos is naturally found in the next chapter, where the reader is reminded of some familiar figures that take the form of theorems and definitions, and where the language of the play is introduced: while Greek tragedies were delivered in the Attic (Ἀττικὴ) and Doric (Δωρισμός) dialects, our play will naturally draw heavily from the mathematical dialect.

The well acquainted reader may skip ahead to the three episodes (ἐπεισόδια) where the story unfolds. As per the standard anatomy of greek tragedies, the three episodes are interspersed with stasima (στάσιμον), choral interludes commenting or explaining the situation. Although a topic in theoretical physics does not make for a very cathartic experience, there are inevitably some components of mimesis (μίμησις) in each of the stasimon, incorporating some re-production of fundamental work upon which the core of the plot is founded.

Our first episode deals with a class of inequalities often said to be the temporal counterpart of Bell's, which are regarded as a necessary condition for macroscopic realism. Their relationship to the classicality of light in the quantum optical sense is investigated. In the second episode, the story revolves around the minimum localization scale of quantum systems imposed by gravitation, and an analysis of how these effects may reveal themselves empirically in a quantum optomechanical experiment. In our final, and longest episode, we explore the possibility of detecting non-classical signatures of gravity which relies on the operational definition of quantum entanglement.

Finally, the exodus (ἔξοδος) marks the end of this play, with general concluding remarks.

2 PROPAEDEUTICS

If I have seen further it is by standing on the shoulder of Giants.

— **Isaac Newton** [63]

This chapter provides the unfamiliar reader with important foundational tools and ideas that will help understand the rest of the thesis. The first section covers core mathematical objects, concepts, and properties which are ubiquitous in quantum theory, such as Hilbert spaces, Lie algebras and tensor products. In the second section, the foundations of quantum mechanics, from the Hamiltonian and Lagrangian formalisms are revisited. In the third section, important tools from quantum optics are presented. The fourth and final section introduces the fascinating language of quantum information theory, and formalizes the notion of quantum entanglement.

2.1 ELEMENTS OF MATHEMATICS

In this opening section, we introduce many mathematical objects and properties which are crucial to quantum theory. The aim is to provide a somewhat self-contained presentation of the most important concepts for the purpose of this thesis. Inevitably, the work presented in the following chapters does involve some other mathematical concepts which, for the sake of conciseness, have not been formalized in this introduction. These include Lebesgue measure theory, probability theory, distribution theory and complex analysis, for which the unversed reader may find helpful introductions in the excellent book by Appel [64].

2.1.1 *Hilbert spaces*

Quantum mechanics speaks of the dynamics and evolution of quantum states, which are commonly represented as projective rays of a Hilbert space. But what does nature have to do with Hilbert spaces? One may argue that the Hilbert space representation seems somewhat artificially *ad-hoc*, and in point of fact it just works and has been working very well for quite some time. It is nonetheless possible to opt for a more general perspective, which is called the algebraic formulation of quantum mechanics, the foundations of which are C^*-algebras, instead of Hilbert spaces. In 1943 however, the Gelfand-Naimark theorem [65] established that there was a representation of any algebra of observables as operators on a Hilbert space. This showed the

Hilbert space description to be a perfectly justified choice of convenience rather than a fundamental natural fact. With this in mind, let us now dedicate some time to the proper definition of Hilbert spaces.

The Hilbert space is a relatively sophisticated mathematical object. Broadly speaking it is a type of vector space that is equipped with a scalar product and which is complete. Let us properly define these concepts (for a basic definition of vector spaces, see Appendix B).

Definition 1 (Scalar products). *A complex scalar product*[1] *on a complex vector space* V *is an external binary operation* $\langle \_|\_ \rangle : V^2 \to \mathbb{C}$ *called a sesquilinear form. It satisfies the five following conditions, the first two being right linearity and left anti-linearity*[2]*:*

1. $\forall (x, y, z) \in V^3, \forall \lambda \in \mathbb{C},\ \langle x|y + \lambda z\rangle = \langle x|y\rangle + \lambda \langle x|z\rangle$.
2. $\forall (x, y, z) \in V^3, \forall \lambda \in \mathbb{C},\ \langle x + \lambda y|z\rangle = \lambda^* \langle x|y\rangle + \langle x|z\rangle$.
3. $\forall (x, y) \in V^2,\ \langle y|x\rangle = \langle x|y\rangle^*$ *(hermitian symmetry).*
4. $\forall x \in V,\ \langle x|x\rangle \geqslant 0$ *(positivity).*
5. $\forall x \in V,\ \langle x|x\rangle = 0 \implies x = 0_V$ *(definiteness).*

In other words, a complex scalar product is a sesquilinear positive definite form on the vector space V. With this definition at hand, we introduce our first important property.

Theorem 1 (Cauchy-Schwarz inequality). *The complex scalar product satisfies the Cauchy-Schwarz inequality*

$$\forall (x, y) \in V^2,\ \langle x|x\rangle \langle y|y\rangle \geqslant |\langle x|y\rangle|^2 ,$$

and the equality is realized if and only if $\exists \lambda \in \mathbb{C},\ x = \lambda y$.

Proof. The case $y = 0$ is trivial. Suppose $y \neq 0$ and let $z = x - \frac{\langle y|x\rangle}{\langle y|y\rangle} y$ be the projection of x onto the hyperplane orthogonal to y. Then we observe that $\langle y|z\rangle = 0$ and $x = \frac{\langle y|x\rangle}{\langle y|y\rangle} y + z$, thus one may establish $\langle x|x\rangle = \left|\frac{\langle y|x\rangle}{\langle y|y\rangle}\right|^2 \langle y|y\rangle + \langle z|z\rangle = \frac{|\langle x|y\rangle|^2}{\langle y|y\rangle} + \langle z|z\rangle$ and the inequality follows from $\langle z|z\rangle \geqslant 0$. Furthermore, if $\exists \lambda \in \mathbb{C},\ x = \lambda y$ then the equality is trivial. Reciprocally the equality is equivalent to having $z = 0$ which immediately implies the colinearity of x and y. □

Another ingredient we need in order to define Hilbert spaces is the notion of completeness. For this, let us briefly go through some rudiments of vector space topology. Basic definitions of metric spaces, normed spaces and Cauchy sequences can be found in Appendix B.

1 Sometimes the scalar product is also called inner product.

2 One may well define the complex scalar product with right anti-linearity and left linearity. We have chosen here to stay consistent with Dirac's notations which are widely employed in the quantum physics community.

Definition 2 (Complete sets). *A metric space E is said to be complete when all Cauchy sequences of the set converge.*

A simple example of set that is not complete is the set of rationals $\mathbb{Q}$ equipped with the distance $d(x, y) = |x - y|$. Indeed, the sequence defined by $u_0 = 1$ and $\forall n \in \mathbb{N}, u_{n+1} = \frac{1}{2}u_n + \frac{1}{u_n}$ is a Cauchy sequence which does not converge in $\mathbb{Q}$.

Definition 3 (Banach spaces). *A normed vector space $(V, \mathcal{N})$ is called a Banach space if it is complete.*

If the Banach space has the structure of an associative algebra (that is an associative inner multiplication which is distributive on its addition), then it is called a Banach algebra. We now arrive at the formal definition of a Hilbert space.

Definition 4 (Hilbert spaces). *A complex vector space $\mathcal{H}$ is said to be a Hilbert space when the two following conditions are satisfied:*

1. *$\mathcal{H}$ is equipped with a complex scalar product.*
2. *$\mathcal{H}$ is complete.*

Let us note that Hilbert spaces are Banach spaces, as they are complete normed spaces. However, not all Banach spaces are Hilbert spaces as there exist norms which cannot be induced from an inner product. A famous class of examples is all vector spaces $\mathbb{C}^n, n \in \mathbb{N}^*$ equipped with the p-norm $\|x\|_p = (\sum_i |x_i|^p)^{1/p}$ for $p > 1$ and $p \neq 2$.

NOTATION Before we move on to further concepts, a vector v of a Hilbert space is often denoted as a *ket* $|v\rangle$, which is the corresponding Dirac notation. The dual element of a ket is called a *bra* and is denoted $\langle v|$. It is worth noting that the application $\varphi_v(x) : x \longmapsto \langle v|x\rangle$ mapping all elements x of a complex Hilbert space $\mathcal{H}$ to their scalar product with the vector v is a linear map from $\mathcal{H}$ to $\mathbb{C}$ and so the shorthand bra notation for this linear form can be seen as simply constructing the scalar product by applying the bra $\langle v|$ to a ket $|x\rangle$.

2.1.2 *Operators on Hilbert spaces*

Orthonormal bases[3] are very useful for representing linear operators (also called morphisms of vector spaces) due to the following important property, that we shall prove using the power of Dirac's notation.

Theorem 2 (Completeness relation). *Let $|i\rangle_{i \in I}$ be an orthonormal basis of a Hilbert space $\mathcal{H}$, then*

$$\sum_{i \in I} |i\rangle\langle i| = \mathbb{1}_{\mathcal{H}}. \tag{1}$$

3 The existence of an orthonormal basis is guaranteed by the Gram-Schmidt procedure in finite dimension and by Zorn's lemma in infinite dimension, we shall take those facts for granted for simplicity.

Proof. Let $|u\rangle \in \mathcal{H}$ then $\exists!(\lambda_i)_{i\in I} \in \mathbb{C}^{|I|}$, $|u\rangle = \sum_{i\in I} \lambda_i |i\rangle$, indeed the coefficients are simply the orthogonal projections onto each basis direction $\lambda_i = \langle i|u\rangle$. We have $|u\rangle = \sum_{i\in I} \langle i|u\rangle |i\rangle = \left(\sum_{i\in I} |i\rangle\langle i|\right) |u\rangle$ by associativity. As this holds for all vector $|u\rangle$, the result follows. □

Let us suppose that we have a morphism $U : E \to F$ where the input and output spaces are two finite dimensional vector spaces of dimensions $n, m \in \mathbb{N}$ over a field $\mathcal{F}$, for which we choose respective orthonormal bases $(v_i)_{1\leqslant i\leqslant n}$ and $(w_i)_{1\leqslant i\leqslant m}$. Then one can fully represent U through its action on the basis vectors. Indeed using two completeness relations one can write

$$U = \mathbb{1}_F U \mathbb{1}_E = \sum_{(i,j)\in(I\times J)} |w_i\rangle\langle w_i| U |v_j\rangle\langle v_j|,$$

from which one can read off the matrix elements of the representation of U in the considered bases as $u_{ij} = \langle w_i|U|v_j\rangle$.

The set of morphisms (of vector spaces) from E to F, denoted $\mathcal{L}(E, F)$ is itself a vector space. We see from the matrix representation that if E and F are n and m dimensional respectively, then $\dim(\mathcal{L}(E, F)) = nm$. In fact it is important to note, for the theory of quantum channels, that the vector space of operators between Hilbert spaces is also a Hilbert space.

Quite often in quantum mechanics, we deal with morphisms the input and ouput spaces of which are the same, they are called endomorphisms, and on a finite dimensional space they can be represented by square matrices. Let us briefly revisit some spectral theory of endomorphisms.

Definition 5 (Trace and determinant). *Let $U \in \mathcal{L}(E)$ be an endomorphism of the finite dimensional vector space E. Then its trace is the sum of its eigenvalues $\mathrm{Tr}(U) = \sum_{x\in\sigma(U)} x.deg(x)$ and its determinant is the product of its eigenvalues*[4] $\det(U) = \prod_{x\in\sigma(U)} x^{deg(x)}$.

Formally, it is possible to generalize the notion of trace to bounded positive-semidefinite endomorphisms (which will be defined shortly) of infinite dimensional Hilbert spaces. The notion of determinant can also be extended to that of functional determinants [66]. While the extension of the trace will be discussed further as it is noteworthy for the density operator formalism, that of the determinant is beyond the scope of this thesis.

Definition 6 (Diagonalizability). *An endomorphism $U \in \mathcal{L}(E)$ of a vector space E over field $\mathcal{F}$ is said to be diagonalizable when there exists a basis $|i\rangle_{i\in I}$ of E in which $U = \sum_{i\in I} \lambda_i |i\rangle\langle i|$ where $(\lambda_i)_{i\in I} \in \mathcal{F}^{|I|}$ are some coefficients.*

4 Note that trace and determinant are defined at the operator level, and as such do not depend an any representation of the operator. They are similarity invariants.

In other words, an endomorphism U is diagonalizable when there exists a basis of vectors which are all eigenvectors of U. On a finite dimensional space $\dim(E) = n \in \mathbb{N}^*$ this can be stated for matrix representations as $\exists P \in GL(n), \exists D \in \mathrm{diag}(n),\ U = PDP^{-1}$, that is, there exists a similarity P transforming U into a diagonal matrix D.

Definition 7 (Boundedness). *A morphism $U \in \mathcal{L}(E, F)$ between two normed vector spaces E, F is said to be bounded when*

$$\exists M \in \mathbb{R}_+^*, \forall x \in E,\ \|U(x)\|_F \leqslant M\|x\|_E.$$

This is denoted $U \in \mathcal{B}(E, F)$.

Definition 8 (Positivity). *A hermitian[5] endomorphism $U \in \mathcal{L}(\mathcal{H})$ of the complex Hilbert space $\mathcal{H}$ is said to be positive-semidefinite (resp. positive definite) when $\forall |x\rangle \in \mathcal{H},\ \langle x|U|x\rangle \geqslant 0$ (resp. $\langle x|U|x\rangle > 0$). One denotes this property $U \geqslant 0$ (resp. $U > 0$).*

One immediately notices that $U \geqslant 0 \implies \sigma(U) \subset \mathbb{R}_+$ and because eigenvectors are non-zero we also have $U > 0 \implies \sigma(U) \subset \mathbb{R}_+^*$. Reciprocally, if an endomorphism of $\mathcal{H}$ is hermitian and has a non-negative (resp. positive) and bounded spectrum, then it is positive semi-definite (resp. positive definite). In order to prove this however, one needs the spectral theorem which will be introduced shortly.

Definition 9 (Adjoint). *Let us consider a linear operator $U \in \mathcal{L}(E, F)$ where E and F are two Hilbert spaces. The adjoint $U^\dagger$ of U is the operator[6] satisfying $\forall (x, y) \in E \times F,\ \langle y|U(x)\rangle = \langle U^\dagger(y)|x\rangle$.*

In the finite dimensional case, the adjoint operator $U^\dagger$ is represented by the hermitian conjugate matrix $M^\dagger$ which is the conjugate transpose of the matrix M representing U. That is, in terms of matrix elements we have $m_{ij}^\dagger = m_{ji}^*$.

Let us note a simple but useful characterisation of positive semi-definite operators.

Claim 1. *Given a complex Hilbert space $\mathcal{H}$, an endomorphism $U \in \mathcal{L}(\mathcal{H})$ is positive semi-definite if and only if there exists an operator $V \in \mathcal{L}(\mathcal{H})$ such that $U = V^\dagger V$.*

Proof. Clearly, if $U = V^\dagger V$ then it is hermitian and satisfies the property $\forall x \in \mathcal{H},\ \langle x|U|x\rangle = \|Vx\|^2 \geqslant 0$. The reciprocal requires the spectral theorem. If U is hermitian then one can write its spectral representation as $U = \sum_{i \in I} \lambda_i |i\rangle\langle i|$, where $\lambda_i \in \mathbb{R}$. The positive-semidefiniteness condition yields $\forall i \in I,\ \lambda_i \geqslant 0$ hence defining $V = \sum_{i \in I} \sqrt{\lambda_i}\, |i\rangle\langle i|$ ends the proof. □

5 Technically it can be shown, from the polarization identity and the Hellinger-Toeplitz theorem, that a positive-semidefinite operator on a complex Hilbert space $\mathcal{H}$ is self-adjoint and bounded.

6 One can prove the existence and uniqueness of such an operator using Riesz's representation theorem, however this is beyond the scope of this summary.

Definition 10 (Remarkable properties). *Let us consider a linear operator* $U \in \mathcal{L}(E, F)$ *where* E *and* F *are two Hilbert spaces.*

1. *If* U *commutes with its adjoint, then it is said to be normal.*
2. *If* U *is equal to its adjoint, then it is said to be hermitian*[7]*.*
3. *If* $U^\dagger U = \mathbb{1}_E$*, then* U *said to be isometric.*
4. *If* $E = F$ *and* U *is isometric, then* U *is said to be unitary.*
5. *If* $U^2 = U$*, then* U *is said to be a projector.*

Note that in cases 1 and 2, we have $E = F$*.*

The set of unitary operators on a n-dimensional Hilbert space equipped with the multiplication, has a group structure, is called the unitary group and is denoted $\mathcal{U}(n)$.

Hermitian operators are of prime importance in the context of quantum theory, let us remind some of their key properties.

Claim 2. *Hermitian operators have real spectra.*

Proof. Given the eigenequation $U|v\rangle = \lambda|v\rangle$ one has $\langle v|U|v\rangle = \lambda\|v\|$ and $\langle v|U^\dagger|v\rangle = \lambda^*\|v\|$. Hermitian symmetry of U and $\|v\| \neq 0$ yields $\lambda = \lambda^*$ which ends the proof. □

Claim 3. *Hermitian operators have mutually orthogonal eigenspaces.*

Proof. Consider two eigenequations $U|v\rangle = \lambda|v\rangle$ and $U|w\rangle = \mu|w\rangle$. Then $\langle w|U|v\rangle = \lambda\langle w|v\rangle$ and $\langle w|U^\dagger|v\rangle = \mu^*\langle w|v\rangle$. If U is hermitian, then the two expressions are equal and the eigenvalues are real, so we arrive at $\lambda\langle w|v\rangle = \mu\langle w|v\rangle$, which implies that either the two eigenvalues are equal, or the eigenvectors are orthogonal. □

Let us now introduce an important type of projector.

Definition 11 (Orthogonal projectors). *A projector* $\Pi \in \mathcal{L}(E)$ *of a Hilbert space* E *is orthogonal when its kernel and support are orthogonal.*

In quantum mechanics non-orthogonal projectors are very rarely encountered, and so the orthogonality is usually omitted. We also have the following important characterization that, in some textbooks, is taken as definition.

Claim 4. *A projector of a Hilbert space is orthogonal is and only if it is hermitian.*

7 More generally it would be said to be self-adjoint, however in the context of a Hilbert space with a hermitian scalar product those two notions coincide.

Proof. Consider a projector $\Pi \in \mathcal{L}(E)$. If it is orthogonal, then its kernel and image are orthogonal supplements of the Hilbert space. Let us now consider two vectors $x, y \in \mathcal{E}$. Then $\langle y|\Pi(x)\rangle = \langle \Pi(y)|x\rangle$ holds on $\ker(\Pi)$ as well as on $\mathrm{supp}(\Pi)$, as it takes the forms $0 = 0$ and $\langle y|x\rangle = \langle y|x\rangle$ respectively. Since $E = \ker(\Pi) \oplus \mathrm{supp}(\Pi)$ the equation holds on E and thus Π is hermitian, by definition of the adjoint. Conversely if Π is hermitian, then its kernel and support are two eigenspaces associated with different eigenvalues, by claim 3. they are thus orthogonal. □

We now come to one of the most important mathematical theorems in quantum mechanics.

Theorem 3 (Spectral decomposition theorem for normal operators). *Any normal operator $U \in \mathcal{L}(E)$ on a finite dimensional*[8] *vector space E can be orthonormally diagonalized. Conversely any orthonormally diagonalizable operator is normal.*

Proof. We begin by the converse which is straightforward. Let U be an orthonormally diagonalizable operator. Then there exists a unitary similarity transformation P such that $U = PDP^\dagger$ where D is a diagonal operator. Then $UU^\dagger = PDP^\dagger PD^* P^\dagger$ and using the unitarity of P and the commutativity of diagonal operators gives the normality of U. Reciprocally, we proceed by induction on the dimension of E. The case $\dim(E) = 1$ is trivial. Let us consider a normal operator U, an eigenvalue $\lambda \in \sigma(U)$, the orthogonal projector Π onto the eigenspace $E_\lambda = \ker(U - \lambda \mathbb{1})$ and the orthogonal projector Ξ onto the orthogonal complement $E_\lambda^\perp$. From $\Pi + \Xi = \mathbb{1}$ one has $U = (\Pi + \Xi)U(\Pi + \Xi) = \Pi U \Pi + \Pi U \Xi + \Xi U \Pi + \Xi U \Xi$. We immediately see that $\Pi U \Pi = \lambda \Pi$ and $\Xi U \Pi = 0$ as the eigenspace is, of course, stable through U. By normality of U the operator commutes with $U^\dagger$ and so the eigenspace is also stable through $U^\dagger$ thus $\Xi U^\dagger \Pi = 0$, taking the hermitian conjugate of this equation yields $\Pi U \Xi = 0$. Hence we are left with $U = \Pi U \Pi + \Xi U \Xi$. Since the first term is already diagonal on E_λ one only needs to prove that the second term is diagonalizable on $E_\lambda^\perp$, and since $\dim(E_\lambda^\perp) \leqslant \dim(E) - 1$ by induction this reduces to proving that $\Xi U \Xi$ is normal. Noting that $\Pi + \Xi = \mathbb{1}$ we see that $\Xi U \Xi = \Xi U$ and $\Xi U^\dagger \Xi = \Xi U^\dagger$. Combining this with the normality of U and the projector property we have $\Xi U \Xi \Xi U^\dagger \Xi = \Xi U U^\dagger \Xi = \Xi U^\dagger U \Xi = \Xi U^\dagger \Xi \Xi U \Xi$, which ends the proof. □

This powerful theorem allows us to have a handy way of writing down all hermitian operators U as $U = \sum_{i \in I} \lambda_i |i\rangle\langle i|$, which is called

8 This can be generalized to infinite dimensional vector spaces, even uncountably infinite dimensions, however it requires the notion of spectral measure which is beyond the scope of this thesis.

the spectral representation. Note that $(\lambda_i)_{i\in I}$ is not necessarily an injective sequence, as there can be degenerate eigenvalues. The spectral representation is simply a real-weighted sum of spectral projectors, the coefficients being the eigenvalues of the operator. An immediate application of such a representation is the extension of numeric functions to normal operators, as long as they are defined on their spectra.

Definition 12 (Functional extensions). *A numeric function* $f : \mathbb{C} \to \mathbb{C}$ *can be extended to all normal operators* U *of a Hilbert space* $\mathcal{H}$ *with spectral representation* $U = \sum_{i\in I} \lambda_i |i\rangle\langle i|$ *as long as* f *is defined on* $\sigma(U)$*, in the following way:* $f(U) := \sum_{i\in I} f(\lambda_i) |i\rangle\langle i|$.

In particular, positive-semidefinite operators have a well defined square root, and a well defined absolute value $|U| = \sqrt{U^\dagger U}$. In order to extend definitions of functions beyond normal operators, one can rely on the analyticity of the function and the Banach algebra structure of operators, making sure that the operator norm does not exceed the function's radius of convergence. In this sense, the exponential function can easily be extended to non-normal or non-diagonalizable operators, however its familiar properties on the real or complex sets will not always carry over, as we shall see at length in the next section.

It would be unbecoming to conclude this section on Hilbert space operators without mentioning some important representations of operators and of the trace. Let us briefly revise these useful tools.

Claim 5. *If* $U \in \mathcal{L}(H)$ *is a normal endomorphism of a Hilbert space* $\mathcal{H}$ *then*

$$\mathrm{Tr}(U) = \sum_{i\in I} \langle i|U|i\rangle \,, \tag{2}$$

for any orthonormal basis $(|i\rangle)_{i\in I}$ *of* $\mathcal{H}$.

Proof. Since U is normal, it is unitarily diagonalizable. That is, there exists a unitary transformation P such that $\forall i \in I$, $|i\rangle = P|i'\rangle$ where $(|i'\rangle)_{i\in I}$ is an eigenbasis of U, i.e. $U = PdP^\dagger$ where d is diagonal. Hence $\sum_{i\in I} \langle i|U|i\rangle = \sum_{i\in I} \langle i'|P^\dagger UP|i'\rangle = \sum_{i\in I} d_i$ describes the sum of eigenvalues of U. □

This expression in fact is not only limited to normal endomorphisms, but to a broader class of operators that play an important role in quantum theory.

Definition 13 (Trace class). *Let* $U \in \mathcal{B}(\mathcal{H})$ *be a bounded endomorphism of the complex Hilbert space* $\mathcal{H}$*. Then* U *is said to be in the trace class if the series* $\sum_{i\in I} \langle i|\sqrt{U^\dagger U}|i\rangle$ *converges, where* $|i\rangle_{i\in I}$ *is an orthonormal basis of* $\mathcal{H}$*. In this case we have*

$$\mathrm{Tr}(U) = \sum_{i\in I} \langle i|U|i\rangle \,.$$

In finite dimension, all endomorphisms are obviously in the trace class and the definition of the trace coincides with the matrix trace. The set of trace class endomorphisms of $\mathcal{H}$ is a vector space denoted $\mathcal{B}_1(\mathcal{H})$. Equipped with the trace norm $\|U\|_1 := \mathrm{Tr}\left(\sqrt{U^\dagger U}\right)$ the trace class set is a Banach space. It is also worth noting that the trace class set is a bilateral ideal in the algebra of bounded endomorphisms, that is, if U is trace class and V is bounded, then UV and VU are trace class. Given this fact, let us briefly review some important properties of the trace.

Claim 6 (Similarity invariance of the trace). *Let $U \in \mathcal{B}_1(\mathcal{H})$ be a trace class operator on the Hilbert space $\mathcal{H}$. Then $\mathrm{Tr}(U)$ is invariant under any similarity (that stabilizes the set of bounded operators).*

Proof. Consider any invertible endomorphism P on the Hilbert space $\mathcal{H}$. By introducing the notation $u_{ij} = \langle i|U|j\rangle$ for operators, and using the inverse property $(P^{-1}P)_{ij} = \delta_{ij}$ one has[9]

$$\begin{aligned}\mathrm{Tr}\left(P^{-1}UP\right) &= \sum_{i\in I} \langle i|P^{-1}UP|i\rangle \\ &= \sum_{(i,j,k)\in I^3} \langle i|P^{-1}|j\rangle\ \langle k|P|i\rangle\, u_{kj} \\ &= \sum_{(j,k)\in I^2} \delta_{k,j} u_{kj} = \mathrm{Tr}(U).\end{aligned}$$

□

This statement is unsurprising in finite dimensions, as the trace of an operator is the sum of its eigenvalues, it is to be invariant under any change of matrix representation basis.

Claim 7 (Symmetry of the trace). *Let $UV \in \mathcal{B}_1(\mathcal{H})$ be a trace class endomorphism of the Hilbert space $\mathcal{H}$ composed of the two endomorphisms U, V on the same Hilbert space. Then one has $VU \in \mathcal{B}_1(\mathcal{H})$ and the identity $\mathrm{Tr}(UV) = \mathrm{Tr}(VU)$.*

Proof. Using two completeness relations in the definition of $\mathrm{Tr}(UV)$ and orthonormality $\langle i|j\rangle = \delta_{i,j}$, one has

$$\mathrm{Tr}(UV) = \sum_{(i,j,k)\in I^3} \langle i|j\rangle\ \langle j|U|k\rangle\ \langle k|V|i\rangle = \sum_{(i,k)\in I^2} u_{ik} v_{ik},$$

which is invariant under the swap operation $u \leftrightarrow v$. □

Claim 8 (Cyclicality of the trace). *$(U_j)_{1\leqslant j\leqslant n} \in (\mathcal{L}(\mathcal{H}))^n$ be a family of endomorphisms of the Hilbert space $\mathcal{H}$ where $n \in \mathbb{N}^*$, such that the ordered product $\prod_{j=1}^n A_j$ is a trace class operator. Then for any cyclic permutation $\sigma \in \mathfrak{S}_n$ of the index set, one has $\mathrm{Tr}\left(\prod_{j=1}^n U_j\right) = \mathrm{Tr}\left(\prod_{j=1}^n U_{\sigma(j)}\right)$.*

9 Let us insist again: in order to write the left-most quantity, one should also require that P and its inverse be bounded.

Proof. The result is trivial for $n = 1$ and already proven for $n = 2$ (symmetry of the trace). Suppose $n \geqslant 3$. The cyclic permutations of the index set $\{1, ..., n\}$ form a monogenous group. A valid generator is the permutation $\sigma = (n, 1, ..., n-1)$, it is thus sufficient to prove the trace invariance through this permutation. Let $V = \prod_{j=1}^{n-1} U_j$, by symmetry of the trace one has $\mathrm{Tr}(VU_n) = \mathrm{Tr}(U_n V)$ which proves that the trace is invariant under σ. □

Last but not least, it is worth mentioning at least three types of matrix decompositions which the quantum theorist may find handy to have kept in mind.

Theorem 4 (Polar decomposition). *Let $A \in \mathcal{M}_n(\mathbb{K})$ be a real or complex square matrix, where $n \in \mathbb{N}^*$. There exists a unitary matrix $U \in \mathcal{M}_n(\mathbb{K})$ and a positive semi-definite matrix $P \in \mathcal{M}_n(\mathbb{K})$ such that $A = UP$, where $P = |A| = \sqrt{A^\dagger A}$. If $A \in GL_n(\mathbb{K})$ then U is unique.*

Proof. $P = |A|$ is positive, by spectral theorem it can be decomposed as $P = \sum_i \lambda_i |i\rangle\langle i|$ where $\forall i, \lambda_i \geqslant 0$ and where $(|i\rangle)_{i \in I}$ is an orthonormal basis. Define $|\psi_i\rangle = A|i\rangle$, then $\langle\psi_i|\psi_i\rangle = \langle i|A^\dagger A|i\rangle = \langle i|P^2|i\rangle = \lambda_i^2$. For indices i such that $\lambda_i \neq 0$, one can define $|e_i\rangle = \lambda_i^{-1}|\psi_i\rangle$. The vectors $(|e_i\rangle)$ thus defined form an orthonormal family of vectors. This family can be extended to a basis by a Gram-Schmidt procedure.

Now let us define $U = \sum_i |e_i\rangle\langle i|$, which is unitary since it maps an orthonormal basis to another. Assuming $\lambda_i \neq 0$ one can establish $UP|i\rangle = \sum_k |e_k\rangle \langle k|P|i\rangle = \lambda_i |e_i\rangle = A|i\rangle$. Otherwise $UP|i\rangle = 0 = A|i\rangle$. Hence $A = UP$ on the orthonormal basis $(|i\rangle_{i \in I})$ which establishes the matrix equation. Finally, if A is invertible, then so is P hence U is uniquely determined as $U = AP^{-1}$. □

Here we have dealt with the left polar decomposition, one has the same results with a right polar decomposition. Let us see an immediate and powerful consequence of this theorem.

Theorem 5 (Singular value decomposition). *Let $A \in \mathcal{M}_n(\mathbb{K})$ be a real or complex square matrix, where $n \in \mathbb{N}^*$. Then there exists two unitary matrices U, V and a non-negative diagonal matrix S such that $A = USV$.*

Proof. By polar decomposition one has $A = WP$ where W is unitary and P is positive semi-definite. By spectral theorem one can write $P = TST^\dagger$ where T is itself unitary and S is diagonal and non-negative. Thus $A = WTST^\dagger$ and the multiplicative group structure of unitary matrices ends the proof. □

Theorem 6 (Cholesky decomposition). *Let $A \in \mathcal{M}_n(\mathbb{K})$ be a positive-definite matrix. There exists a unique lower-triangular matrix L such that $A = LL^\dagger$.*

Proof. Given a positive semi-definite matrix $A \in \mathcal{M}_n(\mathbb{K})$, by claim 1 one can write it as $A = V^\dagger V$ for some square matrix V. A Gram-Schmidt procedure allows to unequivocally write $V = QR$ where Q is unitary and R is upper-triangular. Thus $A = (QR)^\dagger QR = R^\dagger R$, and defining $L = R^\dagger$ yields the result. □

Now that we have reviewed some of the most important results about operators in Hilbert space, let us go back to the extension of familiar functions to operators. One particular function that we can extend to Hilbert space operators is the exponential function. Because of its importance in physics, we shall devote the next section to some of its crucial definitions and properties.

2.1.3 *The exponential map*

Let us go over some important properties of the exponential map. Although the aim is to maintain a certain level of rigour, what is shown here is best formulated within the framework of Lie groups, Lie algebras and representation theory. For our purpose, we shall not delve too deep in the theory, and refer the curious reader to Ref. [67] for a comprehensive introduction. We simply give ourselves the following definitions.

Definition 14 (Lie groups). *A Lie group $\mathcal{G}$ is a group which is also a finite-dimensional real smooth manifold, in which multiplication and inversion are smooth maps, that is $(x, y) \longmapsto x^{-1}y$ is a smooth mapping of $\mathcal{G}^2$ onto $\mathcal{G}$.*

Definition 15 (Lie algebras). *A Lie algebra $\mathfrak{g}$ is a vector space over a field $\mathcal{F}$ equipped with a bilinear operator $[\_,\_] : \mathfrak{g}^2 \to \mathfrak{g}$ called Lie bracket, satisfying the following two properties*

1. $\forall x \in \mathfrak{g},\ [x.x] = 0$ *(alternativity).*
2. $\forall (x, y, z) \in \mathfrak{g}^3,\ [x, [y, z]] + [y, [x, z]] + [z, [x, y]] = 0$ *(Jacobi identity).*

Claim 9. *The Lie bracket is anticommutative, that is*

$$\forall (x, y) \in \mathfrak{g}^2,\ [x, y] = -[y, x].$$

Proof. $\forall (x, y) \in \mathfrak{g}^2$ we have $[x + y, x + y] = [x, y] + [y, x]$ having used the alternativity and bilinearity properties on the right hand side. Using alternativity on the left hand side yields the result. □

For any associative algebra A the commutator $[x, y] = xy - yx$ defines a Lie bracket. In the remainder of this thesis, we shall use the terms commutator and Lie bracket interchangeably, as we will work in the associative algebras of endomorphisms of a vector space, or that of square matrices.

Definition 16 (Adjoint action). *Given a Lie algebra $\mathfrak{g}$ and $x \in \mathfrak{g}$, we define the adjoint action of x on $\mathfrak{g}$ as the map $Ad_x : \mathfrak{g} \to \mathfrak{g},\ y \longmapsto xyx^{-1}$, and its derivative $ad_x : \mathfrak{g} \to \mathfrak{g},\ y \longmapsto [x, y]$.*

As stated in a previous section, one can easily extend the exponential function to normal operators on a Hilbert space, by simply writing down their spectral representation. However there is no reason that the usual morphism realized by the exponential between $(\mathbb{C}, \times)$ and $(\mathbb{C}, +)$ be carried into a group morphism between operator groups. This is exemplified in the following important theorems.

Theorem 7 (Hadamard identity). *For all couple of elements (u, v) of a real Banach algebra*

$$Ad_{e^u}(v) = e^{ad_u}(v). \tag{3}$$

Proof. Consider the function defined on the real set $f : t \longmapsto e^{tu} v e^{-tu}$. One finds its first derivative to take the form $\frac{d}{dt} f(t) = e^{tu}[u, v]e^{-tu}$. It is also straightforward to establish the expression for the n-th derivative $\forall n \in \mathbb{N},\ \frac{d^n}{dt^n} f(t) = e^{tu} \mathrm{ad}_u^n(v) e^{-tu}$. By analyticity of f on the real set, its Maclaurin expansion is $f(t) = \sum_{n=0}^{+\infty} \mathrm{ad}_u^n(v) t^n / n!$ which at $t = 1$ yields the result. □

As a simple but common use case of the Hadamard identity in quantum theory, let us assume that we have two Hilbert space operators $x, p \in \mathcal{L}(\mathcal{H})$ which satisfy the commutation relation $[x, p] = \lambda \mathbb{1}$ for some $\lambda \in \mathbb{C}$, then $e^p x e^{-p} = x + [x, p] = x + \lambda \mathbb{1}$.

Let us further venture in the complications which arise with exponentials on non-commutative algebras. Consider an operator algebra $\mathcal{A}$ and an element $(x, y) \in \mathcal{A}^2$. If $[x, y] = 0$ then we can write[10]

$$\begin{aligned} e^{x+y} = \sum_{n=0}^{+\infty} \frac{(x+y)^n}{n!} &= \sum_{n=0}^{+\infty} \sum_{k=0}^{n} \binom{n}{k} \frac{x^k y^{n-k}}{n!} \\ &= \sum_{n=0}^{+\infty} \sum_{k=0}^{n} \frac{x^k y^{n-k}}{k!(n-k)!} = \sum_{r,s=0}^{+\infty} \frac{x^r y^s}{r!s!} = e^x e^y, \end{aligned}$$

however this simple homomorphism property of the exponential map breaks down when the algebra is not commutative (invalid binomial expansion), as is the case in quantum theory. One may still wonder whether there exists an element $z \in \mathcal{A}$ satisfying $e^z = e^x e^y$. Intuitively, one can opt for $z = \log(e^x e^y)$ and write down the power series $\log(t) = \sum_{n=1}^{+\infty} \frac{(-1)^{n+1}}{n} (t-1)^n$. By substitution one can establish

$$\log(e^x e^y) = \sum_{n=1}^{+\infty} \frac{(-1)^{n+1}}{n} \left(\sum_{k,l=0}^{+\infty} \frac{x^k y^l}{k!l!} - \mathbb{1} \right)^n.$$

10 Writing out the exponent technically assumes an underlying unital field of characteristic 0, which will always be the case in quantum theory. Convergence issues are not a concern when dealing with normal operators.

By noticing that $\sum_{k,l=0}^{+\infty} \frac{x^k y^l}{k!l!} - \mathbb{1} = \sum_{k+l>0} \frac{x^k y^l}{k!l!}$ one arrives at an obscure yet common identity in quantum theory, called the Baker-Campbell-Hausdorff (BCH) formula.

Theorem 8 (Baker-Campbell-Hausdorff formula). *Given two elements x, y of a Banach algebra the exponentials of which are defined, we have*

$$e^x e^y = \exp\left(\sum_{n=1}^{+\infty} \sum_{k_1+l_1>0} \dots \sum_{k_n+l_n>0} \frac{(-1)^{n+1}}{n} \frac{x^{k_1} y^{l_1} \dots x^{k_n} y^{l_n}}{k_1! l_1! \dots k_n! l_n!}\right).$$

The way we arrived at the BCH formula is simply illustrative. This identity has been thoroughly studied in the mathematics community and for a complete picture and several derivations see Ref. [68]. In quantum theory one will not have to deal with the full BCH expansion in general. In order to unpack this formula, it is instructive to inspect the first terms. The $n = 1$ term reads

$$\sum_{k_1+l_1>0} \frac{x^{k_1} y^{l_1}}{k_1! l_1!} = x + y + xy + \frac{x^2 + y^2}{2} + \dots$$

The $n = 2$ term reads

$$\sum_{k_1+l_1>0} \sum_{k_2+l_2>0} \left(\frac{-1}{2}\right) \frac{x^{k_1} y^{l_1} x^{k_2} y^{l_2}}{k_1! l_1! k_2! l_2!} = \left(\frac{-1}{2}\right) (x^2 + y^2 + xy + yx + \dots)$$

One notes that the n-th term contains contributions of order at least n. From those two terms alone, one can write down the order 2 BCH expansion as

$$e^x e^y = \exp\left(x + y + \frac{1}{2}[x, y] + \dots\right),$$

and one can show that terms of order n can be written with n nested commutators. With some more tedious work one can arrive at the order 3 BCH expansion

$$e^x e^y = \exp\left(x + y + \frac{1}{2}[x, y] + \frac{1}{12}([x, [x, y]] + [y, [y, x]]) + \dots\right). \quad (4)$$

In standard quantum theory, it is quite common to have situations where the second order nested commutators vanish, in this case we have the following useful identity.

Theorem 9 (Disentangling theorem). *Given two elements x, y of a Banach algebra, the exponentials of which are defined, if the nested commutators satisfy $[x, [x, y]] = [y, [y, x]] = 0$ and we denote the commutator $[x, y] = c$, then*

$$e^{x+y} = e^x e^y e^{-\frac{1}{2}c} = e^y e^x e^{\frac{1}{2}c}. \quad (5)$$

Before moving on to another topic, let us go through another useful and typical situation where some difficulties may arise when handling the exponential map in non-commutative algebras.

Fundamental physical laws are often expressed as differential equations, the simplest of which are homogeneous linear first order ordinary equations, which take the form $y' = ay$ to be solved on an interval of the real line with some initial condition.

In the case of commutative algebras, there is a well known solution $y(t) = \exp\left(\int_{t_0}^{t} a(s)ds\right)y(t_0)$, which comes from the simple property of the exponential $\frac{d}{dt}e^f = f'e^f$. This property itself can be seen as arising from $\forall n \in \mathbb{N}^*$, $\frac{d}{dt}f^n = nf^{n-1}f'$ combined with the power series definition of the exponential function. However, in the non-commutative case one has $\forall n \in \mathbb{N}^*$, $\frac{d}{dt}f^n = \sum_{k=1}^{n} f^{k-1}f'f^{n-k}$. Therefore

$$\frac{d}{dt}e^f = \lim_{n\to\infty}\frac{d}{dt}\left(1+\frac{f}{n}\right)^n = \lim_{n\to\infty}\sum_{k=1}^{n}\left(1+\frac{f}{n}\right)^{k-1}\frac{f'}{n}\left(1+\frac{f}{n}\right)^{n-k},$$

recognizing the limit of a Riemann sum, this takes the form

$$\frac{d}{dt}e^f = \int_0^1 e^{sf}f'e^{(1-s)f}ds = e^f\int_0^1 \mathrm{Ad}_{e^{sf}}(f')ds = e^f\int_0^1 e^{\mathrm{ad}_{sf}}(f')ds,$$

where we have used the Hadamard identity Eq. (3) in the final step. Hence, when one is faced with the seemingly simple differential equation $y' = ay$, in general the solution will have to take into account non-vanishing commutators between a function and its derivative. This results in the following theorem, which was first put forward in Ref. [69].

Theorem 10 (Magnus' theorem). *Let a be a function of t in an associative ring, and let y be a solution of $y' = ay$ with $y(0) = \mathbb{1}$. Then under certain convergence conditions, y can be written in the form $y(t) = \exp(\Omega(t))$ where Ω satisfies*

$$\frac{d}{dt}\Omega = \sum_{n=0}^{+\infty}\frac{B_n}{n!}ad_\Omega^n a,$$

where $(B_n)_{n\in\mathbb{N}}$ is the Bernouilli sequence.

For a derivation of this theorem and more about its context, see the extensive review Ref. [70]. For our purpose, we can note the three first terms in the Magnus expansion:

$$\begin{aligned}
\Omega_1(t) &= \int_0^t a(t_1)dt_1,\\
\Omega_2(t) &= \int_0^t dt_1\int_0^{t_1} dt_2[a(t_1), a(t_2)],\\
\Omega_3(t) &= \int_0^t dt_1\int_0^{t_1} dt_2\int_0^{t_2} dt_3\Big[a(t_1),[a(t_2),a(t_3)]\Big]\\
&\qquad\qquad + \Big[a(t_3),[a(t_2),a(t_1)]\Big].
\end{aligned}$$

2.1.4 *Tensor products*

One last useful ingredient to formalize quantum theory for the purpose of this thesis, is that of tensor products.

Definition 17 (Tensor products). *A tensor product* $E \otimes F$ *of two vector spaces* E, F *over the same field* $\mathcal{F}$ *is a vector space associated with a bilinear map* $E \times F \to E \otimes F$, $(x, y) \longmapsto x \otimes y$. *A basis of* $E \otimes F$ *is* $(v_i \otimes w_j)_{(i,j)\in I\times J}$ *where* $(v_i)_{i\in I}$ *and* $(w_j)_{j\in J}$ *are respective bases of* E *and* F.

From this construction it is clear that in finite dimensions one has $\dim(E \otimes F) = \dim(E)\dim(F)$.

Definition 18. *A tensor product* $\mathcal{H}_1 \otimes \mathcal{H}_2$ *of two Hilbert spaces* $\mathcal{H}_1, \mathcal{H}_2$ *is the tensor product of the two vector spaces equipped with the inner product*

$$\forall \phi_1, \psi_1 \in \mathcal{H}_1,\ \forall \phi_2, \psi_2 \in \mathcal{H}_2,$$
$$\langle \phi_1 \otimes \phi_2 | \psi_1 \otimes \psi_2 \rangle = \langle \phi_1 | \psi_1 \rangle_1 \langle \phi_2 | \psi_2 \rangle_2 .$$

In quantum theory, it is common practice to omit the tensor multiplication between kets and instead of writing $|\psi_1\rangle \otimes |\psi_2\rangle$ opt for $|\psi_1\rangle |\psi_2\rangle$ and sometimes even $|\psi_1\psi_2\rangle$ when the context is not ambiguous. Tensor products on dual spaces yield the same rules for the tensor product of bras. A noteworthy fact for the study of entanglement theory, is that not all vectors $|v\rangle$ in the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ can be factorized as $|v\rangle = |v_1\rangle \otimes |v_2\rangle$ where $|v_1\rangle \in \mathcal{H}_1$ and $|v_2\rangle \in \mathcal{H}_2$.

Definition 19. *A tensor product* $A \otimes B$ *of two algebras* A, B *is the algebra obtained by the construction*

$$\forall a_1, a_2 \in A,\ \forall b_1, b_2 \in B,\ (a_1 \otimes b_1)(a_2 \otimes b_2) = a_1 a_2 \otimes b_1 b_2.$$

We have some useful identities combining tensor products and previously seen operations. For example, given two algebras $\mathcal{A}_1, \mathcal{A}_2$ and $A \in \mathcal{A}_1$ and $B, C \in \mathcal{A}_2$ one has $[A \otimes B, A \otimes C] = A^2 \otimes [B, C]$. There is also the interesting fact that given an analytic function f we have[11] $f(A \otimes \mathbb{1}) = f(A) \otimes \mathbb{1}$. Finally, one has the following simple identity: $\exp(A \otimes \mathbb{1} + \mathbb{1} \otimes B) = \exp(A) \otimes \exp(B)$.

Let us now see how the trace combines with tensor products.

Definition 20. *Let* $A \in \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ *be an endomorphism of the tensor product Hilbert space* $\mathcal{H}_1 \otimes \mathcal{H}_2$. *The partial trace of* A *over the Hilbert space* $\mathcal{H}_1$ *is the application*

$$\mathrm{Tr}_1(A) : \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2) \to \mathcal{L}(\mathcal{H}_2),\ A \longmapsto \sum_{i\in I} (\langle i| \otimes \mathbb{1}) A (|i\rangle \otimes \mathbb{1}),$$

where $(|i\rangle)_{i\in I}$ *is any orthonormal basis of* $\mathcal{H}_1$.

Let us note that the partial trace of an operator is another operator on a smaller Hilbert space, as this will be important in the formalization of quantum channels.

11 Assuming A is in a Banach algebra and that its norm is less than the radius of convergence of f.

2.2 ELEMENTS OF STANDARD QUANTUM PHYSICS

With all the required mathematical ingredients at hand, we are now ready to revisit some foundations of modern quantum physics. In particular, we review how one builds the quantum counterparts of Hamiltonian mechanics, phase space formulations and Lagrangian mechanics. The Schrödinger and Heisenberg pictures, akin to the Eulerian and Lagrangian specifications of the classical flow field, are also introduced.

2.2.1 *Quantizing Hamiltonian mechanics*

In this section we remind some basics of Hamiltonian quantum mechanics, starting from classical physics and building the canonical commutation relations in quantum mechanics. In Hamiltonian theory, the equations of motion of a system are derived from a Hamiltonian, a function of phase-space variables, through an operation called Poisson bracket. The concept of phase space was developed at the end of the 19th century by Ludwig Boltzmann, Henri Poincaré and Josiah Willard Gibbs, and is a smooth manifold on which every state of a system can be represented. A single classical particle's state is defined by its positions and momenta, which constitute a single point in its 6-dimensional phase space. Let us define the Poisson bracket explicitly.

Definition 21 (Poisson brackets between phase space variables). *Given a single particle with position vector* x *and momentum vector* p*, the Poisson bracket between position and momentum variables satisfies the following three equations:*

1. $\{x_i, p_j\} = \delta_{i,j}$,
2. $\{x_i, x_j\} = 0$,
3. $\{p_i, p_j\} = 0$.

Definition 22 (Poisson brackets between phase space functions). *Given three functions* f, g, h *of phase space and two real numbers* λ, μ*, the Poisson bracket satisfies the following four conditions:*

1. $\{f, g\} = -\{g, f\}$ *(anticommutativity).*
2. $\{\lambda f + g, h\} = \lambda\{f, h\} + \{g, h\}$ *(linearity).*
3. $\{f, gh\} = \{f, g\}h + g\{f, h\}$ *(Leibniz rule).*
4. $\{f, \{g, h\}\} + \{h, \{f, g\}\} + \{g, \{h, f\}\} = 0$ *(Jacobi identity).*

One can notice in fact that the Poisson bracket is a type of Lie bracket, with the additional Leibniz rule. The classical Hamiltonian equations of motion take the simple form

$$\frac{df}{dt} = \{f, H\} + \partial_t f, \tag{6}$$

and one sees that for functions f that do not have explicit time dependence $\partial_t f = 0$, but only depend on time through the phase space variables, the evolution is entirely governed by the Poisson bracket with the Hamiltonian. This case is quite common as it applies to any polynomial of phase space variables with constant coefficients. In particular, Hamiltonians with no explicit time dependence induce dynamics for which the energy is conserved $\{H, H\} = 0$ by anti-commutativity. More generally, any function that does not have explicit time dependence and which commutes with the Hamiltonian, is a conserved quantity, also called a constant of motion.

To sum up, on classical phase space we have a simple multiplication between observables, which are scalar functions of the phase space variables, and a more sophisticated multiplication called the Poisson bracket. In quantum phase space however, the simple multiplication is not commutative. In combination with the Poisson bracket, this imposes a certain form for the non-commutativity as we shall see now.

Let us consider four operator-valued functions a_1, a_2, b_1, b_2 of the phase space variables[12]. Then the Poisson bracket $\{a_1 a_2, b_1 b_2\}$ can be expanded in two ways. One can first expand the product $a_1 a_2$ and then expand $b_1 b_2$:

$$\begin{aligned}\{a_1 a_2, b_1 b_2\} = a_1(b_1\{a_2, b_2\} + \{a_2, b_1\}b_2) \\ + (\{a_1, b_1\}b_2 + b_1\{a_1, b_2\})a_2,\end{aligned}$$

or equivalently expand the $b_1 b_2$ product first, and then $a_1 a_2$:

$$\begin{aligned}\{a_1 a_2, b_1 b_2\} = b_1(a_1\{a_2, b_2\} + \{a_1, b_2\}a_2) \\ + (a_1\{a_2, b_1\} + \{a_1, b_2\}a_2)b_2.\end{aligned}$$

Expanding those two expressions, one sees that second and fourth terms in the first expansion are respectively equal to the second and third term in the second expansion. Equating the two expansions thus imposes the condition

$$(a_1 b_1 - b_1 a_1)\{a_2, b_2\} = \{a_1, b_1\}(a_2 b_2 - b_2 a_2).$$

We recognize a commutator, and we can understand this equation as follows: the operations $\mathcal{L} : (a, b) \longmapsto [a, b]$ and $\mathcal{P} : (a, b) \longmapsto \{a, b\}$, defined on the space of couples of functions of the canonical variables,

12 It is common practice in introductory quantum mechanics to denote operator valued quantities with a hat, however in the same way that vectors were not underlined or denoted with an arrow, we shall omit hats on operators and trust the reader to identify object types from context.

commute. Since this commuting property holds on the whole function space, necessarily there exists a nonzero element κ in the center of the group of functions over phase space (i.e. a scalar operator), such that $\mathcal{L} = \kappa\mathcal{P}$. We shall later justify why it turns out that $\kappa = i\hbar\mathbb{1}$, where $\hbar$ is the reduced Planck constant. In doing so, we will visit the Schrödinger and Heisenberg pictures of quantum dynamics.

In other words, by letting go of the commutativity of the phase space variables, hence making the algebra of functions defined on phase space non-commutative, the Poisson structure is modified in a way that is completely captured by the commutator between functions. In particular, Hamilton's equation (6) for a function with no explicit time dependence can be written down using the commutator as

$$\frac{df}{dt} = \frac{-i}{\hbar}[f, H], \tag{7}$$

which is called Heisenberg's equation of motion. Furthermore, the definition of the Poisson bracket between phase space variables can now be rewritten with commutators as follows.

Claim 10 (Commutator between phase space variables).
Given a single particle with position vector x and momentum vector p, the commutator between position and momentum operators satisfies the following three equations:

1. $[x_i, p_j] = i\hbar\delta_{i,j}$,
2. $\{x_i, x_j\} = 0$,
3. $\{p_i, p_j\} = 0$.

Proof. This immediately follows from the relationship between Poisson bracket and commutator. □

2.2.2 *Schrödinger, Heisenberg and Dirac pictures*

So far, we have seen that the failure of commutativity between functions of phase space variables can only be made compatible with Poisson brackets if the commutators are proportional to the Poisson brackets. We have also shown that functions of phase space variables which do not explicitly depend on time have their dynamics governed by their commutator with the Hamiltonian function. Let us now approach the question of quantum dynamics from the point of view of unitary transformations and Noether's theorem.

The fundamental object in quantum mechanics one is introduced to is the wavefunction $\psi(x, t)$ which is a complex probability amplitude, and belongs in the Hilbert space $\mathcal{H}$ of $\mathcal{L}^2(\mathbb{R}^4, \mathbb{C})$ functions. If ψ is normalized, it is associated to a pure physical state usually denoted with a ket $|\psi\rangle$, of which it is a position space representation. Any unitary operation U defines an automorphism of both the state space

$\mathcal{H}$ and of the space of its endomorphisms $\mathcal{L}(\mathcal{H})$. One can see this through the following construction. Let $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ and $|\psi'\rangle = U|\psi\rangle$, $|\phi'\rangle = U|\phi\rangle$ then

$$\langle\phi'|\psi'\rangle = (U|\phi\rangle)^\dagger U|\psi\rangle = \langle\phi|U^\dagger U|\psi\rangle = \langle\phi|\psi\rangle.$$

For all endomorphism $O \in \mathcal{L}(\mathcal{H})$ let $O' = UOU^\dagger$ so that

$$\langle\phi'|O'|\psi'\rangle = \langle\phi|U^\dagger UOU^\dagger U|\psi\rangle = \langle\phi|O|\psi\rangle.$$

What this means is that the action of a unitary operation leaves the physics unchanged, as the overlaps between states and the expectation values of operators are left invariant. In fact one also has the converse statement: operations under which the physics is left unchanged necessarily leave overlaps between any states invariant, they are isometric endomorphisms, i.e. unitary operations.

We have seen that according to Hamiltonian theory, a closed system's evolution must be governed by its Hamiltonian. For a closed system, this Hamiltonian is conserved, and so the system must be time translation invariant according to Noether's theorem. Let us consider such a closed system the quantum state of which lies in a Hilbert space $\mathcal{H}$. Then time translation symmetry reads

$$\forall |\phi\rangle, |\psi\rangle \in \mathcal{H},\ \forall dt \geqslant 0,\ \langle\phi(t+dt)|\psi(t+dt)\rangle = \langle\phi(t)|\psi(t)\rangle.$$

In light of our previous remark, it follows that there is an automorphism $U(dt)$ of the state space and of the space of its endomorphisms. The set of such unitary operators equipped the operator composition has the structure of an abelian group, which means we can write down $\forall t \geqslant 0, \forall n \in \mathbb{N}^*,\ U(t) = U(t/n)^n$. Taking the limit $n \to +\infty$ and carrying out a quadratic expansion yields

$$\forall t \geqslant 0,\ U(t/n) = \mathbb{1} + \frac{t}{n}U'(0) + O(1/n^2) \sim \exp\left(\frac{t}{n}U'(0) + O(1/n^2)\right),$$

so that one arrives at

$$U(t) \underset{t\to 0}{\sim} \exp\big(tU'(0)\big).$$

A consequence of this final equation is that the unitarity of $U(t)$ for any parameter t implies that the operator $U'(0)$ must be antihermitian. To put it more mathematically, we have characterized the generators of the time translation symmetry group[13].

All things considered, we have established the existence of a hermitian operator, which will turn out to be the Hamiltonian up to a scaling factor $-H/\hbar$, satisfying $U'(0) = -iH/\hbar$. With such a prescription, the unitary time propagator is found to be generated by the

13 We have assumed that this Lie algebra of generators is topologically star-shaped at its identity element.

time independent Hamiltonian: $\forall t \in \mathbb{R},\ U(t) = \exp(-iHt/\hbar)$. We may now look at the action of this operation on the state space. We obtain the simple equation $\forall |\psi\rangle \in \mathcal{H},\ |\psi(t)\rangle = \exp(-iHt/\hbar)\,|\psi(0)\rangle$, from which one establishes the famous Schrödinger equation through a time differentiation

$$\forall t \in \mathbb{R},\ i\hbar \frac{d}{dt}\,|\psi(t)\rangle = H\,|\psi(t)\rangle\,. \tag{8}$$

This formulation of quantum dynamics in which it is the quantum states that evolves in time according to the unitary propagator is called Schrödinger picture. As mentioned previously, one can also adopt the dual point of view, in which the unitary propagator instead conjugates the space of operators, and where the states are constants of time. That is, we now define

$$O_H(t) = \exp(iHt/\hbar)O_S \exp(-iHt/\hbar),$$

where the H index indicates a Heisenberg operator, and the S index indicates a Schrödinger operator. The dynamics of the operators is then simply found to be the adjoint action of the time propagator[14].

$$\begin{aligned}
\frac{d}{dt}O_H(t) &= \frac{iH}{\hbar}\exp(iHt/\hbar)O_S\exp(-iHt/\hbar) \\
&\qquad\qquad - \exp(iHt/\hbar)O_S\exp(-iHt/\hbar)\frac{iH}{\hbar}, \\
&= \frac{i}{\hbar}\exp(iHt/\hbar)[H, O_S]\exp(-iHt/\hbar), \\
&= \frac{-i}{\hbar}[O_H(t), H].
\end{aligned}$$

One recognizes the Heisenberg equation of motion Eq. (7). In deriving this result, we have thus effectively identified the generator of the time propagator as being the Hamiltonian, shown that it must be a hermitian operator, and that the κ coefficient relating the Poisson to the Lie bracket must be purely imaginary. The reduced Planck constant $\hbar$ simply comes as a scaling factor that can be ignored when working in natural units.

A third representation of quantum dynamics worth mentioning for its importance in quantum field theory, is called Dirac picture. It is essentially a hybridization of the Schrödinger and Heisenberg representations when the dynamics is generated by a Hamiltonian that can be split in two parts $H = H_0 + H_1$. In most encountered situations H_0 represents a free Hamiltonian while H_1 is an interaction term, usually a small perturbation. Working in the Dirac representation amounts to having operators evolve through the action of H_0 according to Heisenberg's equation, and have states evolve through the action of H_1 according to Schrödinger's equation. States and operators in the Dirac picture, that we shall denote with a tilde, are then related to those

14 Assuming the Schrödinger operator itself does not carry an extra time dependence.

in the Schrödinger picture via the following automorphisms of state and operator spaces:

$$\left|\tilde{\psi}(t)\right\rangle = \exp(iH_0 t/\hbar)\left|\psi(t)\right\rangle_S\,;\ \tilde{O}(t) = \exp(iH_0 t/\hbar)O_S\exp(-iH_0 t/\hbar).$$

From this one can establish the corresponding equations of motion for states and operators in the Dirac picture

$$i\hbar\frac{d}{dt}\left|\tilde{\psi}(t)\right\rangle = \tilde{H}_1\left|\tilde{\psi}(t)\right\rangle;\ \frac{d}{dt}\tilde{O}(t) = \frac{-i}{\hbar}[\tilde{O}(t), H_0]. \tag{9}$$

2.2.3 *Quantum phase space*

We have reviewed how in relinquishing the commutativity of functions of the phase space variables, Hamilton's equations of motion may be cast into Heisenberg's equations of motion. We have also seen how the Hamiltonian generates a unitary propagator which is an automorphism of the state and operator spaces corresponding to time evolution. One can view the dynamics as arising from the variation of the observables themselves (Heisenberg picture) or of the quantum state itself (Schrödinger picture).

Let us now step away from dynamics and think about quantum states themselves. In classical physics, a single point-like system's (ontic) state can be represented as a single point in phase space. If one does not know precisely the position or momentum of the classical system, then its (epistemic) state will be represented as a probability distribution $f(x,p)$ over phase space which evolves according to Liouville's equation[15] $\partial_t f = -\{f, H\}$. What would then be the quantum counterparts to the ontic and epistemic classical states? In order to determine this, one first needs to represent quantum states in position and momentum spaces.

Consider the position operator X which is self-adjoint. By the spectral theorem, one can find an orthonormal basis of the state space made up of eigenvectors of X, and hence one has the completeness relation $\int_{\mathbb{R}} dx\,|x\rangle\langle x| = \mathbb{1}$, where we have a Dirac overlap between normalized eigenvectors $\langle x|x'\rangle = \delta(x-x')$. One can then write an arbitrary quantum state $|\psi\rangle$ as $|\psi\rangle = \int_{\mathbb{R}} dx\,\langle x|\psi\rangle\,|x\rangle$, and the overlap $\psi(x) := \langle x|\psi\rangle$ is called the wavefunction.

Let us now turn to the momentum operator P, which is by definition the generator of spatial translations $|x+\delta x\rangle = \exp(-iP\delta x/\hbar)\,|x\rangle$. Being a hermitian operator, one also has the completeness relation $\int_{\mathbb{R}} đk\hbar k\,|k\rangle\langle k| = \mathbb{1}$, where we have denoted $đk = dk/2\pi$ and defined $|k\rangle$ so that $P\,|k\rangle = \hbar k\,|k\rangle$. Note that the orthonormality is here written as $\langle k|k'\rangle = 2\pi\delta(k'-k)$. By spectral decomposition of P one can write $\exp(-iP\delta x/\hbar) = \int_{\mathbb{R}} đk\exp(-ik\delta x)\,|k\rangle\langle k|$, and so one has

15 Note that there is an extra sign compared to Hamilton's equations.

$|x+\delta x\rangle = \int_{\mathbb{R}} đk \exp(-ik\delta x)\,|k\rangle\,\langle k|x\rangle$. Applying the bra $\langle k|$ to the previous equation yields

$$\langle k|x\rangle = \int_{\mathbb{R}} đk' \exp(-ik\delta x) 2\pi\delta(k'-k)\,\langle k'|x\rangle = \exp(-ik\delta x)\,\langle k|x\rangle\,.$$

That is, $\langle k|x\rangle = \exp(-ikx)\,\langle k|0\rangle$. Finally the constant factor can be determined by evaluating $\langle x|x'\rangle = \int_{\mathbb{R}} đk\,\langle x|k\rangle\,\langle k|x'\rangle = |\,\langle k|0\rangle\,|^2\delta(x'-x)$, which imposes $\langle k|0\rangle = 1$. We thus arrive at the important relationship

$$\langle k|x\rangle = e^{-ikx}. \tag{10}$$

This indicates that the position and momentum eigenstates are related by a Fourier transformation. As for the wavefunctions on position (or direct) and momentum (or reciprocal) space, they are also related by a Fourier transform

$$\mathcal{F}(\psi)(k) := \langle k|\psi\rangle = \int_{\mathbb{R}} dx\,\langle k|x\rangle\,\langle x|\psi\rangle = \int_{\mathbb{R}} dx\; e^{-ikx}\psi(x).$$

A noteworthy consequence of this, is that the action of a momentum operator in the position representation is simply the application of a gradient $P\psi(x) = -\frac{i}{\hbar}\partial_x\psi(x)$.

We have now characterized representations of quantum states on phase space. But what if, as can be the case in classical statistical physics, one had some imperfect preparation of a quantum state? Then in order to calculate the expectation value of an observable one would have to average over fluctuations in the state preparation itself. This kind of statistical quantum states are captured by what are called density operators. Suppose indeed that a pure quantum state $|\psi_i\rangle$ is prepared with a probability p_i. Then the expectation value of an observable O would take the form

$$\begin{aligned}\langle O\rangle = \sum_i p_i\,\langle\psi_i|O|\psi_i\rangle &= \sum_{ij} p_i\,\langle\psi_i|O|j\rangle\,\langle j|\psi_i\rangle \\ &= \sum_j \langle j|\left(\sum_i p_i\,|\psi_i\rangle\langle\psi_i|\,O\right)|j\rangle = \mathrm{Tr}(\rho O),\end{aligned}$$

where we have introduced an orthonormal basis $(|j\rangle)$, a completeness relation, and the operator $\rho = \sum_i p_i\,|\psi_i\rangle\langle\psi_i|$. This operator is a density operator, and one can easily check that it is hermitian, positive semi-definite with unit trace. A density operator represents a pure quantum state whenever it is itself a projector $\rho^2 = \rho$, otherwise it represents a mixed state. One of the most important mixed state arising in physics is the thermal state, and it takes the form

$$\rho_{th} = \frac{e^{-\frac{H}{k_B T}}}{\mathrm{Tr}\left(e^{-\frac{H}{k_B T}}\right)}, \tag{11}$$

where k_B is Boltzman's constant. This is nothing more than a Boltzman distribution where the classical energy is replaced by the Hamiltonian operator. We will introduce other representations of the thermal state shortly.

The density operator is the quantum counterpart of a classical epistemic state. One first observation supporting this is the form of its evolution. In the Schrödinger picture, taking the Schrödinger equation and its hermitian conjugate yields $\frac{d}{dt}\rho(t) = \frac{i}{\hbar}[\rho, H]$. We notice that, just like Liouville's and Hamilton's equations differ by a sign, this quantum Liouville equation and the Heisenberg equation also differ by a sign. We can now take a further step and write out what is the quantum phase space representation of states, by combining the density operator with our previously established pure state representations on position and momentum space. This phase space representation was first proposed by Wigner and it reads

$$W(x,p) = \int_{\mathbb{R}} ds e^{-ips/\hbar} \left\langle x + \tfrac{s}{2} \middle| \rho \middle| x - \tfrac{s}{2} \right\rangle .$$

Contrary to the classical case, the Wigner distribution is not exactly a probability distribution, but a quasi-probability distribution in that in can take negative values. To convince ourselves that this function behaves as a quasi-probability distribution, let us first note that it is normalized. Indeed $\int đp \frac{W(x,p)}{\hbar} = \int ds \delta(p) \left\langle x + \frac{s}{2} \middle| \rho \middle| x - \frac{s}{2} \right\rangle = \langle x|\rho|x\rangle$, and integrating over x yields $\iint ds đp \frac{W(p,x)}{\hbar} = \mathrm{Tr}(\rho) = 1$. Furthermore, the Wigner function yields expectation values of any functions of phase space, a desirable property for an object that corresponds to a probability distribution. Indeed, for any function f of the position operator X one has

$$\begin{aligned}
\iint_{\mathbb{R}^2} dx \frac{đp}{\hbar} f(x) W(x,p) &= \iiint_{\mathbb{R}^3} dx ds \frac{đp}{\hbar} e^{-ips/\hbar} f(x) \left\langle x + \tfrac{s}{2} \middle| \rho \middle| x - \tfrac{s}{2} \right\rangle \\
&= \iint_{\mathbb{R}^2} dx ds \delta(s) f(x) \left\langle x + \tfrac{s}{2} \middle| \rho \middle| x - \tfrac{s}{2} \right\rangle \\
&= \int_{\mathbb{R}} dx f(x) \langle x|\rho|x\rangle \\
&= \mathrm{Tr}(f(X)\rho) = \langle f(X) \rangle .
\end{aligned}$$

A slightly more contrived but very similar calculation also proves that for any function g of the momentum operator P one has

$$\iint_{\mathbb{R}^2} dx \frac{đp}{\hbar} g(p) W(x,p) = \mathrm{Tr}(g(P)\rho) = \langle g(P) \rangle .$$

There are other ways to represent quantum states in phase space, and in order to build up another convenient representation, we shall later introduce some of the most important quantum states. Before concluding this short introduction to quantum phase space, let us look at one of the most famous consequences of the non-commutativity

between position and momentum operators, from the perspective of measurement statistics.

Consider two hermitian operators A', B' and take their centered counterparts $A = A' - \langle A' \rangle, B = B' - \langle B' \rangle$. One can rewrite the operator product as $AB = \frac{1}{2}([A, B] + [A, B]_+)$ where $[.,.]_+$ denotes an anti-commutator. From this, one has

$$|\langle AB \rangle|^2 = \langle AB \rangle \langle BA \rangle = \frac{1}{4} \langle [A, B] + [A, B]_+ \rangle \langle [B, A] + [B, A]_+ \rangle ,$$

where we have used the hermiticity of the operators. Let us note that for hermitian operators $\langle [A, B] \rangle \in i\mathbb{R}$ and $\langle [A, B]_+ \rangle \in \mathbb{R}$ so that $\langle [B, A] \rangle = -\langle [A, B] \rangle = \langle [A, B] \rangle^*$. By linearity of the expectation value, the cross terms vanish and one is left with

$$|\langle AB \rangle|^2 = \frac{1}{4} \left(|\langle [A, B] \rangle|^2 + |\langle [A, B]_+ \rangle|^2 \right) . \tag{12}$$

Recall the Cauchy-Schwarz inequality $\|X\|^2 \|Y\|^2 \geqslant |X.Y|^2$, where we work with the Hilbert-Schmidt scalar product $X.Y = \mathrm{Tr}\big(Y^\dagger X\big)$ and the associated norm $\|X\| = \sqrt{X^\dagger X}$. Let us now consider an arbitrary quantum state ρ (a hermitian, positive semi-definite operator). Setting $X = \sqrt{\rho} A$ and $Y = \sqrt{\rho} B$ in the Cauchy-Schwarz inequality yields $\mathrm{Tr}(\rho A^2)\,\mathrm{Tr}(\rho B^2) \geqslant |\mathrm{Tr}(\rho AB)|^2$. This relation may be equivalently written as $\langle A^2 \rangle \langle B^2 \rangle \geqslant |\langle AB \rangle|^2$. We can now combine this with Eq. (12) to obtain the following theorem due to Robertson [71]:

Lemma 1 (Robertson's inequality). *For all pair of observables A, B of a quantum system in a given state, the following inequality holds*

$$\langle A^2 \rangle \langle B^2 \rangle \geqslant \frac{1}{4} \left(|\langle [A, B] \rangle|^2 + |\langle [A, B]_+ \rangle|^2 \right) . \tag{13}$$

One arrives at the Heisenberg inequality by dropping the (positive) anti-commutator. For centered observables the variance takes the simple form $\Delta A = \langle A^2 \rangle$, so Roberton's inequality implies the relation $(\Delta A)(\Delta B) \geqslant \frac{1}{4} |\langle [A, B] \rangle|^2$. Note that if we now shift back the operators so they are no longer centered, the inequality still holds, as extra $\langle A \rangle^2 \mathbb{1}$ terms leave the commutator invariant. Square rooting this last inequality yields the Heisenberg uncertainty relations or principle:

Theorem 11 (Heisenberg's uncertainty relations). *For all pair of observables A, B of a quantum system in a given state, the following inequality holds*

$$\sigma_A \sigma_B \geqslant \frac{1}{2} |\langle [A, B] \rangle| . \tag{14}$$

In particular from the canonical commutation relation $[x, p_x] = i\hbar\mathbb{1}$, one obtains the famous relation $\sigma_x \sigma_{p_x} \geqslant \frac{\hbar}{2}$. In the literature, the notation Δ instead of σ is widely adopted, although measurement uncertainties are standard deviations.

The Heisenberg uncertainty relations have a direct consequence on the representation of states on quantum phase space. Contrary to classical physics, where the ontic state of a single particle was represented as a point in phase space, in quantum physics, there must necessarily be a spread of the corresponding probability density. In that sense, the states that minimize the uncertainty relations will be interpreted as being the most classical. Since the Heisenberg uncertainty relations between position and momentum can essentially be seen as a Cauchy-Schwarz inequality linking the position and momentum representations, and that we have shown that they are related to one another by a Fourier transform, it should not come as a surprise that the states saturating Heisenberg's uncertainty relations should be gaussian in some sense. Let us show this explicitly.

If we define the pure state with position representation

$$\psi(x) = (2\pi\sigma_x^2)^{-1/4} \exp\left(\frac{ip_0 x}{\hbar}\right) \exp\left(-\frac{(x-x_0)^2}{4\sigma_x^2}\right),$$

then by construction we have $\langle x \rangle = x_0$ and $\left\langle (x-x_0)^2 \right\rangle = \sigma_x^2$. One can express its Wigner function

$$\begin{aligned} W(x, p_x) &= \int_{\mathbb{R}} ds e^{-ip_x s/\hbar} \psi\left(x + \frac{s}{2}\right) \psi^*\left(x - \frac{s}{2}\right), \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-x_0)^2}{2\sigma^2}} \int_{\mathbb{R}} ds e^{\frac{-i(p_x-p_0)s}{\hbar}} e^{\frac{-s^2}{8\sigma^2}}, \\ &= 2\exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right) \exp\left(-\frac{(p_x-p_0)^2}{2\sigma_p^2}\right), \end{aligned}$$

where $\sigma_p = \hbar^2/(2\sigma^2)$ and given three reals a, b, c with a being strictly positive we have used the formula $\int_{\mathbb{R}} ds e^{-as^2+bs+c} = \sqrt{\frac{\pi}{a}} e^{c-\frac{b^2}{a}}$. We see that in this form, this state which saturates the uncertainty relations has a gaussian phase space representation. The state we have considered here plays an important role in quantum theory, and is called a coherent state. In Sec. 2.3 we will take some time to further develop other representations of coherent states, and in particular shed some light on their relationship to states which are at the other end of the spectrum of classicality, called Fock states.

2.2.4 *Quantizing Lagrangian mechanics*

In Sec.2.2.1 we have seen how to build quantum mechanics from classical Hamiltonian mechanics, by enforcing the compatibility of the Poisson bracket with the Lie bracket. In doing so, we have established Heisenberg's equations of motion as a quantum analogue of Hamilton's classical equations. It is a well known fact that equations of motion can also be built from the Lagrangian formalism, which relies on the principle of stationary action. The action is a functional

defined as the time integral of the Lagrangian $S[q] = \int dt L(q(t), \dot{q}(t))$ and by enforcing stationarity $\delta S = 0$ one arrives at the Euler-Lagrange equations $\partial_q L - \partial_t(\partial_{\dot{q}} L) = 0$.

Quantum mechanics, as it turns out, can also be formulated by taking an action as the fundamental quantity. The notion of quantum mechanical action was first introduced by Dirac, and laid the foundations for what is now called the path integral formalism, a framework that was largely developed by Feynman [72].

The main motivation for us to briefly present the path integral formalism, is that Hamiltonian quantum mechanics is not Lorentz invariant. Taking the Hamiltonian as a fundamental quantity restricts us to working in a given reference frame, whereas starting from an action does not impose such a restriction. The starting point of the path integral formulation is to reflect on the conditional probability amplitude for a particle to find itself in the state $|x + \Delta x\rangle$ at a time $t + \Delta t$ given that it was in the state $|x\rangle$ at time t. Since the generator of spatial translation is the momentum operator P and the generator of time evolution is the Hamiltonian operator H, this two-point correlation function can be cast as

$$K(x + \Delta x, t + \Delta t | x, t) = \langle x + \Delta x | e^{-iH\Delta t/\hbar} | x\rangle = \langle x | U(\Delta x, \Delta t) | x\rangle \,,$$

where the operator $U(x,t) = e^{iPx/\hbar} e^{-iHt/\hbar}$ realizes a spacetime translation. For infinitesimal spacetime intervals, we have the first order expression $U = \mathbb{1} + \frac{i}{\hbar}(P dx - H dt)$ which is the operator form of the infinitesimal action $dS = p dx - E dt$. That is, one can rewrite the action for a path between the spacetime events located at (x,t) and $(x + \Delta x, t + \Delta t)$ as $\Delta S = \int_t^{t+\Delta t} dt (p \frac{dx}{dt} - E) = \int_t^{t+\Delta t} dt L$, where we have recognized the Legendre transform relating the Lagrangian to the Hamiltonian $L = p \frac{dx}{dt} - E$.

Assuming a non-relativistic Hamiltonian $H = \frac{P^2}{2m} + V(x)$ one can then insert a completeness relation, and use Eq.(10) to obtain

$$\begin{aligned}
&K(x + \Delta x, t + \Delta t | x, t) \\
&\quad = \int_{\mathbb{R}} \frac{đp}{\hbar} \langle x | p\rangle \langle p | U(\Delta x, \Delta t) | x\rangle \\
&\quad \underset{\Delta \to 0}{=} \int_{\mathbb{R}} \frac{đp}{\hbar} \left(1 + \frac{i}{\hbar}\left(p\Delta x - \left(\frac{1}{2m}p^2 + V(x)\right)\Delta t\right) + O(\Delta^2)\right) \\
&\quad \underset{\Delta \to 0}{=} \int_{\mathbb{R}} \frac{đp}{\hbar} \exp\left(\frac{i}{\hbar}\left(p\Delta x - \left(\frac{1}{2m}p^2 + V(x)\right)\Delta t\right) + O(\Delta^2)\right) \\
&\quad \underset{\Delta \to 0}{=} \sqrt{\frac{m}{2i\pi\hbar\Delta t}} \exp\left(\frac{i}{\hbar}\Delta S(x + \Delta x, t + \Delta t | x, t) + O(\Delta^2)\right),
\end{aligned}$$

where $\Delta S(x + \Delta x, t + \Delta t | x, t) = L(x, \dot{x}, t)\Delta t = (\frac{1}{2}m\dot{x}^2 - V(x))\Delta t$. In other words, the infinitesimal propagator takes the form of a normalized phase factor, and the phase is given by the infinitesimal change

in the action. In order to propagate this formula to non-infinitesimal spacetime intervals, one notices the decomposition rule

$$\begin{aligned} K(x_f, t_f|x_i, t_i) &= \int_{\mathbb{R}} dx \, \langle x_f|e^{-iH(t_f-t)/\hbar}|x\rangle \, \langle x|e^{-iH(t-t_i)/\hbar}|x_i\rangle \\ &= \int_{\mathbb{R}} dx K(x_f, t_f|x, t) K(x, t|x_i, t_i), \end{aligned}$$

which may be iterated in order to establish

$\forall n \in \mathbb{N}^*$,

$$K(x_n, t_n|x_0, t_0) = \left(\prod_{k=1}^{n-1} \int_{\mathbb{R}} dx_k\right) \prod_{k=0}^{n-1} K(x_{k+1}, t_{k+1}|x_k, t_k),$$

where $\left(\prod_{k=1}^{n-1} \int_{\mathbb{R}} dx_k\right) = \int_{\mathbb{R}} dx_{n-1} \int_{\mathbb{R}} dx_{n-2} ... \int_{\mathbb{R}} dx_2 \int_{\mathbb{R}} dx_1$. If one now fixes a spacetime interval, and uses the n-point decomposition formula where $n \to +\infty$, one can express the total propagator as an infinite product of integrals over infinitesimal propagators, for which we have established a simple form given by Eq. (2.2.4). The product of infinitesimal propagators reads

$$\begin{aligned} &\prod_{k=0}^{n-1} K(x_{k+1}, t_{k+1}|x_k, t_k) \\ &\qquad = \left(\frac{m}{2i\pi\hbar\Delta t}\right)^{\frac{n}{2}} \exp\left(\frac{i}{\hbar} \sum_{k=0}^{n-1} L(x_k, \dot{x}_k, t_k)\Delta t + O(n\Delta t^2)\right), \end{aligned}$$

and carrying out the limit $n \to +\infty$ one obtains

$$\begin{aligned} &\lim_{n\to+\infty} \prod_{k=0}^{n-1} K(x_{k+1}, t_{k+1}|x_k, t_k) \\ &\qquad = \lim_{n\to+\infty} \left(\frac{m}{2i\pi\hbar\Delta t}\right)^{\frac{n}{2}} \exp\left(\frac{i}{\hbar} S(x_n, t_n|x_0, t_0)\right), \end{aligned}$$

where we have used the evident additivity of the actions, and the fact that Δt scales as n^{-1} hence $O(n\Delta t^2) = O(\frac{1}{n})$ ensures convergence. Defining the functional integral, or path integral, as

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} \mathcal{D}x[t] := \lim_{n\to+\infty} \left(\frac{m}{2i\pi\hbar\Delta t}\right)^{\frac{n}{2}} \left(\prod_{k=1}^{n-1} \int_{\mathbb{R}} dx_k\right),$$

one arrives at the simple formula

$$K(x_f, t_f|x_i, t_i) = \int_{x(t_i)=x_i}^{x(t_f)=x_f} \mathcal{D}x[t] e^{\frac{i}{\hbar} S(x_f, t_f|x_i, t_i)}. \tag{15}$$

What this formula says, is that the probability amplitude for a system at position x_i at time t_i to find itself at position x_f at time t_f

is given by a sum over all possible paths the endpoints of which are (x_f, t_f) and (x_i, t_i), each term having a phase given by the classical action associated to the path. This allows, with little effort, to formally quantize any classical theory.

Given the definition of the functional integral, the path integral at this stage looks more like a mathematical subtlety than a practical tool. As it stands, such a complex formula is indeed intractable, however its main interest for our purpose is that it emphasizes the importance of the classical action. Combined with the fact that classical physics is governed by the principle of stationary action, the path integral provides a powerful tool to obtain semi-classical approximations. Using a stationary phase approximation, the leading term of Eq. (15) reads $K(x_f, t_f|x_i, t_i) \approx \mathcal{N} e^{\frac{i}{\hbar} S[x^c]}$, where $\mathcal{N}$ is some normalization factor and x^c is the classical solution.

To show this, let us go back to the case where our time interval is divided into a large number $n \in \mathbb{N}^*$, of regular sub-intervals such that $[0, t] = \bigcup_{k=0}^{n-1} [t_k, t_{k+1}]$, and let us define the sequence of functions $S_n(x) : \mathbb{R}^n \to \mathbb{R}$ by $S_n(x) = \sum_{k=0}^{n-1} L(x_k, \dot{x}_k, t_k)\Delta t$.

Let us fix $n \in \mathbb{N}^*$, and consider the integral $I_n = \int_{\mathbb{R}^n} dx e^{i\nu S_n(x)}$, where $\nu \in \mathbb{R}^*$. Then given a stationary point x^c of S_n, a quadratic expansion reads $S_n(x) \approx S_n(x^c) + \frac{1}{2}(\delta x)^T h(\delta x)$, where the deviation to the stationary point is $\delta x = x - x^c$ and the hessian elements are given by $h_{ij} = \partial_{x_i}\partial_{x_j} S(x = x^c)$. Hence under the stationary phase approximation ($\nu \gg 1$) we establish

$$I_n \approx e^{i\nu S_n(x^c)} \int_{\mathbb{R}^n} d(\delta x) e^{\frac{i\nu}{2}(\delta x)^T h(\delta x)}.$$

The Schwarz theorem ensures symmetry of h, and the spectral theorem yields the decomposition $h = P\omega P^T$ where P is an orthogonal similarity, and $\omega = \mathrm{diag}(\omega_{kk})$ is a diagonal form of the hessian. Hence $(\delta x)^T h(\delta x) = (\delta\phi)^T \omega(\delta\phi)$ where we have defined the normal variable $\delta\phi = P^T \delta x$. By orthogonality of P, this transformation has unit Jacobian determinant, hence carrying out the change of variable in the integral yields

$$I_n \approx e^{i\nu S_n(x^c)} \int_{\mathbb{R}^n} d(\delta\phi) e^{\frac{i\nu}{2}(\sum_{k=1}^n (\delta\phi_k)^2 \omega_{kk})}.$$

This reduces to a product of Gaussian integrals, which can be expressed using standard techniques from complex analysis, and we find

$$I_n \approx e^{i\nu S_n(x^c)} \frac{1}{\sqrt{\det(h)}} \left(\frac{2i\pi}{\nu}\right)^{\frac{n}{2}}.$$

Taking the limit $n \to +\infty$, $I_n(2i\pi)^{-n/2}$ becomes a path integral, x^c becomes the classical path, and S_n becomes an action. The remaining factors simply contribute to the normalization. Hence setting $\nu = \frac{1}{\hbar}$ yields the announced result. This can in fact be interpreted as a proof of the classical least action principle.

2.3 ELEMENTS OF QUANTUM OPTICS

This section introduces a few ideas from the vast field of quantum optics [73], which are of interest for the work presented in the rest of the dissertation. In particular, two types of states which respectively best capture the corpuscular and wavelike features of the electromagnetic quantum field, are presented. The reader is also reminded of some useful phase space representations, and of important properties of the beam splitter.

2.3.1 *Coherent states and Fock states*

In quantum mechanics, a coherent state is loosely speaking the quantum state of a quantum harmonic oscillator that behaves classically, as we have seen, they minimize the uncertainty relations. Coherent states are an accurate description of light at the output of a laser as shown by Glauber [74].

A classical one dimensional harmonic oscillator of mass m and angular frequency ω has Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2,$$

where p_x is its momentum, x its position. Hamilton's equations of motion read $\partial_t x = p_x/m$ and $\partial_t p_x = -m\omega^2 x$. One can symmetrize those equations using the canonical transformation $P = p_x/\sqrt{m\omega}$ and $X = \sqrt{m\omega}x$ leading to $\partial_t X = \omega P$ and $\partial_t P = -\omega X$. This can be combined in a single complex equation via $\alpha := (X + iP)/\sqrt{2}$ so that Hamilton's equations simply read $\partial_t \alpha = -i\omega\alpha$.

Let us now turn to the quantum harmonic oscillator described by the operator valued Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2,$$

which is clearly seen to be positive semi-definite by the evaluation of $\langle\psi|H|\psi\rangle$. Furthermore, Heisenberg's uncertainty relations impose $\langle p_x^2\rangle \geqslant \hbar/(4\langle x^2\rangle)$ so that the expectation value of the Hamiltonian is minimized by $\hbar\omega/2$ called zero-point energy. In contrast with classical physics, the ground state of the quantum harmonic oscillator has non-zero energy. Following what was done for the classical oscillator, we define the dimensionless observables $P = p_x/\sqrt{m\hbar\omega}$ and $X = \sqrt{m\omega/\hbar}x$. Then the commutator reduces to $[X, P] = i\mathbb{1}$ and the Hamiltonian takes the form $H = (\hbar\omega/2)(X^2 + P^2)$. From $(X - iP)(X + iP) = \frac{2}{\hbar\omega}H - \mathbb{1}$ we see that the Hamiltonian can be rewritten in terms of two other operators, called bosonic ladder operators, the annihilation operator $a = (X + iP)/\sqrt{2}$ and the creation

operator which is its conjugate. Using the ladder operators, we can express the Hamiltonian as

$$H = \hbar\omega \left(a^\dagger a + \frac{1}{2}\mathbb{1} \right). \tag{16}$$

The commutation relation between ladder operators $[a, a^\dagger] = \mathbb{1}$ can in fact be taken as the starting point from which the dimensionless position and momentum operators (also called quadrature operators) can be reconstructed. As we can see, the ladder operators are themselves not hermitian, however one can easily construct another hermitian operator called the number operator $N = a^\dagger a$. What can we say of its spectral properties? The spectral theorem tells us that $\sigma(N) \subset \mathbb{R}$. Claim 1 from the mathematical elements gives us $\sigma(N) \subset \mathbb{R}_+$. But let us try to further characterize the spectrum by giving ourselves the $d(n)$ linearly independent normalized eigenvectors $(|n\rangle_i)_{1 \leqslant i \leqslant d(n)}$ that span the eigenspace $\ker(N - n\mathbb{1})$. Then we can write

$$\forall i \in [\![1, d(n)]\!],\ \|a\,|n\rangle_i\|^2 = \langle n|a^\dagger a|n\rangle_i = n\,\langle n|n\rangle_i\,,$$

which gives $n \geqslant 0$, and also $|n\rangle_i \in \ker(a) \iff n = 0$. Using the bosonic commutation relations yields $Na^\dagger\,|n\rangle_i = (n+1)a^\dagger\,|n\rangle_i$ and the normalization condition implies $a^\dagger\,|n\rangle_i = \sqrt{n+1}\,|n+1\rangle_j$. This also gives $a\,|n\rangle_i = \sqrt{n}\,|n-1\rangle_h$ if $n \neq 0$, and $a\,|0\rangle_i = 0$.

With this quick observation, we have already established that the spectrum is positive, and either contains zero and is stable through any translation $n \mapsto n + m,\ m \in \mathbb{N}$, or is stable through any translation $n \mapsto n + m,\ m \in \mathbb{Z}$. The second case is ruled-out as it would contradict positivity. Hence we have identified the spectrum to be exactly $\sigma(N) = \mathbb{N}$, justifying the denomination "number operator". It remains to be shown that the eigenvalues are non-degenerate. We proceed by induction from the non-degeneracy of the ground state $|0\rangle$ that we will demonstrate by proving that $\dim(\ker(N)) = 1$. We have already shown that $|0\rangle_i \in \ker(a)$. Then working in the position representation $\psi_i(x) := \langle x|0\rangle_i$ one has

$$|0\rangle_i \in \ker(a) \implies \langle x|a|0\rangle_i = 0 \iff (x + \partial_x)\psi_i(x) = 0.$$

The equivalence stems from $a = (X + iP)/\sqrt{2}$ and the fact that the action of the momentum operator on wavefunctions is a gradient. That is, the eigenvectors $|0\rangle_i$ in the position representation are solutions of a first order homogeneous linear differential equation, a set that is known to be one dimensional. We may thus drop the degeneracy index for the ground state. For the inductive part, let us suppose that the eigenvalues up to $n \in \mathbb{N}$ are non-degenerate. Then consider two distinct eigenvectors $|n+1\rangle_i$ and $|n+1\rangle_j$ associated to the eigenvalue $n+1$. Then by non-degeneracy of eigenvalue n one has $a\,|n+1\rangle_j = a\,|n+1\rangle_i = \sqrt{n+1}\,|n\rangle$. So one can write

$a^\dagger |n\rangle = \frac{1}{\sqrt{n+1}} a^\dagger a |n+1\rangle_i = \frac{1}{\sqrt{n+1}} a^\dagger a |n+1\rangle_j$. Recognizing the number operator we arrive at $\sqrt{n+1}\,|n+1\rangle_i = \sqrt{n+1}\,|n+1\rangle_j$ which ends the proof. The independent eigenvectors of the number operator form what is called the Fock basis.

Coherent states of light or matter were introduced by Schrödinger in the mid 1920s [75] and are formally defined by the eigenequation $a|\alpha\rangle = \alpha|\alpha\rangle$, where $\alpha \in \mathbb{C}$. According to this definition, $|0\rangle$ is an example of coherent state. In order to find the form of other coherent states, and show that this formal definition is consistent with the minimal uncertainty claim we had formulated in the previous section, let us investigate their expression in the Fock basis. We expand the coherent state as $|\alpha\rangle = \sum_{n=0}^{+\infty} \langle n|\alpha\rangle |n\rangle$ and write out its defining eigenequation in that basis

$$a|\alpha\rangle = \alpha|\alpha\rangle \iff \sum_{n=0}^{+\infty} \alpha \langle n|\alpha\rangle |n\rangle = \sum_{n=0}^{+\infty} \langle n+1|\alpha\rangle \sqrt{n+1}\,|n\rangle\,.$$

This reveals a first order recursive relation between the overlaps $\langle n|\alpha\rangle$, for which the solution is $\forall n \in \mathbb{N}$, $\langle n|\alpha\rangle = (\alpha^n/\sqrt{n!})\langle 0|\alpha\rangle$. The normalization condition allows us to determine the first vacuum overlap as $\langle\alpha|\alpha\rangle = |\langle 0|\alpha\rangle|^2 \sum_{n=0}^{+\infty} \frac{|\alpha|^{2n}}{n!} = 1$, from which we establish the useful expression, up to a global phase factor

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{+\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle\,. \tag{17}$$

An immediate observation is that there is no mutual orthogonality between coherent states $\langle\beta|\alpha\rangle = \exp\big(|\alpha-\beta|^2/2\big)$. Another interesting way of constructing coherent states, is through the application of a displacement operator on phase space defined by

$$D(\alpha) = e^{\alpha a^\dagger - \alpha^* a}. \tag{18}$$

Setting $x = \alpha a^\dagger - \alpha^* a$ and $y = -\alpha a^\dagger + \alpha^* a$ in the BCH identity $e^x e^y = \exp\big(x + y + \frac{1}{2}[x,y] + \frac{1}{12}([x,[x,y]] + [y,[y,x]]) + ...\big)$ makes the unitarity of the displacement operator immediately apparent, as one finds $D^\dagger(\alpha) = D(-\alpha) = D^{-1}(\alpha)$. Furthermore, the disentangling theorem Eq. (5) yields $\exp\big(\alpha a^\dagger\big)\exp(-\alpha^* a) = \exp\big(\alpha a^\dagger - \alpha^* a + |\alpha|^2/2\big)$, which leads to a different form of the displacement operator

$$D(\alpha) = e^{-\frac{|\alpha|^2}{2}} e^{\alpha a^\dagger} e^{-\alpha^* a}.$$

This final expression of the displacement operator elucidates its action on the vacuum: $|\alpha\rangle = D(\alpha)|0\rangle$.

In the spirit of the Schrödinger and Heisenberg pictures of quantum dynamics, one can represent the action of the displacement operator on the vacuum rather from its action on the ladder operators

using the Hadamard lemma $e^{u}ve^{-u} = e^{\mathrm{ad}_u}(v)$. Setting the operators $u := \alpha^* a - \alpha a^\dagger$ and $v := a$ in the Hadamard lemma, yields

$$D^\dagger(\alpha) a D(\alpha) = a + \alpha \mathbb{1},$$

which is a transformation commonly called Bogoliubov shift [76]. As a consistency check, using the unitarity of the displacement operator, we find that the action of the displacement operator on the vacuum state indeed satisfies the defining property of a coherent state: $aD(\alpha)\,|0\rangle = D(\alpha)D^\dagger(\alpha)aD(\alpha)\,|0\rangle = D(\alpha)(a + \alpha\mathbb{1})\,|0\rangle = \alpha D(\alpha)\,|0\rangle$.

The Bogoliubov property also comes in handy when evaluating quadrature moments of coherent states

$$\begin{aligned}\langle X\rangle &= \frac{1}{\sqrt{2}}\,\langle 0|D^\dagger(\alpha)(a^\dagger + a)D(\alpha)|0\rangle \\ &= \frac{1}{\sqrt{2}}\,\langle 0|a^\dagger + \alpha^* I + a + \alpha\mathbb{1}|0\rangle = \sqrt{2}\,\mathrm{Re}(\alpha),\end{aligned}$$

and similarly

$$\langle P\rangle = \frac{i}{\sqrt{2}}\,\langle 0|D^\dagger(\alpha)(a^\dagger - a)D(\alpha)|0\rangle = \sqrt{2}\,\mathrm{Im}(\alpha).$$

From the unitarity of the displacement operator and the bosonic commutation relations, the second order quadrature moments of coherent states can also be established:

$$\left\langle X^2\right\rangle = \frac{1}{2}\left\langle a^{\dagger 2} + 2aa^\dagger + \mathbb{1} + a^2\right\rangle = \frac{1}{2}(\alpha^{*2} + 2|\alpha|^2 + \alpha^2 + 1),$$

and

$$\left\langle P^2\right\rangle = \frac{1}{2}(2|\alpha|^2 + 1 - \alpha^2 - \alpha^* 2).$$

We finally recover our very first statement about coherent states, as the uncertainties turn out to satisfy $\sigma_X\sigma_P = \frac{1}{2}$, they indeed saturate the Heisenberg bound. As such, coherent states are minimal uncertainty states, and for this reason[16] they are commonly considered to be the most classical quantum states.

2.3.2 *The Glauber-Sudarshan P representation*

The relationship between coherent states and the classicality of quantum states does not merely stop at our previous observations. One can in fact build another representation of quantum states on phase space, based on coherent states themselves, as an alternative to the powerful Wigner representation. Such a representation is called the Glauber-Sudarshan P function [77, 78]. The main interest of the P

16 Other noteworthy reasons include the associated field expectation value which corresponds to the classical form, and the good phase localization for high photon numbers.

function for the purpose of this thesis is that its non-negativity[17] is a necessary and sufficient condition for classicality, whereas the non-negativity of the Wigner function is not sufficient to infer classicality.

To construct the P representation of a state, one must have a completeness relation with coherent states. Let us evaluate the integral over the complex plane $\int_{\mathbb{C}} d^2\alpha\, |\alpha\rangle\langle\alpha|$, where $d^2\alpha = d\mathrm{Re}(\alpha)d\mathrm{Im}(\alpha)$. Using the Fock representation Eq. (17) one has

$$\int_{\mathbb{C}} d^2\alpha\, |\alpha\rangle\langle\alpha| = \int_{\mathbb{C}} d^2\alpha\, e^{-|\alpha|^2} \sum_{(n,m)\in\mathbb{N}^2} \frac{\alpha^n \alpha^{*m}}{\sqrt{n!m!}} |n\rangle\langle m| .$$

In polar coordinates $\alpha = re^{i\theta}$ the surface element may be rewritten as $d^2\alpha = r dr d\theta$, and using Fubini's theorem one arrives at

$$\begin{aligned}&\int_{\mathbb{C}} d^2\alpha\, |\alpha\rangle\langle\alpha| \\ &= \sum_{(n,m)\in\mathbb{N}^2} \frac{|n\rangle\langle m|}{\sqrt{n!m!}} \left(\int_{\mathbb{R}_+} dr\, e^{-r^2} r^{n+m+1}\right) \left(\int_0^{2\pi} d\theta\, e^{i(n-m)\theta}\right).\end{aligned}$$

The integral over θ is simply $2\pi\delta_{n,m}$ so this simplifies to

$$\int_{\mathbb{C}} d^2\alpha\, |\alpha\rangle\langle\alpha| = 2\pi \sum_{n\in\mathbb{N}} \frac{|n\rangle\langle n|}{n!} \int_{r\in\mathbb{R}_+} dr\, e^{-r^2} r^{2n+1}.$$

Finally by introducing the bijective change of variable $s = r^2$ one obtains

$$\int_{\mathbb{C}} d^2\alpha\, |\alpha\rangle\langle\alpha| = \pi \sum_{n\in\mathbb{N}} \frac{|n\rangle\langle n|}{n!} \int_{r\in\mathbb{R}_+} ds\, e^{-s} s^n = \pi\mathbb{1},$$

where in the last step we have identified the gamma function which cancels out the factorial in the denominator, and used the completeness of the Fock states. That is, one can now decompose a density operator into matrix elements using coherent states by inserting two completeness relations

$$\rho = \frac{1}{\pi^2} \iint_{\mathbb{C}^2} d^2\alpha d^2\beta\, \langle\alpha|\rho|\beta\rangle\, |\alpha\rangle\langle\beta| .$$

One can finally arrive at the P-representation of a quantum state, defined as satisfying

$$\rho = \int_{\mathbb{C}} d^2\alpha P(\alpha)\, |\alpha\rangle\langle\alpha| . \tag{19}$$

The P distribution, like Wigner's, is only a quasi-probability distribution, as it can take on negative values. States for which it is positive are called classical, and are non-classical otherwise. The normalization of the P distribution follows from $\mathrm{Tr}(\rho) = \int_{\mathbb{C}} d^2\alpha P(\alpha) = 1$.

17 If the P-function can be expressed as a standard function, which as we shall see is not always the case.

Extracting the P function from its defining equation requires a little bit of work. One way to arrive at it is to consider the "coherent state matrix element"

$$\begin{aligned}\langle -\beta|\rho|\beta\rangle &= \int_{\mathbb{C}} d^2\alpha P(\alpha)\,\langle -\beta|\alpha\rangle\,\langle\alpha|\beta\rangle \\ &= e^{-|\beta|^2}\int_{\mathbb{C}} d^2\alpha P(\alpha) e^{-|\alpha|^2} e^{\alpha^*\beta-\beta^*\alpha},\end{aligned}$$

where we have used the result $\langle\alpha|\beta\rangle = e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)+\alpha^*\beta}$. A two-dimensional inverse Fourier transform, when there is convergence of the integral, yields the result

$$P(\alpha) = \frac{e^{|\alpha|^2}}{\pi^2}\int_{\mathbb{C}} d^2\beta\; e^{|\beta|^2}\,\langle -\beta|\rho|\beta\rangle\, e^{\beta^*\alpha-\beta\alpha^*}. \tag{20}$$

Let us now devote some time to the determination of some important P-representations corresponding to common states, such as the coherent states themselves, Fock states and the thermal state.

For the coherent state the result is straightforward. The coherent state overlap equation gives $\langle -\alpha|\beta\rangle\,\langle\beta|\alpha\rangle = e^{-(|\alpha|^2+|\beta|^2)-u^*\beta+u\beta^*}$, hence

$$P(\alpha) = \frac{e^{|\alpha|^2-|\beta|^2}}{\pi^2}\int_{\mathbb{C}} d^2s\; e^{s^*(\alpha-\beta)-s(\alpha^*-\beta^*)} = \delta^{(2)}(\alpha-\beta),$$

as expected from the fact that the P representation is a decomposition on the set of coherent states. For Fock states the overlaps read $\langle -\beta|n\rangle\,\langle n|\beta\rangle = e^{-|\beta|^2}(-\beta^*\beta)^n/n!$ so that one recognizes n-th order derivatives of the integrand exponential factor of Eq. (20). Hence

$$P(\alpha) = \frac{e^{|\alpha|^2}}{\pi^2}\frac{\partial_\alpha^n\partial_{\alpha^*}^n}{n!}\int_{\mathbb{C}} d^2\beta e^{\beta^*\alpha-\beta\alpha^*} = \frac{e^{|\alpha|^2}}{\pi^2 n!}\partial_\alpha^n\partial_{\alpha^*}^n\delta^{(2)}(\alpha).$$

Finding the P-representation of the thermal state requires more effort, and we shall take it as an opportunity to view phase space representations of states from a more global perspective.

In the same way classical probability distributions $f(x)$ on the real space can be represented by their characteristic function, which is their inverse Fourier transform $C(k) = \int_{\mathbb{R}} dx\; e^{ikx}f(x)$, one can introduce a class of quantum mechanical characteristic functions called the Cahill-Glauber functions

$$C(\alpha,\tau) = \mathrm{Tr}\left(\rho\exp\left(\alpha a^\dagger - \alpha^* a + \frac{1}{2}\tau|\alpha|^2\right)\right). \tag{21}$$

Let us focus on the case $\tau = 1$ for which the characteristic function is said to be normally ordered and denoted $C_N(\alpha) = \mathrm{Tr}\left(\rho e^{\alpha a^\dagger}e^{-\alpha^* a}\right)$. Using Eq. (19) one sees that

$$C_N(\alpha) = \int_{\mathbb{C}} d^2\beta P(\beta)\,\langle\beta|e^{\alpha a^\dagger}e^{-\alpha^* a}|\beta\rangle = \int_{\mathbb{C}} d^2\beta P(\beta) e^{\beta\alpha^*-\beta^*\alpha},$$

so we identify the Fourier transform of the P-distribution. Inverting this transformation yields a handy formula

$$P(\alpha) = \frac{1}{\pi^2} \int_{\mathbb{C}} d^2\beta \; e^{\beta^*\alpha - \beta\alpha^*} C_N(\beta). \tag{22}$$

In the case $\tau = -1$ one obtains what is called the anti-normally ordered characteristic function $C_A(\alpha) = \mathrm{Tr}\left(\rho e^{-\alpha a^\dagger} e^{\alpha^* a}\right)$, which happens to be the Fourier transform of another phase space representation, called the Husimi Q-function, and defined by $Q(\alpha) = \frac{1}{\pi}\langle\alpha|\rho|\alpha\rangle$. Using the disentangling theorem Eq. (5) we see that the normally ordered and anti-normally ordered characteristic functions[18] are simply related through $C_N(\alpha) = C_A(\alpha)e^{|\alpha|^2}$.

We are now in a good position to work out the P-representation of a thermal state. Recall the form of the thermal state Eq. (11). Combined with the Hamiltonian expression Eq. (16), the insertion of two completeness relations in the Fock basis allows to express the thermal state as $\rho_{\text{th}} = Z^{-1}\sum_{n\in\mathbb{N}} \exp(-E_n/k_B T)\,|n\rangle\langle n|$ where the energies read $E_n = \hbar\omega(n + \frac{1}{2})$ and $Z = \sum_{n\in\mathbb{N}} \exp(-E_n/k_B T)$ in order for the state to have unit trace. For ease of reading, let us introduce the dimensionless variable $\lambda = \hbar\omega/k_B T \in \mathbb{R}_+^*$. Then we have $Z = \sum_{n\in\mathbb{N}} e^{-\lambda(n+\frac{1}{2})} = \frac{e^{-\lambda/2}}{1-e^{-\lambda}}$, having detected a geometric sum. We have therefore determined that the thermal state is simply a statistical mixture of Fock states that can be written as $\rho_{\text{th}} = \sum_{n\in\mathbb{N}} p_n\,|n\rangle\langle n|$ where $p_n = (1-e^{-\lambda})e^{-n\lambda}$. It is useful to note that this can be entirely expressed using the expected photon number. Indeed, one notices that

$$\begin{aligned}
\overline{n} = \sum_{n\in\mathbb{N}} n p_n &= (1-e^{-\lambda}) \sum_{n\in\mathbb{N}} n e^{-n\lambda} \\
&= (1-e^{-\lambda}) \left(-\partial_\lambda \sum_{n\in\mathbb{N}} e^{-n\lambda}\right) \\
&= (1-e^{-\lambda}) \frac{e^{-\lambda}}{(1-e^{-\lambda})^2} \\
&= \frac{1}{e^{\lambda}-1},
\end{aligned}$$

and observing that $e^{-\lambda} = \frac{\overline{n}}{1+\overline{n}}$ one finds

$$\rho_{\text{th}} = \frac{1}{1+\overline{n}} \sum_{n\in\mathbb{N}} \left(\frac{\overline{n}}{1+\overline{n}}\right)^n |n\rangle\langle n|. \tag{23}$$

18 Let us simply mention that the case $\tau = 0$ gives the Weyl ordered characteristic function, and it corresponds to the Fourier transform of the Wigner distribution.

From this one can establish the thermal state's Husimi-Q representation as follows

$$\begin{aligned} Q(\alpha) &= \frac{1}{\pi}\langle\alpha|\rho_{\text{th}}|\alpha\rangle \\ &= \frac{1}{\pi}e^{-|\alpha|^2}\sum_{(n,m)\in\mathbb{N}^2}\langle m|\rho_{\text{th}}|n\rangle\,\frac{\alpha^{*m}\alpha^n}{\sqrt{m!n!}} \\ &= \frac{e^{-|\alpha|^2}}{\pi(1+\overline{n})}\sum_{n\in\mathbb{N}}\left(\frac{\overline{n}}{1+\overline{n}}\right)^n\frac{|\alpha|^{2n}}{n!}. \end{aligned}$$

We arrive at the simple expression $Q(\alpha) = \frac{1}{\pi(1+\overline{n})}\exp\left(-\frac{|\alpha|^2}{1+\overline{n}}\right)$. The relationship to the P function is simple in Fourier space, as the characteristic functions are simply related by an exponential factor. Carrying out a Fourier transform, we find the corresponding anti-normally ordered characteristic function

$$C_A(\beta) = \frac{1}{\pi(1+\overline{n})}\int_{\mathbb{C}} d^2\alpha\ \exp\left(-\frac{|\alpha|^2}{1+\overline{n}}\right)e^{\beta\alpha^*-\beta^*\alpha} = e^{-(1+\overline{n})|\beta|^2},$$

where the final equality was obtained by explicitly writing out the algebraic forms of the dummy variable $\alpha = (q+ip)/\sqrt{2}$ and the function variable $\beta = (x+iy)/\sqrt{2}$, as well as the differential element $d^2\alpha = \frac{1}{2}dqdp$. Doing so reveals gaussian integrals from which the result is deduced. The normally ordered characteristic function thus takes the very simple form $C_N(\beta) = \exp\left(-\overline{n}|\beta|^2\right)$ and inverting the Fourier transform yields

$$P(\alpha) = \frac{1}{\pi^2}\int_{\mathbb{C}} d^2\beta\ \exp\left(-\overline{n}|\beta|^2\right)e^{\beta^*\alpha-\beta\alpha^*} = \frac{1}{\pi\overline{n}}\exp\left(-\frac{|\alpha|^2}{\overline{n}}\right). \quad (24)$$

We see that the P-representation of the thermal state is a gaussian, being positive it is thus a classical state. This concludes our overview of the Glauber-Sudarshan P representation.

2.3.3 *The beam splitter operator*

This short section is devoted to the beam splitter, because of its importance and its ubiquity in applied and fundamental physical experiments. Its function is unimpressive: a beam splitter quite simply splits light beams. This simple function is in fact one of the building blocks of all sorts of interferometric protocols. Classically, it is an elementary object that is usually made up from a transparent glass slide with some coating on one side. A cube formed by two pyramidal glass pieces is also a common implementation of beam splitters. In quantum optics, the beam splitter is also of special interest for its role in simple yet subtle experiments testing the non-classicality of light [79]. Depending on the nature of the incident light, it was shown that the beam splitter can act as a simple entangling device [80]. Its quantum

mechanical description was at the center stage in the second half of the 1980s [81]. We shall represent the beam splitter with the sketch in Fig. 1 where light propagates from bottom to top. Let us first exhibit

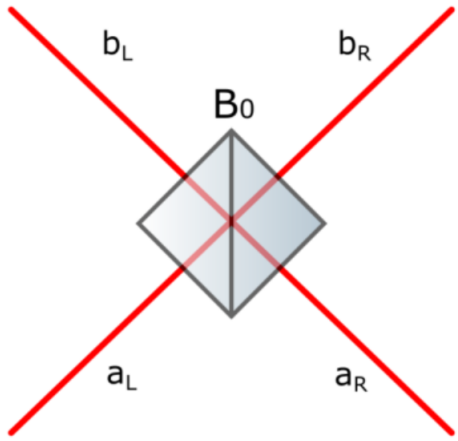


Figure 1: The beam splitter B_0 and its two input mode annihilation operators a and its two output mode annihilation operators b.

some simple properties of the beam splitter. The general quantum operator corresponding to the beam splitting operation reads

$$B = e^{\frac{\theta}{2}(a_L^\dagger a_R - a_L a_R^\dagger)}, \tag{25}$$

where $\theta \in \mathbb{R}$. We evidently have unitarity of B. Hadamard's lemma gives the evolution of annihilation operators under the beam splitter transformation

$$B a_L B^\dagger = \exp\left(\mathrm{ad}_{\frac{\theta}{2}(a_L^\dagger a_R - a_L a_R^\dagger)}\right)(a_L).$$

Using the bosonic commutation relations, one notices the following pattern:

$$\forall n \in \mathbb{N}, \begin{cases} \mathrm{ad}^{4n}(a_L) & = & \left(\frac{\theta}{2}\right)^{4n} a_L \\ \mathrm{ad}^{4n+1}(a_L) & = & \left(\frac{\theta}{2}\right)^{4n+1} a_R \\ \mathrm{ad}^{4n+2}(a_L) & = & -\left(\frac{\theta}{2}\right)^{4n+2} a_L \\ \mathrm{ad}^{4n+3}(a_L) & = & -\left(\frac{\theta}{2}\right)^{4n+3} a_R \end{cases}$$

where we have omitted the index of the adjoint operation for legibility. Thus we can write down the previous equation as

$$B a_L B^\dagger = \sum_{n=0}^{+\infty} \frac{(-1)^n \left(\frac{\theta}{2}\right)^{2n}}{(2n)!} a_L + \sum_{m=0}^{+\infty} \frac{(-1)^m \left(\frac{\theta}{2}\right)^{2m+1}}{(2m+1)!} a_R,$$

and by recognizing the power series, this translates into a friendlier expression

$$Ba_L B^\dagger = \cos\left(\frac{\theta}{2}\right) a_L + \sin\left(\frac{\theta}{2}\right) a_R.$$

A similar derivation also yields

$$Ba_R B^\dagger = \cos\left(\frac{\theta}{2}\right) a_R - \sin\left(\frac{\theta}{2}\right) a_L.$$

Noteworthy is the unit value of the quadratic sum of the coefficients, which is consistent with the fact that those coefficients represent the transmissivity and reflectivity of the lossless beam splitter. In the remainder of this thesis we limit ourselves to 50:50 beam splitters. This amounts to choosing[19] $\theta = \pi/2$ in Eq. (25). The beam splitter transformations in this case take the following form

$$\begin{cases} Ba_R^\dagger B^\dagger &= \frac{1}{\sqrt{2}}(a_L^\dagger + a_R^\dagger) \\ Ba_L^\dagger B^\dagger &= \frac{1}{\sqrt{2}}(a_L^\dagger - a_R^\dagger) \end{cases} \tag{26}$$

Now that we have characterized the action of the beam splitter operator on the bosonic operators, let us take a closer looks at some basic situations. Consider an input state which is a single photon in the left mode $|\psi\rangle_{in} = |1\rangle_L \otimes |0\rangle_R$ then the output state reads

$$|\psi\rangle_{out} = B\,|10\rangle = Ba_L^\dagger\,|00\rangle\,.$$

By unitarity of B and by the fact that its maps the vacuum to itself (which is consistent with a passive component), we can write

$$|\psi\rangle_{out} = Ba_L^\dagger B^\dagger B\,|00\rangle = Ba_L^\dagger B^\dagger\,|00\rangle\,,$$

thus Eqs.(26) give

$$|\psi\rangle_{out} = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle).$$

We observe that the output modes are entangled, but so far the result is not very impressive, the output is a superposition of the photon being in each one of the two output modes, the other being in the vacuum state. What is perhaps more interesting is the Hong-Ou-Mandel effect [82] which arises when the two input modes of the beam splitter are in the single photon Fock state $|\psi\rangle_{in} = |11\rangle$. Then $|\psi\rangle_{out} = Ba_L^\dagger a_R^\dagger\,|00\rangle$. Inserting two $B^\dagger B = \mathbb{1}$ factors and using Eqs. (26) gives

$$|\psi\rangle_{out} = \frac{1}{2}(a_L^\dagger - a_R^\dagger)(a_L^\dagger + a_R^\dagger)\,|00\rangle\,.$$

The commutation of bosonic operators acting on different modes results in the destructive interference of two paths, given by the cross

19 Letting $\theta = -\pi/2$ was also possible but we have, quite arbitrarily, chosen the opposite. Changing sign is simply equivalent to flipping the beam splitter around its phase-asymmetry plane.

terms. The only terms that remain correspond to the two photons emerging in the same mode, that is

$$|\psi\rangle_{\text{out}} = \frac{1}{2}(a_L^{\dagger 2} - a_R^{\dagger 2})\,|00\rangle = \frac{1}{\sqrt{2}}(|20\rangle - |02\rangle).$$

Let us now turn to an important case where the beam splitter does not generate entanglement. Consider the situation where the input state is a coherent state in the left mode, and the vacuum state in the right mode $|\psi\rangle_{\text{in}} = |\alpha\rangle_L \otimes |0\rangle_R$, this reads

$$|\psi\rangle_{\text{in}} = D_L(\alpha)\,|00\rangle = e^{\alpha a_L^\dagger - \alpha^* a_L}\,|00\rangle\,.$$

Expanding the exponential and inserting $B^\dagger B$ gives a workable expression for the output state

$$|\psi\rangle_{\text{out}} = \sum_{n=0}^{+\infty} \frac{1}{n!} B(\alpha a_L^\dagger - \alpha^* a_L)^n B^\dagger\,|00\rangle\,.$$

By inserting n times a $B^\dagger B$ factor and using Eqs. (26) we obtain

$$|\psi\rangle_{\text{out}} = e^{\alpha \frac{1}{\sqrt{2}}(a_L^\dagger - a_R^\dagger) - \alpha^* \frac{1}{\sqrt{2}}(a_L - a_R)}\,|00\rangle = \left|\frac{\alpha}{\sqrt{2}}\right\rangle_L \left|\frac{-\alpha}{\sqrt{2}}\right\rangle_R. \tag{27}$$

As we can see, the output state consists of two coherent states and the intensity in each mode is halved, as expected from a lossless beam splitter, however in this case there is no entanglement whatsoever.

This concludes our short overview of useful results and definitions from quantum physics. In the next section, we will take a step away from standard quantum physics where quantum states and Hamiltonians are take the center stage, and instead introduce a more modern framework in which it is the probabilities and measurements that become the fundamental objects.

2.4 ELEMENTS OF QUANTUM INFORMATION THEORY

In the final section of this chapter, we present the basics of quantum information theory. We briefly revise notions of classical states, measurements and channels, and generalize these to their quantum versions. We formalize the notion of quantum channels, and present the theory of entanglement for pure and mixed states, along with important criteria and measures.

2.4.1 *Quantizing information theory*

The information theoretic and operationalist approach to physics consists in taking measurement results as central objects. After all, they are the fundamental events on which the agent bases any ontological model governing observed correlations between preparations and

measurement outcomes. Let us in this perspective consider a physical system $\mathcal{S}$ on which we choose to measure the property P. We will shortly give a formal definition of a measurement, but for now we can formulate the most basic requirement that a measurement result is a random variable which takes values on a set $\{e_1, e_2, ..., e_n\}$ of n outcomes that can very well be infinite. One may object that in this notation we are limiting ourselves to countably infinite outcomes, however one should remember that the temptation for continuity stems from an ontological postulate. Regardless of this postulate's validity, all measurements and operations are coarse grained and so any feature that hinges on the continuity assumption cannot be physical[20].

This being said, a state S of the system $\mathcal{S}$ is a probability distribution over these measurement outcomes. Using a subtle argument of finite speed of dynamical evolution [83], one may assume that carrying out a second measurement of the property P on the system $\mathcal{S}$ *immediately after* having obtained a first measurement outcome e_i, would certainly yield the same outcome[21]. Hence, all singular probability distributions on the set of possible outcomes are special states of perfect knowledge, called pure states. By contrast, all probability distributions which have support on more than one outcome are called mixed states. It is not difficult to see that all distributions over the set of outcomes can be expressed as a (normalized) linear combination of singular distributions, which are orthogonal to one another. As such, the set of pure states spans the state space $\mathfrak{S}$. Let us formalize this concept through the following definition.

Definition 23 (Classical states and n-level systems). *The classical states of a system $\mathcal{S}$ are given by the vectors $x^T = (x_1, ..., x_n)$ for[22] $n \in \overline{\mathbb{N}^*}$, where $\forall i \in [\![1, n]\!]$, $x_i \geqslant 0$ and $\|x\|_1 = 1$, and where the canonical representation basis is the set of pure states. Such systems are called n-level systems.*

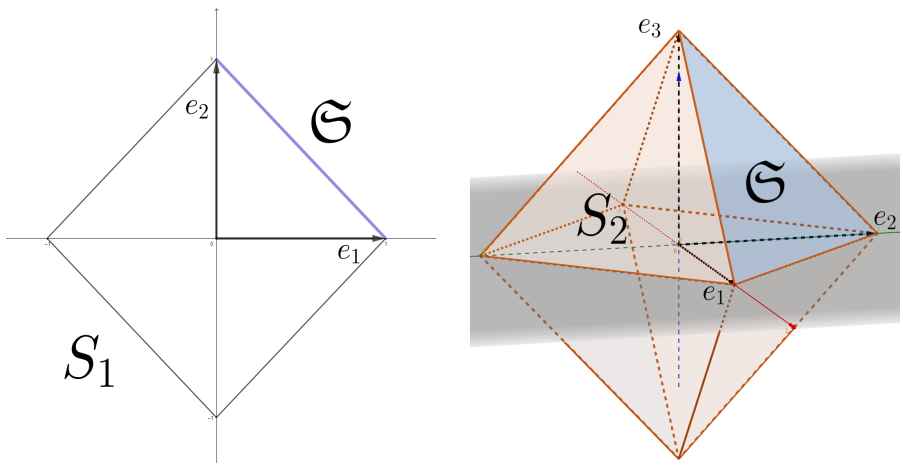
The positivity and ℓ^1 normalization amounts to having the state represent a probability distribution over $n \in \overline{\mathbb{N}^*}$ outcomes. One notices that a state x is a pure state if and only if it is normalized for the ℓ^2 norm, or equivalently, that its entrywise square represented by $(x^2)^T = (x_1^2, ..., x_n^2)$ satisfies $\left\|x^2\right\|_1 = 1$. The complete state space is then given by the closed convex hull of the set of pure states.

Before moving on to evolutions and measurements, let us briefly clarify the geometry of the state space. It is worth noting that pure

20 Any feature that would be parametrized by a strictly continuous variable $\theta \in \mathbb{R}$ is indistinguishable from its restriction to the discrete set of rationals, as the topological distance of $\mathbb{Q}$ to $\mathbb{R}$ is zero.

21 One may not even need to refer to dynamics, but invoke only the consistency in time of measurement results, however this raises the delicate question of the very definition and functions of a measurement.

22 Throughout this section we use the standard notations $\overline{\mathbb{N}} = \mathbb{N} \cup \{+\infty\}$ to denote the topological closure of $\mathbb{N}$, and $\mathbb{N}^* = \mathbb{N} \backslash \{0\}$.



(a) State space for a 2-level classical system.

(b) State space for a 3-level classical system.

Figure 2: Representations of the unit 1-sphere S_1 and 2-sphere S_2 for the ℓ^1 norm. The respective state space simplicies $\mathfrak{S}$ are shown in blue.

states span the state space $\mathfrak{S}$, but *do not* form a basis of $\mathfrak{S}$. Although they naturally form a basis of the vector space $\mathcal{V}$ they span, the state space is a projective space, obtained by projecting the non-negative orthant of $\mathcal{V}$ onto the unit sphere for the ℓ^1 norm. To make this clear, if one considers for example a set of two classical pure states spanning a plane, the ℓ^1 unit sphere is a square, and the state space is simply a one dimensional line which corresponds to the part of the square which is included in the non-negative quadrant of the plane, as represented in Fig. 2a. Similarly, for three pure states spanning a whole volume, the ℓ^1 unit sphere is an octahedron, and its intersection with the non-negative octant gives a triangle, as shown in Fig. 2b. For four pure states, the state space would be a tetrahedron. In general the state space spanned by $n \in \overline{\mathbb{N}^*}$ pure states is an $n-1$ dimensional simplex.

Now that we have characterized states of physical systems, let us turn to their evolution and formalize the meaning of a measurement. One basic requirement that can be enforced on a classical evolution operator $\mathcal{E}$ is that it must transform valid states to other valid states, that means that $\mathcal{E}$ must preserve the ℓ^1 norm and stabilize the non-negative orthant. An additional requirement, which is necessary in order to avoid faster-than-light signalling [84], is that evolutions $\mathcal{E}$ must be compatible with convex mixtures. Explicitly, this requirement takes the form

$$\forall (x,y) \in \mathfrak{S}^2, \forall \lambda \in [0,1],\ \mathcal{E}(\lambda x + (1-\lambda)y) = \lambda \mathcal{E}(x) + (1-\lambda)\mathcal{E}(y).$$

From those two basic requirements taken together one can establish the following simple definition.

Definition 24 (Classical evolutions). *Evolutions $\mathcal{E}$ of a classical system $\mathcal{S}$ are ℓ^1 norm preserving positive linear operators of the vector space $\mathcal{V}$ spanned by the pure states of $\mathcal{S}$.*

Since evolutions must be linear, they admit matrix representations in the basis of pure states. The set of evolution matrices are called stochastic matrices, transition matrices, or Markov matrices. They transform probability vectors into other probability vectors.

We now turn to measurements. Operationally, a measurement $\mathcal{M}$ is what gives answers to questions asked about a system $\mathcal{S}$. Some questions may have few outcomes, such as yes or no questions. For example, one may ask whether the physical system $\mathcal{S}$ is in the state e_1. A more extreme and trivial example would be to ask if the system is itself, for which there is technically only one outcome. On the other end of the spectrum, one may ask a more general question such as which of the states e_i the system is in. This measurement $\mathcal{M}_0$ has as many outcomes as there are degrees of freedom, and as such constitutes the sharpest possible measurement. If one chooses to label the measurement outcomes of $\mathcal{M}_0$ by the natural number $k \in [\![1, n]\!]$, then it is a random variable K satisfying $\mathbb{P}(K = k) = e_k^T x$. We see that the measurement outcomes are represented by the elements e_i themselves. Any question about the system which admits $m \in [\![1, m]\!]$ possible answers can in fact be formulated as a partition[23] of the set of pure states[24], mapping each pure state to the set of outcomes $[\![1, m]\!]$. This means that any m-outcome measurement $\mathcal{M}$ can be represented by a set of m vectors of the form $\forall k \in [\![1, m]\!],\ \mu_k = \sum_{i \in I_k} e_i$, where $\forall k \in [\![1, m]\!],\ I_k \subset [\![1, n]\!]$ is a set of indices labelling pure states on which the measurement outcome is constant and equal to k[25]. The probability that measurement $\mathcal{M}$ on the system S in the state x yields outcome k is then $\mathbb{P}(K = k) = \mu_k^T x$. The normalization condition then reads $\sum_{k=1}^m \mu_k^T x = (\sum_{k=1}^m \mu_k^T) x = 1$, which is always satisfied as $\sum_{k=1}^m \mu_k^T = \sum_{i=1}^n e_i^T = (1, ..., 1)$. In light of those remarks, let us formally define a measurement on a classical n-level system.

Definition 25 (Classical measurements). *Let $\mathcal{S}$ be an n-level classical system where $n \in \overline{\mathbb{N}^*}$ and let us denote its set of pure states $(e_i)_{1 \leqslant i \leqslant n}$. For all $m \in [\![1, n]\!]$, any m-outcome measurement $\mathcal{M}$ is uniquely described by a family of m vectors $(\mu_k)_{1 \leqslant k \leqslant m}$ which have non-negative components and which satisfy $\sum_{k=1}^m \mu_k = \sum_{i=1}^n e_i$. Furthermore when the system $\mathcal{S}$ is in state x, the measurement outcome is a random variable K satisfying $\mathbb{P}(K = k) = \mu_k^T x$.*

We are now ready to formulate the quantum counterparts of the classical definitions. To do so, we need only replace any state vec-

23 Reminder: a partition of a set E is a set of mutually exclusive subsets of E the union of which is E.

24 This can be understood by the fact that any boolean function can be built from the logical disjunction $\vee$ and the logical negation $\neg$.

25 The sets (I_k) form a partition of $[\![1, n]\!]$.

tor x of the real Hilbert space $\mathcal{V}$ by a hermitian operator ρ on the complex Hilbert space $\mathcal{H}$. The non-negativity of x will be taken into account by enforcing the positive semi-definiteness of the operator $\sigma(\rho) \subset \mathbb{R}_+$. The inner product between vectors $\mu_k^T x$ is replaced by the Hilbert-Schmidt inner product $\mathrm{Tr}(M_k^\dagger \rho)$. Correspondingly the ℓ_1 normalization of the vector x translates to the Hilbert-Schmidt normalization $\sqrt{\mathrm{Tr}(\rho^\dagger \rho)} = 1$, which in the hermitian case reduces to $\mathrm{Tr}(\rho) = 1$, and which means that ρ must be in the trace class, as per Def. 13. Analogous to the classical state where a state x is pure if and only if $\|x^2\|_1 = 1$, a quantum state ρ is pure if and only if $\mathrm{Tr}(\rho^2) = 1$. This leads to the following three fundamental quantum information theoretic definitions.

Definition 26 (Quantum states). *The quantum states of a system $\mathcal{S}$ are given by unit trace hermitian positive-semidefinite operators ρ of a complex Hilbert space $\mathcal{H}$. Such objects are called density operators.*

Definition 27 (Quantum evolutions). *Evolutions $\mathcal{E}$ of a quantum system $\mathcal{S}$ are linear super-operators, or maps, that stabilize the quantum state space.*

Definition 28 (Quantum measurements). *Let $\mathcal{S}$ be a quantum system with $n \in \overline{\mathbb{N}^*}$ pure states. For all $m \in [\![1, n]\!]$, any m-outcome measurement $\mathcal{M}$ is uniquely described by a family of m hermitian positive semi-definite operators $(M_k)_{1 \leqslant k \leqslant m}$ which satisfy $\sum_{k=1}^{m} M_k = \mathbb{1}$. Furthermore when the system $\mathcal{S}$ is in state ρ, the measurement outcome is a random variable K satisfying $\mathbb{P}(K = k) = \mathrm{Tr}(M_k \rho)$.*

At this point we have laid out a convenient extension of classical theory, and these definitions alone already lead to some interesting questions. Although the transition from vectors to operators for states and measurements may neatly account for the fact that quantum theory is non-abelian, one may wonder why we are working on a complex Hilbert space, rather than a real Hilbert space. One may also ask what does the quantum state space look like, and how does its dimension scale with the number of pure states. Another question is the possibility of having a more explicit definition of a quantum evolution. While we shall discuss the two former questions, the latter requires more formalism and will be the topic of our next section.

An explanation for the necessity of complex Hilbert spaces, as opposed to real Hilbert spaces, lies within the continuity of quantum evolutions. The continuity requires, for instance, all quantum evolutions to admit n-th roots which are also valid evolutions. This is only possible if the underlying field contains $\mathbb{R}$ and is algebraically closed. A simple but illustrative example is the existence of square roots of the negation for a single quantum bit, whereas no such operation is possible on a single classical bit, or without using the imaginary unit i. More remarkably, the use of complex numbers in physical theories is not a mere mathematical convenience or requirement, but was recently shown to be a genuine empirical constraint [85].

Before moving on to the characterization of quantum evolutions, let us say a few words about quantum state spaces and introduce a useful representation for the states of two-level quantum systems. It is clear that classical information theory can be embedded into quantum information theory, by simply taking classical state vectors to be diagonal density operators, and classical measurement vectors to be diagonal quantum measurement operators. Because of this, the fact that quantum state spaces have higher dimensionality than classical state spaces should not come as a surprise.

Explicitly, the set $\mathcal{M}_n(\mathbb{C})$ of complex $n \times n$ matrices is a $2n^2$ dimensional real vector space. Hermitian symmetry reduces the dimension by $n(n-1)+n = n^2$ and the unit trace constraint further fixes one degree of freedom. In total the state space of an n-level quantum system has dimension $2n^2 - n^2 - 1 = n^2 - 1$. As a consequence, a two-level quantum system, called qubit, has state space dimensionality 3 whereas the classical bit has state space dimensionality 1. For three level systems, we have seen that the classical state space is 2-dimensional and can be drawn as a triangle, while its quantum counterpart, being 8-dimensional, cannot be drawn.

Let us turn to the simplest non-trivial quantum system, called qubit. As per our previous remarks, qubit states are represented by 2×2 hermitian matrices. One can opt for a natural representation using the canonical (or computational) basis of the complex vector space of such matrices and write

$$\rho = a\,|0\rangle\langle 0| + c\,|0\rangle\langle 1| + c^*\,|1\rangle\langle 0| + b\,|1\rangle\langle 1| = \begin{pmatrix} a & c \\ c^* & b \end{pmatrix},$$

where $a, b \in \mathbb{R}$ and $c \in \mathbb{C}$. This representation is quite straightforward, however it does not fully exploit the hermitian symmetry or the unit trace, and the states in this basis have a complex coordinate, which does little to help gain intuition about the state space.

One may instead embed the complex component into the basis elements themselves, and use a basis made up of a collection of matrices that are already hermitian. One such basis is called the Pauli basis, and is built from the unit matrix and the three Pauli matrices or operators. Explicitly in the computational basis, the Pauli basis elements are given by

$$(\mathbb{1}, X, Y, Z) = \left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right). \tag{28}$$

By defining the index notation $(\sigma_0, \sigma_1, \sigma_2, \sigma_3) = (\mathbb{1}, X, Y, Z)$ one can check that $\mathrm{Tr}(\sigma_i \sigma_j) = 2\delta_{ij}$, which makes this basis orthogonal. We note that the three Pauli operators share the same spectrum $\{-1, 1\}$, and are all traceless. If we now examine the quantity

$$\rho = \frac{1}{2}(\mathbb{1} + \mu_1 X + \mu_2 Y + \mu_3 Z) = \frac{1}{2}(\mathbb{1} + \mu^T \sigma), \tag{29}$$

where $\mu \in \mathbb{R}^3$ and $\sigma^T = (X, Y, Z)$ then ρ has unit trace and is hermitian. Furthermore, the spectrum of such quantity is found to be $\sigma(\rho) = \{\frac{1}{2}(1 - \|\mu\|), \frac{1}{2}(1 + \|\mu\|)\}$ where the norm is the Euclidean $\mathbb{R}^3$ norm. Thus, the positiveness of ρ simply requires $\|\mu\| \leqslant 1$. The vector μ representing the quantum state is called Bloch vector, and for valid states it must lie in the closed unit ball. One can easily check that the state ρ is pure if and only if $\|\mu\| = 1$, that is to say that the pure states lie on the Bloch sphere. The maximally mixed state is at the center of the Bloch ball.

Worth noting, is that a qubits admit an infinite number of pure states, whereas classical bits only admit two pure states. This gives quantum theory an important feature that is not present in classical theory, called ensemble ambiguity. Specifically, there are infinitely many ways to mix different pairs of pure states, to arrive at the same mixed state.

The state space for a single qubit is, as we have seen, somewhat more complicated than that of the classical bit, and already features operational properties that are absent from classical theory. Let us now complete this short overview on quantum states with an even more interesting example, which is the composite system of two qubits.

Given two qubits with respective pure state spaces in two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, the pure state of the composite system lives in the tensor product space $\mathcal{H}_{12} = \mathcal{H}_1 \otimes \mathcal{H}_2$. As previously defined, the general quantum state ρ_{12} of two qubits is simply a unit trace, positive-semidefinite operator of $\mathcal{H}_{12}$. The set of such operators constitutes a 15-dimensional space. One can identify three important types of bipartite states, which do not limit to qubits.

Definition 29 (Factorizable quantum states). *A bipartite quantum state $\rho_{12} \in \mathcal{B}_1(\mathcal{H}_{12})$ is said to be factorizable when there exists two local states $\rho_1 \in \mathcal{B}_1(\mathcal{H}_1)$ and $\rho_2 \in \mathcal{B}_1(\mathcal{H}_2)$ such that $\rho_{12} = \rho_1 \otimes \rho_2$. These are also known as product states.*

Definition 30 (Separable and entangled quantum states). *A bipartite quantum state $\rho_{12} \in \mathcal{B}_1(\mathcal{H}_{12})$ is said to be separable when it can be written as a convex combination of product states. This is denoted $\rho \in \mathcal{D}_{sep}$ when there is no ambiguity on the underlying Hilbert space. Otherwise, the state is said to be entangled.*

While factorizable and separable states correspond to either uncorrelated or classically correlated states, there is no classical counterpart to entangled states. We have unveiled our very first definition of entanglement, from which it is clear that a pure state is entangled if it cannot be written as a product state. This negative definition of entanglement is unfortunately all but practical, as the factorization may not be obvious. We will later define entanglement in a much more powerful framework, but for now, we can briefly work out a more convenient representation to determine entanglement.

Claim 11. *All bipartite pure states $|\psi\rangle$ may be decomposed in the form $|\psi\rangle = \sum_k \sqrt{\lambda_k}\,|\psi_k\rangle\,|\phi_k\rangle$, where $(|\psi_k\rangle)_k$ and $(|\phi_k\rangle)_k$ are orthonormal sets of states.*

Proof. Any bipartite pure state can be written in the computational bipartite orthonormal basis as $|\psi\rangle = \sum_{ij} a_{ij}\,|i\rangle\,|j\rangle$, where $A = (a_{ij})$ is its matrix representation. By singular value decomposition Th. 5, one may write $A = USV$ where U, V are unitary matrices and S is diagonal and non-negative, and we shall denote its coefficients $\sqrt{\lambda_k}$. Thus $a_{ij} = u_{ik}\sqrt{\lambda_k}v_{kj}$ and we may rewrite our bipartite pure state as $|\psi\rangle = \sum_k \sqrt{\lambda_k}\,(\sum_i u_{ik}\,|i\rangle)\,(\sum_j v_{kj}\,|j\rangle)$. Setting $|\psi_k\rangle = \sum_i u_{ik}\,|i\rangle$ and $|\phi_k\rangle = \sum_j v_{kj}\,|j\rangle$ ends the proof. □

This way of expressing bipartite pure states is sometimes called Schmidt decomposition. The $\sqrt{\lambda_k}$ numbers are called Schmidt coefficients, and the number of non-zero Schmidt coefficients defines the Schmidt rank. With this handy decomposition, a bipartite entangled pure state is simply a state which has Schmidt rank greater than 1. This is of course only a first glimpse at entanglement theory, as the Schmidt rank does not tell us how much entanglement there is in a bipartite state, and does not work for mixed bipartite states. A deeper investigation will be carried out in a later section.

Now that we have defined notable bipartite states, one may be interested in knowing the state of only one of the subsystems. This is done by tracing-out the system that is not of interest.

Definition 31 (Reduced quantum states). *Given a bipartite quantum state $\rho_{12} \in \mathcal{B}_1(\mathcal{H}_{12})$, the reduced state ρ_1 is defined by taking the partial trace*

$$\rho_1 = \mathrm{Tr}_2(\rho_{12}) = \sum_k (\mathbb{1}_1 \otimes \langle k|_2)\rho_{12}(\mathbb{1}_2 \otimes |k\rangle_2),$$

where $(|k\rangle)$ is an orthonormal basis of the Hilbert space $\mathcal{H}_2$.

One can readily check that given an arbitrary bipartite separable state $\rho = \sum_k p_k \rho_1^{(k)} \otimes \rho_2^{(k)}$ where p_k is a probability distribution and $\rho_{1,2}^{(k)}$ are local states, we have consistency $\mathrm{Tr}_2(\rho_{12}) = \sum_k p_k \rho_1^{(k)}$.

A noteworthy characterization of entangled states, is that a pure entangled bipartite state has mixed reduced states. This is strongly at odds with classical information theory, where one expects a composite system to be in a pure state if and only if its subsystems are also in pure states. An extreme example is the Bell state $|\phi^+\rangle\langle\phi^+|$, written as $\rho_{12} = \frac{1}{2}(|00\rangle + |11\rangle)(\langle 00| + \langle 11|)$ in the computational basis, for which the reduced local states are maximally mixed $\rho_{1,2} = \frac{1}{2}\mathbb{1}_{1,2}$. In order to gain deeper insight on quantum entanglement, we first need to spend some time on quantum channels, and different types of quantum operations.

2.4.2 *Quantizing information channels*

We have so far introduced quantum states and measurements, and only superficially mentioned quantum evolutions, which quite trivially must map quantum states to other valid quantum states. Let us now delve slightly further into the characterization and different representations of quantum evolutions, also called quantum channels. A formal definition of quantum channels is given by the Kraus representation [86], sometimes also called operator-sum representation.

Theorem 12 (Kraus representation for quantum channels). *Valid quantum operations (evolutions or channels) are (super-)operations $\mathcal{E} \in \mathcal{L}(\mathcal{B}_1(\mathcal{H}), \mathcal{B}_1(\mathcal{H}'))$ of the form*

$$\mathcal{E} : \rho \longmapsto \sum_{i=1}^{n} A_i \rho A_i^\dagger, \tag{30}$$

where $n \in \mathbb{N}$ and $\{A_i\}_{1 \leqslant i \leqslant n}$ is a set of operators in $\mathcal{L}(\mathcal{H}, \mathcal{H}')$ that obey the following condition

$$\sum_{i=1}^{n} A_i^\dagger A_i = \mathbb{1}_{\mathcal{L}(\mathcal{H})}. \tag{31}$$

Proof. We begin by noting that for $n, p \in \mathbb{N}$ any linear super-operation $\mathcal{E} : \mathcal{B}(\mathcal{H}) \longrightarrow \mathcal{B}(\mathcal{H}')$ from a n-level quantum state space to a p-level quantum state space can be written as $\mathcal{E} : \rho \longmapsto \sum_{ij} \lambda_{ij} \mu_i \rho \mu_j^\dagger$, where λ_{ij} are complex numbers, and (μ_i) is an orthonormal basis of the space of rectangular complex matrices $\mathcal{M}_{p,n}(\mathbb{C})$ equipped with the Hilbert-Schmidt inner product. Enforcing that $\mathcal{E}(\rho)$ be hermitian amounts to the requirement $\forall i, j, \lambda_{ij} = \lambda_{ji}^*$. We may define another basis of $\mathcal{M}_{p,n}(\mathbb{C})$ by constructing $D_p = \sum_i U_{ip} \mu_i$. If we require this new basis to be orthonormal then the transformation U must be a unitary endomorphism of $\mathcal{M}_{p,n}(\mathbb{C})$. In this case we can also write the reciprocal relation as $\sum_p [U^\dagger]_{pj} D_p = \sum_i \left(\sum_p [U^\dagger]_{pj} U_{ip} \right) \mu_i = \mu_j$. Substituting this back into the expression of $\mathcal{E}(\rho)$ one can establish

$$\begin{aligned}
\mathcal{E}(\rho) &= \sum_{ij} \lambda_{ij} \left(\sum_p [U^\dagger]_{pi} D_p \right) \rho \left(\sum_q U_{jq} D_q^\dagger \right) \\
&= \sum_{pq} \left(\sum_{ij} [U^\dagger]_{pi} \lambda_{ij} U_{jq} \right) D_p \rho D_q^\dagger \\
&= \sum_{pq} \left(U^\dagger \Lambda U \right)_{pq} D_p \rho D_q^\dagger,
\end{aligned}$$

and since we require the evolved state to be hermitian, Λ itself must be hermitian, hence by spectral theorem, the unitary change of basis matrix U can be chosen to be diagonalizing, that is the vectors

(D_p) can be chosen to be eigenvectors of Λ associated to a set of real eigenvalues γ_p. With this choice $\mathcal{E}(\rho) = \sum_p \gamma_p D_p \rho D_p^\dagger$. If the eigenvalues γ_p are non-negative then defining $A_p = \sqrt{\gamma_p} D_p$ gives (30). If one eigenvalue is negative, then we cannot have Kraus representation, and it turns out in this case that the superoperator represented by Λ is no longer valid as it may transform states into matrices with negative eigenvalues when embedded into a larger system. With the positivity and hermiticity, we have shown that quantum maps admit the Kraus form (30). The final requirement is trace preservation. This reads

$$\mathrm{Tr}(\mathcal{E}(\rho)) = \sum_{i=1}^{n} \mathrm{Tr}\left(A_i \rho A_i^\dagger\right) = \mathrm{Tr}\left[\left(\sum_i A_i^\dagger A_i\right)\rho\right] := \mathrm{Tr}(\rho),$$

which must hold for any unit trace matrix ρ, hence the requirement (31). □

In our proof of the Kraus representation, we have mentioned that negative eigenvalues for the super-operator Λ lead to non-positivity-preserving maps. To prove this, let us consider the general super-operator Λ that we may embed into a bigger bipartite super-operation $\Lambda \otimes \mathbb{1}$. Considering a Bell-type state $|\psi\rangle = d^{-1/2} \sum_{i=1}^{d} |ii\rangle$, we have

$$(\Lambda \otimes \mathbb{1})(\rho) = \sum_i \gamma_i D_i |\psi\rangle\langle\psi| D_i^\dagger = \sum_i \gamma_i |\psi_i\rangle\langle\psi_i|,$$

from which we see that the γ_i are precisely the eigenvalues of $\mathcal{E}(\rho)$, hence they must all be non-negative for the map to be valid. As a final remark on the Kraus representation, let us note that it is not unique, as any unitary mixing $B_i = \sum_k u_{ik} A_k$ also provides a valid Kraus representation.

We shall refer to those quantum operations or quantum maps as Completely Positive Trace-Preserving (CPTP) maps. Explicitly, the set of valid quantum operations is a subset denoted $\mathbf{CPTP}(\mathcal{H}, \mathcal{H}')$ of $\mathcal{L}(\mathcal{B}_1(\mathcal{H}), \mathcal{B}_1(\mathcal{H}'))$.

There are other important representations of CPTP maps. While they shall not be of immediate use for the results presented in this thesis, two conceptually rich representations deserve a brief mention. The first one is the Choi matrix

$$J(\mathcal{E}) = (\mathcal{E} \otimes \mathbb{1}) \sum_{ij} |ii\rangle\langle jj|,$$

which is constructed via the Choi-Jamiolkowski isomorphism [87]. Among its many strengths, the Choi representation makes transparent the fundamental state-operation equivalence. It also helps provide a straightforward proof of the unitary mixing freedom of the Kraus representation.

The second one worth a mention is the Stinespring representation [88], which relies on more general results from the structure of

C^*-algebras, and the fact that any quantum operation can be seen as a partial trace on the unitary evolution of a larger state in a larger Hilbert space

$$\mathcal{E}(\rho) = \mathrm{Tr}_C[U(\rho \otimes |\psi\rangle\langle\psi|)U^\dagger].$$

The Kraus formalism is sufficient however to establish with little effort some general properties of quantum maps. We shall now touch on two properties that one can consider to be very basic requirements that quantum channels should satisfy. Namely, that evolving a quantum state through two channels sequentially, and that randomly selecting a quantum channel to evolve a state through, should both constitute valid quantum operations.

Claim 12. *The sequential composition of two quantum channels is a quantum channel. Explicitly:*

$$\forall(\mathcal{E},\mathcal{F}) \in \boldsymbol{CPTP}(\mathcal{H}_1,\mathcal{H}_2) \times \boldsymbol{CPTP}(\mathcal{H}_2,\mathcal{H}_3),\ \mathcal{F}\circ\mathcal{E} \in \boldsymbol{CPTP}(\mathcal{H}_1,\mathcal{H}_3).$$

Proof. Given three Hilbert spaces $(\mathcal{H}_i)_{1\leqslant i\leqslant 3}$ and two CPTP maps $\mathcal{E} : \mathcal{B}_1(\mathcal{H}_1) \longrightarrow \mathcal{B}_1(\mathcal{H}_2)$ and $\mathcal{F} : \mathcal{B}_1(\mathcal{H}_2) \longrightarrow \mathcal{B}_1(\mathcal{H}_3)$, there are Kraus operators $\{A_i\}_{1\leqslant i\leqslant n}$ and $\{B_i\}_{1\leqslant i\leqslant m}$, where $(n,m) \in \mathbb{N}^2$, representing those two maps. We can then write the compound action $\forall\rho \in \mathcal{B}_1(\mathcal{H}_1),\ \mathcal{F}\circ\mathcal{E}(\rho) = \sum_{ij} B_j A_i \rho A_i^\dagger B_j^\dagger$, which suggests to define $C_{ij} = B_j A_i$ as the Kraus operators for the compound map. It is readily checked that $\sum_{ij} C_{ij}^\dagger C_{ij} = \sum_i A_i^\dagger \left(\sum_j B_j^\dagger B_j\right) A_i = \mathbb{1}_{\mathcal{L}(\mathcal{H}_1)}$, hence the compound map is a valid quantum operation. □

Claim 13. *The set of quantum channels is convex. Explicitly:*

$$\forall p \in [0,1], \forall\mathcal{E},\mathcal{F} \in \boldsymbol{CPTP}(\mathcal{H}_1,\mathcal{H}_2),\ p\mathcal{E} + (1-p)\mathcal{F} \in \boldsymbol{CPTP}(\mathcal{H}_1,\mathcal{H}_2).$$

Proof. Let us keep the Kraus representations of $\mathcal{E}$ and $\mathcal{F}$ introduced in the previous proof, and consider the map $\mathcal{G} \in \mathcal{L}(\mathcal{B}_1(\mathcal{H}_1),\mathcal{B}_1(\mathcal{H}_2))$ defined by the Kraus operators

$$C_i = \begin{cases} \sqrt{p}A_i & \text{if} \quad 1 \leqslant i \leqslant n \\ \sqrt{1-p}B_i & \text{if} \quad n+1 \leqslant i \leqslant n+m \end{cases},$$

then we have

$$\forall\rho \in \mathcal{B}(\mathcal{H}_1),$$
$$\sum_{i=1}^{n+m} C_i\rho C_i^\dagger = \sum_{i=1}^{n} A_i\rho A_i^\dagger + \sum_{i=n+1}^{n+m} B_i\rho B_i^\dagger = p\mathcal{E}(\rho) + (1-p)\mathcal{F}(\rho),$$

and

$$\sum_{i=1}^{n+m} C_i^\dagger C_i = p\left(\sum_{i=1}^{n} A_i^\dagger A_i\right) + (1-p)\left(\sum_{i=n+1}^{n+m} B_i^\dagger B_i\right) = \mathbb{1}_{\mathcal{L}(\mathcal{H}_1)},$$

which ends the proof. □

To illustrate the generality of this formalism, we can cast fundamental operations in the Kraus representation. The Kraus representations for the preparation $\mathcal{P}$ of an n-level quantum state with spectrum (λ_i) from the absence of any system, for the addition $\mathcal{A}$ of a system in such state to a given system, and for the discarding $\mathcal{D}$ of that sub-system from a bipartite system, are shown in Tab. 1.

Operation and Kraus operators	Input-output spaces
$\mathcal{P} : (P_i)_{1\leqslant i\leqslant n} = (\sqrt{\lambda_i}\,\lvert\psi_i\rangle)_{1\leqslant i\leqslant n}$	$\{0\} \to \mathcal{B}_1(\mathcal{H})$
$\mathcal{A} : (A_i)_{1\leqslant i\leqslant n} = (\mathbb{1}_1 \otimes \sqrt{\lambda_i}\,\lvert\psi_i\rangle)_{1\leqslant i\leqslant n}$	$\mathcal{B}_1(\mathcal{H}_1) \to \mathcal{B}_1(\mathcal{H}_1 \otimes \mathcal{H}_2)$
$\mathcal{D} : (D_i)_{1\leqslant i\leqslant n} = (\mathbb{1}_1 \otimes \langle\psi_i\rvert)_{1\leqslant i\leqslant n}$	$\mathcal{B}_1(\mathcal{H}_1 \otimes \mathcal{H}_2) \to \mathcal{B}_1(\mathcal{H}_1)$

Table 1: Kraus representations of state preparation, addition and discarding.

We have established a formal criterion for quantum operations, seen that they can be conveniently represented in the Kraus formalism, and that state preparation, addition and discarding can all be seen as quantum channels. To conclude our overview of quantum operations, we now turn to three very important classes of quantum operations, that will serve as foundation on which the theory of entanglement is built.

Definition 32 (Local operations). *Given three Hilbert spaces $(\mathcal{H}_i)_{1\leqslant i\leqslant 3}$ the set of local operations denoted $\boldsymbol{LO}(\mathcal{H}_1 \otimes \mathcal{H}_2, \mathcal{H}_3)$ is the subset of all operations $\mathcal{E} \in \boldsymbol{CPTP}(\mathcal{H}_1 \otimes \mathcal{H}_2, \mathcal{H}_3)$ that admit a tensor product decomposition as operations acting on each subsystem. Formally:*

$$\begin{aligned}&\mathcal{E} \in \boldsymbol{LO}(1 \otimes 2, 3)\\ &\qquad\qquad \iff \exists(\mathcal{E}_1, \mathcal{E}_2) \in \boldsymbol{CPTP}(1,3) \times \boldsymbol{CPTP}(2,3),\ \mathcal{E} = \mathcal{E}_1 \otimes \mathcal{E}_2,\end{aligned}$$

where we have only shown Hilbert space indices as a shorthand notation.

We remind that dimensions need not be preserved as discarding and adding systems are valid channels. The above definition can naturally be extended to a countable number $n \in \overline{\mathbb{N}^*}$ of systems the state spaces of which are $(\mathcal{B}(\mathcal{H}_i))_{1\leqslant i\leqslant n}$. Local operations are all channels that can be written as

$$\mathcal{E} = \bigotimes_{i=1}^{n} \mathcal{E}_i \text{ where } \forall i \in [\![1, n]\!],\ \mathcal{E}_i \in \mathbf{CPTP}(\mathcal{H}_i, \mathcal{H}_i').$$

Another important class of operations is called Classical Communication (CC). Classical states are the diagonal density operators in the computational basis, and communication is captured by the relabelling of the system in which this information is contained.

A simple example to start with, is the case where system 1 is described by a quantum system and a classical register and system 2 is just a quantum system. Then the transfer of classical information

from system 1 to system 2 is simply written as the transformation $(|\psi\rangle\langle\psi|_1 \otimes \rho_1) \otimes \rho_2 \longmapsto \rho_1 \otimes (\rho_2 \otimes |\psi\rangle\langle\psi|_2)$, where $|\psi\rangle_i$ is a computational basis state for system i. In general CC operations between two systems i and j are all maps of the form

$$C_{ij} : \rho \longmapsto \sum_n |\psi_n\rangle\langle\psi_n|_j \, (\langle\psi_n|\rho|\psi_n\rangle_i),$$

where $|\psi_n\rangle_{i,j}$ are computational basis states for systems i and j.

Combining the two previous concepts, we arrive at a crucial class of operations called Local Operations and Classical Communication (LOCC).

Definition 33 (LOCC channels). *The set of local-operations with classical communication* ***LOCC*** *is the subset of* ***CPTP*** *of all operations $\mathcal{E}$ which are finite combinations of* LO *and* CC *operations.*

From this definition, it is immediate that **LOCC** is closed under composition. As a basic example of LOCC operation between two parties, one can consider the scenario where agent 1 performs a measurement on his system, classically communicates the measurement outcome to agent 2 who performs a unitary transformation on his part of the system conditioned on the classical he received from agent 1. This sequence of operations reads

$$\rho \mapsto (M_k \otimes \mathbb{1})\rho(M_k^\dagger \otimes \mathbb{1}) \mapsto (\mathbb{1} \otimes U(k))(M_k \otimes \mathbb{1})\rho(M_k^\dagger \otimes \mathbb{1})(\mathbb{1} \otimes U^\dagger(k)),$$

where M_k are measurement operators used by agent 1 and $U(k)$ is the conditional local unitary applied by agent 2, which depends on the classical parameter k.

With the proper definition of LOCC channels at hand, we are now ready to formally establish the definition of entanglement, and to explore some important properties of this non-classical class of correlation.

2.4.3 *Entanglement theory of pure states*

In Sec. 2.4.1 we have briefly touched upon entanglement using the Schmidt decomposition, and seen that pure bipartite entangled states have mixed reduced states. Quantum entanglement is in fact one of the most widely studied features of quantum information theory, and is at the core of most non-classical effects that are sought after in platforms for quantum computation, as well as in experimental tests of fundamental physics. Because of its importance, let us take this section to formalize the notion of quantum entanglement.

The traditional way the notion of entanglement is introduced in late undergraduate courses, is in the context of violations of Bell-type inequalities [24], which are a class of constraints on correlations between pairs of observables, that must hold in any objective-local

Figure 3: Setup of the CHSH experiment as illustrated in Ref. [1], where Alice and Bob can each locally measure two different physical properties of a system, which for simplicity are assumed to take values in $\{-1, 1\}$.

frameworks [89], such as hidden local variable theories. The simplest example are the Clauser-Horne-Shimony-Holt (CHSH) inequalities [25] which can be established by a simple thought experiment.

Consider a bipartite system, with two agents Alice and Bob that can act on each sub-part of the system. We suppose that each agent has two measurement devices to measure two properties of the system they have, say Q, R for Alice and S, T for Bob, as sketched in Fig. 3. To simplify calculations, one can assume without loss of generality that the measurement outcomes are included in the set $\{-1, 1\}$. Let us further assume that Alice and Bob can select their measurement devices randomly and independently of one another[26], then under the realism assumption, the quantity $QS + RS + RT - QT$ is well defined even if some measurements of those quantities are not performed. Because this quantity takes values in the set $\{-2, 2\}$, if Alice and Bob repeat the experiment many times, the empirical average will converge to a true expectation value which must satisfy $\langle QS + RS + RT - QT \rangle \leqslant 2$. However, it is apparent that if Alice and Bob share a bell state such as $|\psi_-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ and choose their measurement devices to measure the observables defined by $(Q, R, S, T) = \left(Z_A, X_A, \frac{-1}{\sqrt{2}}(Z_B + X_B), \frac{1}{\sqrt{2}}(Z_B - X_B)\right)$, then the expectation values satisfy $\langle QS \rangle = \langle RS \rangle = \langle RT \rangle = -\langle QT \rangle = \frac{1}{\sqrt{2}}$, so that the CHSH inequality no longer holds.

The violation of Bell-CHSH inequalities are witnesses of non-classical behavior, and imply that the state on which the bipartite local measurements were performed must be entangled. While it is an important test of entanglement, Bell inequality violations do not quite give the full picture of quantum entanglement. An obvious limitation to such an approach of quantum entanglement is that it only yields a "yes or maybe-not" answer about the presence of entanglement. It turns out that Bell inequality violations are only witnesses of entanglement for pure states. If we more generally consider mixed states, it was shown that some states that do not violate a CHSH inequality can be LOCC-purified to be violating [90], a feature known as hidden non-locality. Furthermore, those violations do not involve any notion

26 This can be ensured if the measurement device selection events are spacelike separated, under the locality assumption.

of degree of entanglement, and the amplitude of the violation does not give a reliable measure of entanglement. In order to have robust criteria and sufficient conditions to certify entanglement, or to establish a measure of it, we shall introduce a different framework.

We recall that physical observables X in quantum theory are hermitian operators, and measuring the physical property X of a system in state ρ amounts to randomly applying one of the spectral projectors P_k of X to the state ρ and renormalizing the result. The probability of applying P_k is given by $\mathrm{Tr}(P_k\rho)$. This formalism, called Positive Operator Valued Measurement (POVM) allows for a simple and practical theory of measurements, but it is not hard to imagine why it does not quite capture all possible properties of physical systems: common physical properties such as mass, entropy or temperature, do not have associated quantum operators and so do not fit within the POVM formulation. Let us now introduce the much more general operational framework of resource theories.

Consider a general set S of states and a class of allowed operations F, called *free-operations*. One can build an oriented graph in which an edge s_i is linked to s_j when it is possible to go from s_i to s_j using only operations in F. This defines a partial order on S that we can reformulate and denote as

$$s_i \succ s_j \iff \exists f \in F,\ s_j = f(s_i).$$

Definition 34 (Free and resource states). *The set $S_{free} \subset S$ that is left invariant under free operations is called the set of free states. States that are not free are called resource states.*

Free states are the minimum of the state space for the partial order. Now that we have defined resource states, let us also define an object that quantifies the amount of resource in a resource state.

Definition 35 (Resource measures). *Any function $\mu : S \longmapsto \mathbb{R}$ satisfying the condition $\forall i, j,\ s_i \succ s_j \implies \mu(s_i) \leqslant \mu(s_j)$ is called a resource measure.*

It is not hard to establish that there are as many non-equivalent measures as there are permutations of incomparable states s_i. Let us give a simple example in order to make things clear.

Consider the set $S = \{1, 2, ..., 16\}$ and let us define the free operation $f : n \longmapsto n/2$ if n is even, $f : n \longmapsto n$ if n is odd. The set of free states is $S_{\text{free}} = \{1, 3, 5, 7, 9, 11, 13, 15\}$ and the non-trivial chains of ordering are $(16 \succ 8 \succ 4 \succ 2 \succ 1)$; $(12 \succ 6 \succ 3)$; $(10 \succ 5)$ and $(14 \succ 7)$. A valid measure μ for this resource is, for instance, the distance to the set of free states, in the sense of the number of required applications of f. We have $\mu(16) = 4$, and in this theory 16 is the most resourceful state.

Resource theories have bloomed in the late 2000s and have since been applied to give a grounded framework for various physical

quantities that are not suited for POVM descriptions. Resource formulations have been established for entanglement [91], asymmetry [92], state gaussianity [93], coherence [94] among others.

Let us now focus on the resource theory of entanglement, which falls under the class of quantum resource theories. Quantum resource theories are specified by a set of free quantum operations F which is stable under composition and which contains the discarding channel. Because state preparation is a quantum operation, there is a subset of F called free states and denoted F_{states}.

Definition 36 (Quantum resource measures). *If $\mathcal{S}$ denotes the set of quantum states, any function $\mu : \mathcal{S} \to \mathbb{R}$ which satisfies*

$$\forall \mathcal{E} \in F,\ \forall \rho \in \mathcal{S}, \mu(\rho) \geqslant \mu(\mathcal{E}(\rho)),$$

is called a resource measure.

In other words, free operations always decrease the resource of a state. It is clear that the resource measure must be a constant function on F_{states}. Let us now be more specific.

Definition 37 (Resource theory of entanglement). *The resource theory of entanglement is the quantum resource theory in which the free operations are the LOCC operations.*

Given this definition, the free states are called separable and the resource states are called entangled. So far, we have simply redefined entanglement in the framework of quantum resource theories: it is the property that is not increasing through LOCC operations.

In order to have a clearer picture of what this means, one may wonder under which conditions on the states ρ_{12} and σ_{12} there exist LOCC operations realizing $\rho_{12} \longmapsto \sigma_{12}$. This question is unfortunately quite difficult to answer in general. To begin our investigation, we shall tackle a less ambitious question, by restricting ourselves to the case of pure bipartite states. To this end we introduce the concept of majorization.

Definition 38 (Majorization). *For any two real vectors $(u, v) \in \mathbb{R}^n$ where $n \in \mathbb{N}^*$, we say that v majorizes u, which is denoted $v \succ u$, when*

$$\forall k \in [\![1, n]\!],\ \sum_{i=1}^{k} v_i^{\downarrow} \geqslant \sum_{i=1}^{k} u_i^{\downarrow} \text{ and } \sum_{i=1}^{n} v_i = \sum_{i=1}^{n} u_i,$$

where the arrow superscript indicates that the vector components have been sorted in decreasing order.

The majorization defines a partial preorder on $\mathbb{R}^n$. It is trivially reflexive, and easily checked to be transitive. It is only a preorder as antisymmetry is not satisfied, given that two vectors that differ by a nontrivial permutation of components majorize one another. While

the majorization realizes a total preorder for $n \in \{1, 2\}$, this fails for $n \geqslant 3$ as can be seen by taking $u^T = (5, 2, 1)$ and $v^T = (4, 4, 0)$.

Let us apply this relation to the space of vectors of $[0, 1]^n$ that lie on the unit ℓ^1 sphere, that is, to probability vectors. We define the two vectors m and M such that $\forall i \in [\![1, n]\!]$, $m_i = \frac{1}{n}$, $M_i = \delta_{i,1}$, which correspond to a uniform distribution and to a point-like distribution on the first index.

Claim 14. *All probability vectors* p *satisfy* $M \succ p$ *and* $p \succ m$.

Proof. For all probability vector p, and by definition of M, it is clear that $\forall k \in [\![1, n]\!], \sum_{i=1}^{k} M_i = 1 \geqslant \sum_{i=1}^{k} p_i^{\downarrow}$, hence $M \succ p$. Let us now show by contradiction that $p \succ m$. Suppose that p is not equal to m, then

$$\exists k \in [\![1, n]\!], \sum_{i=1}^{k} p_i^{\downarrow} < \frac{k}{n} \implies \exists i \in [\![1, k]\!], p_i^{\downarrow} < \frac{1}{n},$$

but we also have the implications

$$\begin{aligned} &\exists k \in [\![1, n]\!], \sum_{i=1}^{k} p_i^{\downarrow} < \frac{k}{n} \\ &\implies \sum_{i=k+1}^{n} p_i^{\downarrow} = 1 - \sum_{i=1}^{k} p_i^{\downarrow} > \frac{n-k}{n} \implies \exists i \in [\![k+1, n]\!], p_i^{\downarrow} > \frac{1}{n}, \end{aligned}$$

which contradicts the fact that $p^{\downarrow}$ is ordered in decreasing values. □

Although what we have shown may seem as yet another mathematical curiosity, the following theorem actually gives a relationship between majorization and convertibility through LOCC operation [1], and is owed to Nielsen.

Theorem 13 (Nielsen's theorem). *There exists a deterministic channel* $\mathcal{E} \in$ ***LOCC*** *realizing the evolution* $|\phi\rangle\langle\phi| = \mathcal{E}(|\psi\rangle\langle\psi|)$ *if and only if one has the majorization* $\lambda(|\phi\rangle\langle\phi|) \succ \lambda(|\psi\rangle\langle\psi|)$, *where*

$$\lambda : \mathcal{H}_1 \otimes \mathcal{H}_2 \longrightarrow [0, 1]^{dim(\mathcal{H}_1)}, |\psi\rangle\langle\psi| \longmapsto \vec{\sigma}(\mathrm{Tr}_2\, |\psi\rangle\langle\psi|),$$

is a function that maps pure bipartite states to the vectorized spectrum[27] *of their reduced density operator on system* 1.

In other words, the partial order induced by the existence of an LOCC operation converting a state to another coincides, on the subspace of pure bipartite states, with the majorization partial preorder on vectorized spectra of partial states. Returning to Claim 14, it is now manifest why d-level Bell states $|\psi\rangle = d^{-1/2} \sum_{i=0}^{d-1} |ii\rangle$, $d \geqslant 2$, are said to be maximally entangled. The corresponding reduced state

27 The vectorized spectrum is simply the representation of the spectrum as a vector, where degenerate eigenvalues are repeated.

reads $\rho_1 = d^{-1} \sum_{i=0}^{d-1} |i\rangle\langle i|$, and its associated λ is the uniform probability vector, which is majorized by all other probability vectors. As a consequence, Nielsen's theorem implies that any bipartite pure state can be constructed from Bell states $|\psi\rangle$ using LOCC operations.

While we shall not make use of it in the work presented in the rest of this thesis, it is worth mentioning that there is a unique measure of pure bipartite state entanglement [95] satisfying[28] $\mu(|\phi^+\rangle) = 1$ and extensivity $\forall k \in \mathbb{N}^*,\ \mu(|\phi\rangle^{\otimes k}) = k\mu(|\phi\rangle)$, which is the Von Neumann entropy of the state $S(\rho) = -\operatorname{Tr}\big[\rho \log_2(\rho)\big]$. This is proven using the fact that there exists an asymptotic LOCC interconversion rate between any bipartite state $|\psi\rangle$ and the Bell pair $|\phi^+\rangle$ [96]. That is, one can reversibly transform the state $|\psi\rangle^{\otimes n}$ to $|\phi^+\rangle^{\otimes nS(\rho_1)}$ for $n \to +\infty$ using LOCC operations, where $S(\rho_1)$ is the Von-Neumann entropy of the reduced state $\operatorname{Tr}_2(|\psi\rangle\langle\psi|)$.

Thus far, we have managed to properly characterize and define a measure for entanglement, by having restricted our analysis to pure states. As announced previously, generalizing our results to mixed states is not a simple matter. Yet, since physical experiments take place in laboratories, not in Hilbert spaces, one never deals with rigorously pure states, and it is therefore of critical importance to extend our criteria and measures of entanglement to mixed states. Before we embark on the quest for general entanglement measures and criteria, let us start with a simple example that serves to show how one should exercise caution when relinquishing state purity. Let us consider two Bell states[29] $|\phi_+\rangle\langle\phi_+|$ and $|\phi_-\rangle\langle\phi_-|$. With a simple coin toss, one can construct the mixed bipartite state

$$\rho_{12} = \frac{1}{2}(|\phi_+\rangle\langle\phi_+| + |\phi_-\rangle\langle\phi_-|).$$

We notice that in the computational basis, this state takes the form

$$\begin{aligned}\rho_{12} &= \frac{1}{4}[(|00\rangle + |11\rangle)(\langle 00| + \langle 11|) + (|00\rangle - |11\rangle)(\langle 00| - \langle 11|)] \\ &= \frac{1}{2}(|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|),\end{aligned}$$

so ρ_{12} turns out to be a separable state that merely exhibits classical correlations! By writing the state in two unitarily equivalent ensemble decompositions, we can view it as the mixing between two states that are maximally costly in resource, but at the same time, the resulting state is clearly a free state. In other words, the way entanglement behaves through state mixing is all but straightforward. So much so, that determining whether two systems are entangled in the most general setting has been shown to be a full-blown NP-hard problem [97]. Fortunately, topological properties will happen to help design sufficient conditions for entanglement, as we shall see in the following

28 We remind a common notation for one of the Bell states $|\phi^+\rangle = 2^{-1/2}(|00\rangle + |11\rangle)$.
29 We use the common notation $|\phi^-\rangle = 2^{-1/2}(|00\rangle - |11\rangle)$.

section where we delve deeper into the theory of mixed state entanglement.

2.4.4 *Entanglement theory of mixed states*

There are essentially two approaches to dealing with the presence of entanglement in mixed state, with their own strengths and weaknesses. The first one that we shall now introduce, is called entanglement witnessing, and consists in giving a sufficient condition for the state to be entangled. The second, less practical but more reliable one, is to build a measure of entanglement.

Entanglement witnessing relies on the fact that entanglement is convex resource theory.

Claim 15. *The set $\mathcal{D}_{sep}$ of separable states is convex.*

Proof. Recall that $\mathcal{D}_{\text{sep}} = \{\sum_{k=1}^{n} p_k \sigma_k \otimes \mu_k\}$, for some $n \in \overline{\mathbb{N}^*}$ where (p_k) is a discrete probability distribution and $(\sigma_k), (\mu_k)$ are sequences of local states. Consider $\lambda \in [0,1]$ and $\rho_1, \rho_2 \in \mathcal{D}_{\text{sep}}$, then there exists $n, m \in \mathbb{N}^*$ and two probability distributions p, q and pairs of sequences of local states $(\sigma), (\pi)$ and $(\mu), (\tau)$ such that

$$\rho_3 := \lambda\rho_1 + (1-\lambda)\rho_2 = \lambda \sum_{k=1}^{n} p_k \sigma_k \otimes \mu_k + (1-\lambda) \sum_{l=1}^{m} q_l \pi_l \otimes \tau_l.$$

By constructing the triplet of sequences, of coefficients and local states $((r_i), (\alpha_i), (\beta_i)) \in ([0,1] \times \mathcal{B}_1(\mathcal{H}_1) \times \mathcal{B}_1(\mathcal{H}_2))^{n+m}$ satisfying

$$(r_i, \alpha_i, \beta_i) := \begin{cases} (\lambda p_i, \sigma_i, \mu_i) & \text{if} \quad 1 \leqslant i \leqslant n \\ ((1-\lambda) q_i, \pi_i, \tau_i) & \text{if} \quad n+1 \leqslant i \leqslant n+m \end{cases},$$

we see that the convex sum takes the form $\rho_3 = \sum_i r_i \alpha_i \otimes \beta_i$ where (r_i) is a probability distribution and $(\alpha_i), (\beta_i)$ are local states, thus $\rho_3 \in \mathcal{D}_{\text{sep}}$. □

This topological property, which on its own does not seem to simplify the task at hand, in fact allows to use the geometric Hahn-Banach theorem, also known as Mazur's theorem.

Theorem 14 (Geometric Hahn-Banach theorem). *In any Banach space E with a non-empty closed convex subspace $\mathcal{C} \subset E$, if an element $x \in E$ is not in $\mathcal{C}$ then there exists a hyperplane $\mathfrak{H}$ that separates x from $\mathcal{C}$, in the sense that any continuous function taking value x and taking a value in $\mathcal{C}$ must also take a value in $\mathfrak{H}$.*

A formal proof of this theorem may be arrived at from elementary functional analysis [98]. In the case of interest to us, since $\mathcal{D}_{\text{sep}}$ is a closed convex subspace of the Banach space $\mathcal{BH}(\mathcal{H})$ of bounded self-adjoint operators acting on the Hilbert space $\mathcal{H}$, according to Th. 14,

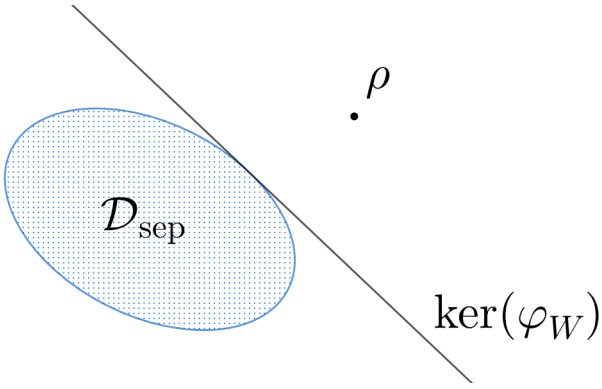


Figure 4: An illustration of the Hahn-Banach separation theorem applied to the resource theory of entanglement.

for any entangled state ρ there must exist a hyperplane $\mathfrak{H} \subset \mathcal{BH}(\mathcal{H})$ separating ρ from $\mathcal{D}_{\text{sep}}$, as illustrated in Fig. 4. Since in the Banach space $\mathcal{BH}(\mathcal{H})$, any hyperplane can be expressed as the kernel of a linear form, and that inner-products $\varphi_y : x \longmapsto \langle y|x\rangle$ with hermitian parameter y span the dual Banach space $(\mathcal{BH}(\mathcal{H}))^*$, one can always find an element $W \in \mathcal{BH}(\mathcal{H})$ such that $\mathfrak{H} = \ker(\varphi_W)$. By choosing the sign of W accordingly, this leads to the important definition.

Definition 39 (Entanglement witnesses). *For any given entangled state $\rho \in \mathcal{B}_1(\mathcal{H})$, any hermitian operator W satisfying both $\mathrm{Tr}(W\rho) < 0$ and $\forall \sigma \in \mathcal{D}_{sep}$, $\mathrm{Tr}(W\sigma) \geqslant 0$, is called an entanglement witness for the state ρ.*

The practical advantage of entanglement witnesses is quite straightforward: one only needs to evaluate the expectation value of one observable W in order to infer the entanglement of ρ. As we have said however, entanglement witnesses cannot detect all entangled states. The negativity of their expectation value constitutes only a sufficient condition for the entanglement of a state. Furthermore, the amplitude of this expected value's negativity does not provide any information about the degree of entanglement of a state.

We will shortly come to the construction of quantities that allow to make quantitative statements about entanglement, however at this stage, we have only shown the existence of entanglement witnesses and have yet to propose a practical construction. While the construction of witnesses is not always a simple matter, the following theorem, sometimes referred to as the Positive Partial Transpose (PPT) criterion, by Peres and Horodecki [99], often comes handy, and will in fact help pave the way to measuring entanglement beyond witnesses.

Theorem 15 (Peres-Horodecki criterion). *The partial transpose ρ^Γ of a separable state ρ is positive.*

Proof. Consider a separable state $\rho_{12} = \sum_{k=1}^{n} p_k \sigma_k \otimes \mu_k$ for some $n \in \overline{\mathbb{N}^*}$ and some sequence of local states (σ_k) and (μ_k). Taking the partial transpose on the space $\mathcal{H}_2$ one has $\rho_{12}^{\Gamma_2} = \sum_{k=1}^{n} p_k \sigma_k \otimes \mu_k^T$.

Because μ_k^T is a hermitian, positive semi-definite, unit trace operator, it is also a valid state. $\rho_{12}^{\Gamma_2}$ is thus a valid state and must therefore have non-negative eigenvalues. □

The set of PPT states is denoted $\mathcal{D}_{\text{PPT}}$. What the PPT criterion states, is that we have the inclusion $\mathcal{D}_{\text{sep}} \subset \mathcal{D}_{\text{PPT}}$. The contrapositive yields a very approachable sufficient condition for entanglement: if the partial transpose of a state has a negative eigenvalue, then it must be entangled! It was shown that for a system of two qubits, or of a qubit and a qutrit, the PPT criterion is a necessary and sufficient condition for entanglement. For pairs of systems with more levels, such as a pair of qutrits, there exist entangled states the partial transpose of which do not have negative eigenvalues, a phenomenon called bound entanglement [100].

While the PPT criterion gives a handy entanglement condition on the paper, what can we say of its experimental implementation to test mixed state entanglement in the laboratory? Partially transposing a state cannot be physically done, as it is not a completely positive map. To give an experimentally fitting condition, it would be desirable to relate the PPT criterion to entanglement witnessing.

Claim 16. *If ρ is an entangled state, then the projector $|\chi_-\rangle\langle\chi_-|^{\Gamma_2}$ on an eigenvector of ρ^{Γ_2} associated with a negative eigenvalue, is an entanglement witness for ρ.*

Proof. Consider an entangled state ρ. Its partial transpose admits a negative eigenvalue, according to the PPT criterion, associated to an eigenstate $|\chi_-\rangle$. The projector onto this eigenvector constitutes an observable which has a negative expectation value on the partial transpose $\text{Tr}\big(|\chi_-\rangle\langle\chi_-|\,\rho^{\Gamma_2}\big) < 0$. Because the trace is invariant under partial transposition, we arrive at $\text{Tr}\left(|\chi_-\rangle\langle\chi_-|^{\Gamma_2}\,\rho\right) < 0$. Furthermore, for any separable state σ, the positivity of its partial transpose gives $\text{Tr}\big(|\chi_-\rangle\langle\chi_-|\,\sigma^{\Gamma_2}\big) \geqslant 0$ thus $\text{Tr}\left(|\chi_-\rangle\langle\chi_-|^{\Gamma_2}\,\sigma\right) \geqslant 0$. □

This construction of an entanglement witness, based on the PPT criterion, will turn out to be useful in a future chapter where we shall present an investigation on the entangling capacity of the gravitational interaction.

We close this short overview of mixed state entanglement with the notion of entanglement monotone. Referring to our previous definition of a general resource measure Def. 36, an entanglement monotone is typically defined in the following way.

Definition 40 (Entanglement monotones and measures). *An entanglement monotone is a real valued function μ defined on the quantum state space $\mathcal{D}$ satisfying the following three conditions:*

1. *μ is positive: $\forall \rho \in \mathcal{D},\ \mu(\rho) \geqslant 0$.*

2. *μ is vanishing on the separable set: $\forall \sigma \in \mathcal{D}_{sep},\ \mu(\sigma) = 0$.*

3. μ *is monotonically decreasing on average under LOCC:*

$$\forall \rho \in \mathcal{D},\ \mu(\rho) \geqslant \sum_i p_i \mu\left(\frac{A_i \rho A_i^\dagger}{p_i}\right),$$

where $\{A_i\}$ *are the Kraus operators associated to an LOCC channel, and* $p_i = \mathrm{Tr}\left(A_i \rho A_i^\dagger\right)$.

If furthermore, the entanglement monotone coincides with the Von Neumann entropy on the set of pure states, and that it is monotonically decreasing under deterministic LOCC, then it is called an entanglement measure.

In some instances, additional properties are embedded into the definition, such as convexity and extensivity. While there exists a large zoo of entanglement measures and monotones [101], it will be sufficient in the context of this thesis to define a particular function which is in the natural continuation of our presentation around the PPT criterion, called negativity.

Definition 41 (Negativity). *The quantity* $\mathcal{N}(\rho) = \frac{1}{2}(\left\|\rho^{\Gamma_2}\right\|_1 - 1)$ *defined for all quantum states* ρ*, is called negativity.*

State negativity has been proven to constitute an entanglement monotone. Because it is quite involved, the interested reader is invited to consult Ref. [102] for a detailed proof. The somewhat obscure definition of negativity, involving the trace norm of a partial transpose, hides a much more workable formulation, as we shall see now.

Claim 17. *The negativity* $\mathcal{N}(\rho)$ *of a state* ρ *is the absolute sum of the negative eigenvalues of its partial transpose* ρ^{Γ_2}.

Proof. The spectral decomposition of the partially transposed state can be written as $\rho^{\Gamma_2} = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$, where $\sum_i \lambda_i = 1$ by invariance of the trace under partial transposition. One can now express the negativity as $\mathcal{N}(\rho) = \frac{1}{2}(\sum_i |\lambda_i| - 1) = \frac{1}{2}\sum_i |\lambda_i| - \lambda_i$ and one recognizes the negative part function. □

As an entanglement monotone, compared to entanglement witnessing, the state negativity provides a much finer picture of the entanglement of a given state. Experimentally however, evaluating the negativity of a state requires to reconstruct it via state tomography, which is a much more costly procedure than the measurement of an entanglement witness. We will have the opportunity to discuss entanglement estimation and the value of tomography in Sec. 5.2.

Part II

EPISODES

3 REALISM AND CLASSICALITY

Reality exists in the human mind, and nowhere else.

— **George Orwell** [103]

One of the hallmarks of quantum theory is the existence of coherent superposition of states. States which have coherence [94, 104] are an important resource in applied physics, notably for the development of quantum information and its applications [1], such as metrology [105–107] or computation [108–112]. Despite their attractive operational properties, quantum superpositions, which are absent from classical physics, have long been at the core of fundamental issues, famously illustrated by Schrödinger's cat gedankenexperiment [113]. Making sense of the disconnect between quantum microscopic and classical macroscopic regimes has resulted in the development of different models for and interpretations of open-system quantum dynamics [114–118]. To clarify the distinction between classical macroscopic regimes and quantum microscopic regimes, the Leggett-Garg Inequalities (LGIs) were devised as a test of macroscopic-realistic theories, generally regarded as a suitable class of description of classical dynamics. In spite of this, it is unclear whether their violation is related to non-classicality.

In this chapter, we begin with a short review of LGIs from the foundations of physics perspective. We then demonstrate that the Leggett-Garg inequalities may not hold for the most classical states of light in the quantum optical sense. After introducing a simple Mach-Zehnder setup and showing how to obtain a violation with a single photon using negative measurements, we focus on classical states of light. By using an appropriate assignment of variables, we show how one is still able to perform negative measurements, and obtain a meaningful violation in the presence of coherent states. Finally, we abandon initial phase reference and demonstrate that the violation is still possible, in particular with thermal states of light, and we investigate the effect of intermediate dephasing.

3.1 REALISM AND THE LEGGETT-GARG INEQUALITIES

In this section, we present the LGIs through a simple derivation, which relies on three fundamental assumptions, which together constitute the macroscopic realism hypothesis. We also introduce a powerful framework to clarify, from a fundamental point of view, what is really tested by the LGIs. In doing so, we will touch upon some important nuances of macroscopic realism.

3.1.1 *The Leggett-Garg inequalities*

Similar to Bell's inequalities, which are based on correlations between spatially separated systems and are a necessary condition for local realism [24], the LGIs test the validity of classical descriptions through the correlations between successive measurements in time of a single system [119]. The LGIs are a consequence of macroscopic realism. As we shall see in Sec. 3.1.3, since the LGIs were first proposed, several subtleties regarding what is meant by macroscopic realism and the precise significance of an LGI violation have been clarified [120–122].

As we have seen in Sec. 2.4.3, Bell's inequalities were established as a necessary condition for local realism, a philosophical position that can be resumed in the conjunction of the following three assumptions:

1. **(A1) Realism**. This first assumption signifies that physical systems contain the information of the probability distribution of outcomes of any measurements performed upon them. As a consequence, this stance takes measurements to simply reveal pre-existing physical values.

2. **(A2) Locality**. This second assumption is the postulate that event A may only influence event B if B is in the light cone of A.

3. **(A3) Induction**. This third assumption presumes that an event A cannot be influenced by future events.

Assumptions **(A2)** and **(A3)** are sometimes joint into what is called local-causality. In a similar fashion, the LGIs are a necessary condition for Macroscopic Realism (MR), which is often defined as the conjunction of **(A3)** along with the two following assumptions:

1. **(B1) Macroscopic Realism *per se* (MRps)**. This assumption states that any macroscopic system having access to a set of distinct macroscopic states must always be in one of those states at any given time. This is quite an intuitive assumption, and a famous example of its failure is illustrated by Schrödinger's cat thought experiment.

2. **(B2) Noninvansive Measurability (NIM)**. This assumption posits that the macroscopic state of a system can be measured while inducing an arbitrarily little perturbation on that state.

In order to show how the LGIs must hold in any framework where MR is assumed to be true, Leggett and Garg, in the same fashion as Bell, invite us to consider a physical system which has a physical property P_Q, the measurement of which has two possible outcomes $Q \in \{-1, +1\}$. Let us suppose that this property is measured at three instants $t_1 < t_2 < t_3$. The measurement outcomes can be respectively

Q_1Q_2	Q_2Q_3	$-Q_1Q_3$	Q_{LG}
$+$	$+$	$-$	1
$+$	$-$	$+$	1
$-$	$+$	$+$	1
$-$	$-$	$-$	-3

Table 2: All possible situations for charges in $\{-1, +1\}$.

denoted Q_i, $i \in \{1, 2, 3\}$. By repeating the preparation process, one can prepare multiple copies of the initial system, and label those initial systems with the letter $r \in \mathbb{N}^*$. The outcome of the measurement at time t_i for system number r can be written as $Q_r(t_i)$. For any given copy of the system (or trial) let us define the following function

$$Q_{LG} = Q_1Q_2 + Q_2Q_3 - Q_1Q_3. \tag{32}$$

All the possible measurement outcomes are recapitulated in Tab. 2. We notice that the Q_{LG} function is less than or equal to 1 in all cases. If we suppose that for each system, all of the three measurements were effectively carried out, then one can build up the average values for each term in Eq. (32), and it follows that

$$\langle Q_{LG}\rangle_{1,2,3} = \langle Q_1Q_2\rangle_{1,2,3} + \langle Q_2Q_3\rangle_{1,2,3} - \langle Q_1Q_3\rangle_{1,2,3} \leqslant 1. \tag{33}$$

The indices under the expectation value brackets indicate that we are taking the statistical average over r when all of the three measurements in time are carried out on each system, and the inequality naturally follows from $Q_{LG} \leqslant 1$ for each trial.

Inequality (33), which also has a lower bound of -3 that shall not be of use to us, may seem to be a strong statement, and deceitfully looks like an LGI, yet as noted in [123, 124], neither realism nor non-invasive measurability were necessary in our derivation. To be more specific, whether the charge values Q_i were measurement outcome values or intrinsic values prior to measurement, Q_{LG} is always well defined and the inequality will hold. However the significance of the inequality is not the same in those two interpretations of the charge values. Indeed, if the Q_i merely designate measurement outcome values, the inequality is so weak that it will hold in any general theory, classical or quantum, in which there are joint probability distributions of repeated measurement outcomes.

This being said, let us suppose that assumptions **(B1)** and **(B2)** hold. Then in this macro-realistic view in which Q_i are the intrinsic values that the measurements merely reveal, the two first measurements (should they be performed or not) do not affect the result of the final measurement (as under NIM the intrinsic value of Q prior to the fi-

nal measurement is unaffected). In this case, we have the following equalities

$$\langle Q_1 Q_3 \rangle_{1,2,3} = \langle Q_1 Q_3 \rangle_{1,3} \quad \text{and} \quad \langle Q_2 Q_3 \rangle_{1,2,3} = \langle Q_2 Q_3 \rangle_{2,3} \,. \tag{34}$$

Finally, under the induction hypothesis, a system is not influenced by the future measurements it may be subjected to, which translates to

$$\langle Q_1 Q_2 \rangle_{1,2,3} = \langle Q_1 Q_2 \rangle_{1,2} \,. \tag{35}$$

Consequently, the weak inequality Eq. (33) takes the following form under the MR assumption

$$\langle Q_1 Q_2 \rangle_{1,2} + \langle Q_2 Q_3 \rangle_{2,3} - \langle Q_1 Q_3 \rangle_{1,3} \leqslant 1. \tag{36}$$

For legibility we will rewrite this LGI with correlation coefficients as

$$K = C_{12} + C_{23} - C_{13} \leqslant 1.$$

Let us bring up some important aspects of this deceptively simple inequality and its derivation.

Though the LGI may look very much like inequality Eq. (33), the statement of Eq. (36) is much more sophisticated and is not as trivial as it looks. In particular, whereas the weak inequality Eq. (33) only involves a single experimental setup, where Q is measured three times, the LGI gives constrains expectation values that are obtained via three completely distinct experimental configurations, in each of which Q is only measured twice per trial. As far as the assumptions go, let us mention that macroscopicity is in fact not a direct requirement for the derivation of the LGI [125]. The reason macroscopicity comes into play is that otherwise noninvasive measurability cannot hold, as it would contradict quantum mechanical rules. Finally, it is worth noting that Q_i was assumed to take values in $\{-1, +1\}$, however this assumption can be relaxed. The LGIs can be derived without dichotomic charges, they can in fact take values in a continuous set. It is only required that $\forall i$, $|Q_i| \leqslant 1$ as shown in Ref. [124].

This simple version and its derivation will suffice at this stage, but we shall later carry out a more general derivation, as we will need to loosen some assumptions on the observable Q, namely its dichotomic property.

In the same way as the CHSH inequalities, the LGIs have been experimentally violated on a variety of platforms, such as superconducting qubits or atomic quantum walks [89, 126]. However, the conclusive invalidation of macroscopic realism through an LGI violation is more delicate to reach than the invalidation of local realism via a Bell-CHSH violation. In the Bell test, one important loophole to address is the communication loophole, which can be closed using space-like separated measurement events. In the Leggett-Garg test however, successive measurement events carried out on the same system may only

be time-like separated, and as such macroscopic noninvasiveness cannot be guaranteed in the same way. Earlier measurements could very well be noninvasive directly, yet affect some hidden variables that may affect the free evolution of the system until the next measurement, an issue referred to as clumsiness loophole. Progress in recent years have reduced the clumsiness loophole to the much less likely collusion loophole [127]. Clumsiness-loophole free experimental protocols were implemented with superconducting qubits [128] and have shown effective violation of the LGIs.

3.1.2 *The ontic models framework*

As previously defined, MRps seems to be a straightforward and unambiguous statement: macroscopic systems must at all times be in one of their accessible macroscopically distinct states. While the notion of macroscopicity itself is not clear-cut, one may more importantly question the meaning of "state" the realism of which is being referred to, as this is framework dependent. In the original formulation by Leggett and Garg, the framework is quantum theory, hence macroscopic realistic states are taken to be incoherent. In other words, the realistic stance as formulated by Leggett and Garg amounts to postulating that some states in the Hilbert space are not allowed by some sort of superselection rule, namely those which would be superpositions of macroscopic states. The relationship between negating superpositions and realism is however not as simple. Let us summarize an interesting investigation from Ref. [123].

The first objection one can make, is that there is nothing realistic about forbidding (macroscopic or non-macroscopic) superpositions. Realism simply requires that quantum theory be taken as representing (mind-independent) facts about the physical world. Denying superpositions does not imply the endorsement of realism, as one can claim that quantum theory with a superselection rule preventing superpositions merely describes measurement outcomes, that is, one can have an instrumentalist interpretation of a theory in which superpositions are forbidden.

As such, denying superpositions is not a sufficient condition to have a realist stance. It turns out that it is not a necessary condition either, for superpositions in the quantum state do not necessarily lead to indefiniteness of physical variables in the de Broglie-Bohm pilot wave theory [129]. The pilot-wave model describes how the wavefunction of a system (up to and including the entire universe) always evolves unitarily, but also specifies the precise position of particles at any given time. All particles also have well-defined momenta at all times, and hence move along smooth deterministic trajectories. These momenta are determined by taking the gradient of the phase of the manybody wavefunction; to put it informally, particles are pushed

around directly by the wavefunction. Based on the hypothesis (which may be assumed or derived) that the probability distribution over initial configurations is determined by the Born rule, the pilot-wave theory is a deterministic hidden variable theory (the hidden variables being configurations of the physical degrees of freedom, for instance, particle positions). In this model, measurement results are uniquely determined by the initial configuration of the total system, the initial wavefunction, and the interaction Hamiltonian between the measuring device and the system being measured. In this framework, physical quantities for a system can take on definite values even when their wavefunctions are in superposition states.

Another stance which may fall under quantum mechanical realism, and most likely corresponds to what Leggett and Garg had in mind, is one in which the wavefunction is taken to be a physical object the collapse of which is a genuine physical process. This class of models, such as the Diosi-Penrose model [130–132], or the Ghirardi–Rimini–Weber theory [33], postulate the existence of additional terms modifying the Schrödinger equation that must be stochastic in order to avoid faster than light signalling [84], so that wavefunctions sponatenously collapse. In the original argument by Leggett and Garg, the realistically forbidden states would be superpositions of two classical Superconducting Quantum Interference Device (SQUID) states. Since the distinct classical states of a SQUID spatially overlap, spontaneous collapse theories which rely on spatial localisation would not rule out LGI violations [133, 134].

In short, the pilot-wave theory, which is compatible with MR as previously cast, would predict LGI violations whenever standard quantum theory does, and in the original setting of Leggett and Garg, spontaneous collapse models would not rule out LGI violations. In light of those observations, it is unclear whether the LGI violation allows to invalidate a class of realist interpretations. The relationship between LGIs and MR deserves more caution, and in order to clarify our statements we will shortly introduce the ontic models framework [135].

Before presenting this framework, it is useful to frame the LGI setup in the language of operationalism. Any experimental process can be divided into a preparation P, an evolution E and a measurement M operation with outcomes $Q = q_i$, and the whole experiment is operationally defined by the conditional probability distribution $\mathbb{P}(Q|P, E, M)$. Whenever two preparations or two transformations yield the same probability distribution, they are said to be operationally equivalent. Measurement procedures are operationally equivalent when there is a bijection between their set of outcomes, and that they have the same probability distribution.

In the setup considered to derive Eq. (33), we have considered the preparation P of an initial state, and three measurement processes

$M_{1,2,3}$ with two intermediate evolutions E_1, E_2. The entire experimental procedure thus may be described by the joint probability distribution $\mathbb{P}(Q_1, Q_2, Q_3|P, M_1, E_1, M_2, E_2, M_3)$, from which one can extract any marginal and correlation. Let us note that marginalizing over one variable *does not* change the conditions, that is, for instance

$$\langle Q_1 Q_3 \rangle_{M_1 M_2 M_3} = \sum_{q_i, q_j} q_i q_j \mathbb{P}(Q_1 = q_i, Q_3 = q_j|P, M_1, E_1, M_2, E_2, M_3) \neq \langle Q_1 Q_3 \rangle_{M_1 M_3} .$$

As shown previously, the LGIs follow from the much more constraining conditions which relate joint probability distributions in processes where only two measurements are carried out, to marginal distributions for pairs of outcomes when all measurements are performed. Explicitly (and omitting the preparation and evolutions for legibility), the two conditions Eq. (34), can be written as

$$\begin{cases} \mathbb{P}(Q_2, Q_3|M_2, M_3) &= \sum_{Q_1} \mathbb{P}(Q_1, Q_2, Q_3|M_1, M_2, M_3) \\ \mathbb{P}(Q_1, Q_3|M_1, M_3) &= \sum_{Q_2} \mathbb{P}(Q_1, Q_2, Q_3|M_1, M_2, M_3) \end{cases} ,$$

and together represent a hypothesis that is referred to as Operational Nondisturbance (OpND). The third condition Eq. (35) is simply time ordering $\mathbb{P}(Q_1, Q_2|M_1, M_2) = \sum_{Q_3} \mathbb{P}(Q_1, Q_2, Q_3|M_1, M_2, M_3)$.

In the previous section, we had simply assimilated OpND to NIM, and as we see, the LGI violation can be viewed as a simple violation of OpND. What requires more caution however, is the relationship between MR and OpND, as OpND may come in different flavours. A measurement M might be OpND for all posterior measurement given a specific preparation P, or be OpND for a given posterior measurement for any preparation P, in which case we have specific OpND, denoted $\text{OpND}_{\text{specific}}$. In the strongest case, a measurement can be OpND for all posterior measurements regardless of preparation P, and is then said to satisfy complete OpND, denoted $\text{OpND}_{\text{complete}}$.

Let us now finally introduce the ontic models framework [135]. It is a framework in which the system of interest is associated with an ontic state $\lambda \in \Lambda$ representing some ontological, intrinsic property, independent of measurements. In the case of classical Hamiltonian mechanics, this ontic state for a single particle is a point in phase space. In ψ-ontic interpretations of quantum mechanics, this ontic state is taken to be the wavefunction itself.

The preparation P of a system is represented by a probability distribution μ_P on the ontic state space. Evolutions are stochastic maps $\tau_E(\lambda|\lambda_0)$ of the ontic state space, giving the conditional probability distribution to be in ontic state λ given an original ontic state λ_0. The sequential composition of a preparation and an evolution gives another valid preparation $\mu_{E \circ P}(\lambda) = \int_\Lambda d\lambda' \mu_P(\lambda')\tau_E(\lambda|\lambda')$. Measurements M are described by a *response function* $\xi_M(Q|\lambda)$, giving the

probability of having outcome Q given the ontic state λ. One may complement the description of a measurement to account for its ontic disturbance, by associating to it an evolution map $\tau_M(\lambda|Q, \lambda_0)$. Two operationally equivalent measurements may not have equal response functions, or equal ontic disturbance maps, a situation termed *measurement contextuality*.

With this framework at hand, it becomes evident that there are two ways to understand NIM. In its weaker version, NIM can be viewed as OpND. In the stronger version, NIM corresponds to Ontic Noninvasiveness (ONI). A measurement M of the physical property Q is ontically noninvasive for outcome q_i when its associated evolution map satisfies $\tau_M(\lambda|Q = q_i, \lambda_0) = \delta(\lambda - \lambda_0)$. If M is ONI then regardless of the preparation procedure P, any measurements posterior to M will have the same statistics whether or not M was carried out. Hence ontic nondisturbance is stronger than the strongest form of OpND. In short, we have the chain of implications

$$\text{ONI} \implies \text{OpND}_{\text{complete}} \implies \text{OpND}_{\text{specific}} \implies \text{LGI}.$$

At this stage we have still not invoked any notion of MR. The point of Leggett and Garg's argument, is that combining MR with negative measurements yields the strong ONI condition. In order to investigate this more specifically, one first needs to have a proper definition of MR.

In the ontic models framework, if M is the macroscopic measurement of the physical property Q of a system in ontic state λ, then MR is simply the requirement that the response function for any such measurements $\xi_M(Q|\lambda)$ takes values in $\{0, 1\}$, and coincides for operationally equivalent macroscopic measurements (i.e. the physical presence of the moon does not depend on how we look at it). In turn, this means that the physical property Q is non-contextually value definite. While this looks at odds with the Kochen-Specker theorem [136], MR does not require the definiteness of all the system's properties, but only of its macroscopic ones.

We shall say that an ontic state is macroscopically definite when all observable macroscopic properties are non-contextually value definite, and two ontic states of such system are macroscopically distinct when there exists at least one macroscopic property on which the two ontic states have zero overlap. We are now ready to define different flavours of MR and show which one in particular the LGI violation may rule out.

3.1.3 *Classes of macroscopic realism*

As stated previously, MR regarding a macroscopic physical property Q is a stance in which all ontic states are supposed to be macroscopically definite for Q. Let us consider the sequence of processes

(P, M_1, E_2, M_2) consisting of a preparation, a measurement of Q, an evolution, and a second measurement of Q. Suppose that it is well established that M_1 is OpND for preparations giving rise to definite values of Q. Then the macroscopic realist would expect identical measurement statistics for M_2 in the sequence (P, E_2, M_2).

Should there be a discrepancy, then it would seem like MR must be false. Indeed, the existence of ontic states which are not macroscopically definite for Q, can explain why M_1 could be disturbing even if it is OpND for preparations giving definite values of Q. Yet, with closer inspection, not all versions of MR can be ruled out, as we shall now discuss.

To present the three versions of MR, it is useful to introduce the notion of operational eigenstate. Given an equivalence class of measurements $\tilde{M}$ for the corresponding physical quantity $\tilde{Q}$, an operational eigenstate of $\tilde{Q}$ is the equivalence class of preparations $\tilde{P}$ giving the same point-like (i.e. Dirac delta for an uncountably infinite number of outcomes, and Kronecker delta otherwise) probability distribution over the set of measurement outcomes. Specifically, if a system is prepared in the q operational eigenstate of $\tilde{Q}$, then all measurements $M \in \tilde{M}$ will have outcome probability distribution $\mathbb{P}(\tilde{Q} = q') = \delta_{q,q'}$. If we denote the q_i operational eigenstate equivalence class as $\tilde{P}_{q_i} = \{P_{q_i} | \, \forall M \in \tilde{M}, \, \mathbb{P}(Q = q | P_{q_i}, M) = \delta_{q,q_i}\}$, and define $\mu_{P_{q_i}}$ as the probability distribution that P_{q_i} gives rise to, then for all ontic state $\lambda \in \Lambda$, for any measurement $M \in \tilde{M}$, and any q_i operational eigenstate preparation $P_{q_i} \in \tilde{P}_{q_i}$ we have the characterization $\lambda \in \text{supp}(\mu_{P_{q_i}}) \iff \xi_M(Q = q|\lambda) = \delta_{q,q_i}$.

The most general version of MR, called Supra Eigenstate Support Macroscopic Realism (SESMR), regarding the property Q, simply postulates that all ontic states are macroscopically definite for Q, and that all preparations can be written as convex mixtures of distributions σ_{q_i} over the ontic state space, explicitly $\mu(\lambda) = \sum_{q_i} \alpha_{q_i} \sigma_{q_i}(\lambda)$, which satisfy the condition $\lambda \in \text{supp}(\sigma_{q_i}) \implies \xi_M(Q = q|\lambda) = \delta_{q,q_i}$. SESMR does not imply LGI, as verifying that M_1 is OpND for all operational eigenstate preparations, does not mean that it cannot be disturbing for other macroscopically definite ontic states. That is, there are ontic states $\lambda \in \Lambda$ which do not belong to $\cup_{q_i} \text{supp}(\mu_{P_{q_i}})$.

One can define a more constrained version of MR, which is termed Operational Eigenstate Support Macroscopic Realism (OESMR). This view assumes SESMR, but further posits that there are no ontic states that cannot be accessed by an operational eigenstate preparation. That is, $\Lambda \subset \cup_{q_i} \text{supp}(\mu_{P_{q_i}})$. While more constraining, OESMR still does not imply LGI. Even if M_1 is OpND for all operational eigenstate preparations, some unavoidable evolutions occurring after an operational eigenstate preparation may give rise to a valid ontic space distribution $\mu_{E \circ P_{q_i}}(\lambda)$ which cannot be expressed as some mixture of operational eigenstate preparations. As such, the prepared state may

evolve into a new distribution that can be, at least ontically, disturbed by M_1. In other words, the set of possible probability distributions over the ontic state space is larger than the set of convex combinations of operational eigenstate preparations. Within OESMR, LGI violations are allowed, not because there should be an ontic state that is not macroscopically definite, nor because some ontic states cannot be expressed as operational eigenstate preparations (like in SESMR), but rather because some probability distributions over ontic states may not be expressed as convex mixtures of operational eigenstates.

Finally, one can add to OESMR the assumption under which any probability distribution over the state space may be expressed as $\mu(\lambda) = \sum_{q_i} \alpha_i \mu_{q_i}(\lambda)$. This posture is called Operational Eigenstate Mixture Macroscopic Realism (OEMMR). OEMMR for the macroscopic variable $\tilde{Q}$ essentially consists in asserting that all preparations P of a system S can be written as mixtures of operational eigenstates of $\tilde{Q}$.

Macroscopic realists appear to be very naturally inclined to think this way, and it implies that, whatever happens microscopically, macroscopic properties of unobserved systems will behave similarly to those of observed systems. OEMMR implies LGI, as there exist no preparation states which cannot be expressed as mixtures of operational eigenstates, meaning that M_1 can never be operationally disturbing if proven to be OpND for all operational eigenstates.

In light of these nuances of MR, it is apparent that, barring any scenario where the measurements are proven to not be merely OpND but fully ONI, an LGI violation may only rule out the strongest form, OEMMR. To close our short presentation on foundational aspects of the LGI, let us note that in their original argument, Leggett and Garg claimed that MR entails ONI, which implies any form of NIM. Should this be the case, then LGI violations would effectively invalidate MRps. This would put MR (regardless of its flavours, the discussion of which were brought about by different implications of the weaker OpND condition) in jeopardy. Leggett and Garg's argument essentially consists in invoking negative-measurements (e.g. the absence of detection of a particle emerging from a double-slit) and a post-selection, which under MR may be considered as forming an ONI measurement procedure for certain outcomes. However, this consideration cannot be framed in a model independent way. In the eyes of a ψ-ontologist, for instance, negative measurements are as ontically invasive as standard measurements.

3.2 VIOLATING THE LGIS WITH CLASSICAL STATES OF LIGHT

To no surprise, the LGIs have been experimentally violated with microscopic systems such as superconducting qubits and atomic quantum walks [89, 126]. While the LGI violation is considered a relevant witness of quantumness, and finding such violations is still an ac-

tive area of interest [137–141], there exists another well established notion of non-classicality of a state, in quantum optics. A state of light ρ can be represented by a distribution in the complex plane as $\rho = \int P(\alpha) |\alpha\rangle\langle\alpha| \, d^2\alpha$ where $|\alpha\rangle$ are coherent states [77, 78]. The state is said to be classical whenever P is a probability density function on phase space [142], and non-classical otherwise. This criterion is justified by the fact that a coherent state is considered a classical pure state [143], in the sense that it minimizes uncertainty relations and is robust against decoherence [144]. By contrast, a superposition of coherent states $|\alpha\rangle$ and $|\beta\rangle$, is non-classical, and when the displacement parameters α, β differ considerably, we obtain what is termed a Schrödinger cat state [145]. Such a non-classical state, whose P representation is not a probability density function, is a valuable resource for quantum information tasks [146, 147], as indicators of quantum behaviour. However, it turns out that classical states can very well have quantum properties, as we shall show.

In this section, we show that classical states of light can violate LGI inequalities. Violations of the LGI with light have already been established [148–153], although with manifestly non-classical states such as single photons Fock states. Violations based on the polarization degree of freedom of a laser field were more recently shown to be possible [154], but constitute nothing more than a specific implementation of a qubit to violate the LGI. By contrast we shall present a protocol which uses measurements on the coherent state itself to achieve the violation. More importantly, the previously established violations have not determined to what degree phase reference, which plays a central role in the decoherence model explaining the quantum-classical transition [155], governs the possibility of LGI violations. Here, we demonstrate a violation of the LGI with a particularly simple setup in which light is classical at each stage and the measurement itself is not weak [156].

3.2.1 *Setup and single photon quantum random walk*

Before introducing the setup and illustrating an LGI violation, let us briefly show how to establish the LGIs, and introduce useful notations as well as the notion of negative measurement. Following review [124] we present a brief derivation of the LGIs.

Using the ontic models framework [135], let us suppose that the system under study is prepared in the ontic state λ with a probability density $\mu(\lambda)$. A measurement that is performed at instant t_i results in the outcome function $\xi_i(Q_i|\lambda)$ which gives the probability of obtaining the value Q_i given the ontic state λ. Induction guarantees that preparing a measurement setup does not influence the initial ontic state distribution $\mu(\lambda)$. Then $\mathbb{P}(Q_i) = \int d\lambda \xi_i(Q_i|\lambda)$. Assuming NIM, the joint probability distribution for the two measure-

ments reads $\mathbb{P}_{ij}(Q_i, Q_j) = \int d\lambda \xi_j(Q_j|\lambda)\xi_i(Q_i|\lambda)\mu(\lambda)$. Let us now restrict to $(Q_i, Q_j) \in S_i \times S_j \subset [-1, 1]^2$. S_i and S_j are the sets of values that Q_i and Q_j can respectively take, and those values are real and absolutely less than or equal to unity. Then the correlation coefficient reads $C_{ij} = \langle Q_i Q_j \rangle = \sum_{(Q_i,Q_j)\in S_i\times S_j} Q_i Q_j \mathbb{P}_{ij}(Q_i, Q_j)$. Inserting the joint probability expression into the last equation gives $C_{ij} = \int d\lambda \langle Q_i \rangle_\lambda \langle Q_j \rangle_\lambda \mu(\lambda)$, where the expectation value is explicitly $\langle Q \rangle_\lambda = \sum_{Q\in S} Q\mathbb{P}(Q)$. Thus

$$\begin{aligned} K &= C_{12} + C_{23} - C_{13} \\ &= \int d\lambda \Big(\langle Q_1 \rangle_\lambda \langle Q_2 \rangle_\lambda + \langle Q_2 \rangle_\lambda \langle Q_3 \rangle_\lambda - \langle Q_1 \rangle_\lambda \langle Q_3 \rangle_\lambda \Big) \mu(\lambda). \end{aligned}$$

Therefore, having $S_1 \times S_2 \times S_3 \subset [-1, 1]^3$ yields

$$K = C_{12} + C_{23} - C_{13} \leqslant 1, \tag{37}$$

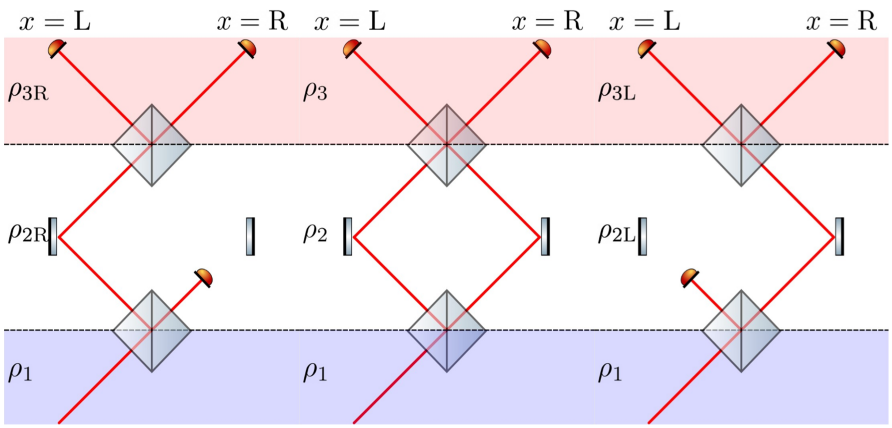
regardless of the cardinality of the sets S_i. In particular, it will be useful in Sec. 3.2.2 to note that if $(S_1, S_2, S_3) = (\{+1\}, \{0, +1\}, \{-1, 0, +1\})$ then the LGI (37) still holds.

Let us now show a simple violation in a Mach-Zehnder interferometer. Mach-Zehnder setups have been considered to test LGIs with dichotomic variables [157], and featured for detailed proposals of LGI violations with single electron transport [158]. We present the three Mach-Zehnder setups, along with the notations and observable definition, and give an example of LGI violation with macroscopic observables and negative measurement in the case of a single photon input state.

We consider three setups as illustrated in figures 5a, 5b and 5c. All in all, the ideal setup consists of two perfect mirrors, two or three photon detectors and two identical 50:50 lossless beam splitters. For our purpose the detectors need not be photon counters, but rather simply detect the presence or absence of photons in the mode. The general beam splitter operator is defined as $B = e^{\frac{\theta}{2}(a_L^\dagger a_R - a_L a_R^\dagger)}$ where $a_L^\dagger$ and $a_R^\dagger$ are bosonic creation operators in the left-hand and right-hand field modes, and we shall fix $\theta = \pi/2$ throughout this study. Using Hadamard's lemma and bosonic commutation relations, the 50:50 beam splitter acts upon photonic modes according to the following rules (see Sec. 2.3.3 for details):

$$\begin{cases} B a_R^\dagger B^\dagger &= \frac{1}{\sqrt{2}}(a_L^\dagger + a_R^\dagger) \\ B a_L^\dagger B^\dagger &= \frac{1}{\sqrt{2}}(a_L^\dagger - a_R^\dagger) \end{cases}. \tag{38}$$

There are two setups for the intermediate measurement, and this is a requirement for ideal negative measurements, also known as interaction-free measurements [159, 160]. Such measurements are important in order to have a meaningful LGI violation, as direct measurements disturb the state and immediately invalidate the NIM hypothesis. The idea of a negative measurement, in the single photon



(a) Detector in the right intermediate mode.

(b) No intermediate detector.

(c) Detector in the left intermediate mode.

Figure 5: Three setups for the two step quantum random walk. The states in each space (input, intermediate, and output) are labelled according to the intermediate detector's position. Photons are detected at the output of the Mach-Zehnder interferometer at two distinct positions $x = \mathrm{L}$ and $x = \mathrm{R}$.

case, is to say that by not observing a photon in one of the two detectors, one can conclude its presence in the other mode without having destroyed it. If an intermediate detector clicks, the trial is discarded, but this case is accounted for when the detector is in the other mode. Of course, even negative measurements do disturb the quantum state, however from a realist's point of view, it is but an update of an agent's knowledge of the state of the system.

Let us note that this measurement method is straightforward only when the beam splitters are lossless and the detectors are ideal (no dark current, and unity quantum efficiency), which we assume in this work. We briefly discuss in the next section why this assumption does not prevent our proposal from being viable.

This being said, let us consider a single photon arriving on the first beam splitter from the left, so $|\psi_1\rangle = |10\rangle$ is the input state. With no intermediate detection, the intermediate state between the two beam splitters is the Bell pair $|\psi_2\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle)$, and the output state is $|\psi_3\rangle = -|01\rangle$. If the intermediate detector is placed on the right hand intermediate mode, then the only state that one can measure negatively is $|\psi_2\rangle_{\mathrm{R}} = |10\rangle$. Similarly, we will denote $|\psi_2\rangle_{\mathrm{L}} = -|01\rangle$ the only negatively measurable state when the detector is placed on the left intermediate mode.

Those are negatively measured states in the sense that one can deduce their form from the absence of a click on the intermediate detector, which is a pivotal point to make in order to even consider NIM. Hence all trials where the intermediate detector clicks have to be discarded. The output states after negative intermediate measurement

are then $|\psi_3\rangle_R = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle)$ and $|\psi_3\rangle_L = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle)$, where the index is a label for the position of the intermediate detector, and is absent if no intermediate measurement is performed.

It should be stressed that discarding trials where the intermediate measurement was not negative (i.e. a detector clicked) does not affect the resulting statistics only if the discarded cases can be picked up in the statistics in the symmetric setup, as illustrated with atomic quantum random walks in [126].

We now define the Q_i values to obtain a violation as follows. We set $Q_1 = +1$ when there is a photon in the left input mode and none in the right input mode. This corresponds to the preparation. We trivially set $Q_2 = +1$ whenever the photon finds itself in either of the intermediate modes. Finally, we set $Q_3 = +1$ when the left output detector clicks, and $Q_3 = -1$ if the right output detector clicks.

Then it is straightforward to establish $\langle Q_3\rangle = -1$ and $\langle Q_3\rangle_{R,L} = 0$. Trivially $C_{12} = +1$, and $C_{13} = \langle Q_3\rangle = -1$. Finally, as $Q_2 = +1$ always holds and trials where the intermediate detector clicks are discarded (i.e. half of the trials for each intermediate detector position), one has $C_{23} = \frac{1}{2}(\langle Q_3\rangle_R + \langle Q_3\rangle_L)$. All in all $K = +2$ which violates (37).

3.2.2 *Violation with coherent states*

We now consider a coherent state impinging on the first beam splitter from the left $|\psi_1\rangle = |\alpha\rangle_L |0\rangle_R = D_L(\alpha) \otimes \mathbb{1}_R |00\rangle$, where we have defined the displacement operator $D(\alpha) = e^{\alpha a^\dagger - \alpha^* a}$. At the output of the first beam splitter, the state of light is $|\psi_2\rangle = \left|\alpha/\sqrt{2}\right\rangle \otimes \left|-\alpha/\sqrt{2}\right\rangle$. Hence, the state at the output of the interferometer with no intermediate measurement is given by $|\psi_3\rangle = |0\rangle \otimes |-\alpha\rangle$. In setups with intermediate measurement where any detected flux results in a discarded experiment, the negatively obtained states at the output are $|\psi_3\rangle_{R,L} = \left|\pm\alpha/\sqrt{2}\right\rangle \otimes \left|\pm\alpha/\sqrt{2}\right\rangle$.

Given the different output states, it may seem at first sight that the LGI violation will immediately follow from what was already shown for the single photon. However, the initial assignment for the observables Q_i that lead to the single photon LGI violation, despite being a good starting point, is problematic. The issue is twofold: the observables as defined previously are no longer well determined, and their values can no longer be negatively measured with a state-selective discarding. Let us explicitly make those points and present a solution.

First, keeping $Q_3 = +1$ when photons impinge on the left detector at the output, and none to the right, and $Q_3 = -1$ when photons impinge to the right and none to the left, would result in an observable that does not have distinct states. Since there is not just a single photon, both modes could carry photons at the same time, in which case Q_3 would have two simultaneous values.

The second point is more troublesome. While with a single photon, trials that are discarded are picked up in the statistics using the symmetric setup, this no longer holds with multiple photons. Indeed, when a flux is detected at t_2 then two cases arise: either there are no photons in the other mode, or there are.

In the first case, the discarded trial is accounted for in the symmetric setup. In the second case, however, the trials in which there were photons in both output modes of the first beam splitter are simply lost. This poses an issue with noninvasiveness as artificially selecting only cases where all the flux is in one mode would completely alter the C_{23} correlator.

We propose a way to solve this issue by choosing the set of values for Q_2 to be $\{0, +1\}$. In particular, we include 0 specifically as a possible value and will make use of its annihilating property. The assignments are summed up in Tab. 3 and the corresponding quantum operators for observables Q_2 and Q_3 are shown in Eqs. (41) and (42). Such an assignment was obtained as follows.

L	R	Q_1	Q_2	Q_3
Vacuum	Vacuum	$+1$	0	-1
Vacuum	Photons	N.A.	$+1$	-1
Photons	Vacuum	$+1$	$+1$	$+1$
Photons	Photons	N.A.	0	0

Table 3: Assignment of values for the observables, with respect to mode states. L and R indicate modes that are respectively on the left hand side and on the right hand side. For Q_1 those are the input modes, for Q_2 those are the intermediate modes and for Q_3, the output modes. As the preparation of the experiment sets the right input mode in the vacuum state, no values need to be assigned in other cases for Q_1, though any arbitrary value would be valid.

We set $Q_1 = +1$ when there are no photons in the right input mode. Other cases concerning the first beam splitter's input states never occur as this is the way the experiment is prepared. The preparation process results in $Q_1 = +1$ constantly.

We furthermore set $Q_3 = -1$ when the left detector does not click, $Q_3 = +1$ when the right detector does not click and the left detector clicks, and $Q_3 = 0$ when both detectors click. Note that when no detectors click at all, $Q_3 = -1$.

Finally we must be careful with the assignment of Q_2. In an attempt to salvage noninvasive measurability, we will define $Q_2 = +1$ when all photons are in the same intermediate mode. Perhaps the most important choice, and what saves the negative measurement method, is the assignment $Q_2 = 0$ if there are photons in both intermediate modes or if there are no photons at all. This way, $Q_2 = +1$ will be

realized as long as exactly one of the two intermediate modes is in the vacuum state, and $Q_2 = 0$ otherwise.

Setting $Q_2 = 0$ in the case where there are photons in both modes may seem to make it so that the discarded trials, which are permanently lost, in fact would not have had any impact on the C_{23} correlation coefficient as $C_{23} = \langle Q_2 Q_3 \rangle = \sum Q_2 Q_3 \mathbb{P}_{23}(Q_2, Q_3)$. So, be they discarded or not, instances in which photons are in both intermediate modes would not contribute to C_{23}.

However, this reasoning is too hasty, as discarding cases when $Q_2 = 0$, while having no effect on the number of nonzero terms in the sum defining C_{23}, does nonetheless change the joint probability distribution $\mathbb{P}(Q_2, Q_3)$.

Nevertheless, setting $Q_2 = 0$ when both intermediate modes contain photons does make it possible to save noninvasive measurability, but in fact without discarding any trials that cannot be negatively distinguished. To show this, let us observe the four following cases that make up all possible situations :

1. If the detector at t_2 does not click, then
   a) Either no photons are detected at t_3 which means there were no photons at all, so $Q_2 = 0$.
   b) Or photons are detected at t_3, so $Q_2 = +1$ because all photons are in the other mode, then $Q_2 = +1$ is known via a negative measurement.
2. If the detector at t_2 does click then
   a) Either no detectors click at t_3 in which case $Q_2 = +1$ but we can discard the trial, and this situation is taken into account in the other setup where the intermediate detector is positioned on the other mode.
   b) Or detectors do click at t_3 in which case $Q_2 = 0$ because there were photons in both modes. Then by having chosen $Q_2 = 0$ we do not need to actually take into account the measurement at time t_3 because $Q_2 Q_3 = 0$ in any case. This means that whether the t_2 measurement was invasive or not does not matter at all. Whether the Q_3 value that is obtained was a possessed value or a measured value plays no role either. What matters is that at least one detector clicks at t_3, but the measurement outcome value is of no importance.

In this manner, direct invasive measurements at t_2 are either discarded but not permanently lost, or a rigorously noninvasive t_2 measurement would contribute to C_{23} in the exact same way as the possibly invasive real t_2 measurement. Another way of phrasing what we have done is that by setting $Q_2 = 0$ when there are photons in both intermediate modes, the only measurements that contribute to C_{23} are

the negative measurements, which can be seen as noninvasive. All in all, the whole argument to salvage noninvasive measurability hinges on the use of the value 0 which is absorbing (or annihilating) for the multiplication.

One point worth discussing is the exposure to a fair sampling loophole. We have assumed here that all detectors are ideal, however our assignment does not absolutely require unity quantum efficiencies and noiseless dynamics. To show that the experiment can work in principle with imperfect detectors, consider an overall error rate e and let us suppose all errors give the worst outcome (i.e. skews the average K value the most towards an LGI violation) in which $Q_1Q_2 + Q_2Q_3 - Q_1Q_3 = 3$. Then under macroscopic realism the highest attainable value for K is $(1+2e)$. If each of the three detectors used to establish the Q values has a generic error rate (in telling apart the vacuum from a non-vacuum state) ε, then the overall error rate will be $e = 1-(1-\varepsilon)^3$. Taking $\varepsilon = 5\%$ yields $e = 0.15$ so that the K function threshold for an LGI violation may be shifted to 1.3. As we shall see, this new threshold can be exceeded with a coherent state input, as well as with a thermal state.

Let us now show that the violation is indeed achieved. To this end, recall that the probability of detecting n photons in a coherent state $|\alpha\rangle$ is Poissonian

$$p_n(\alpha) = e^{-|\alpha|^2}\frac{|\alpha|^{2n}}{n!}. \tag{39}$$

First $C_{12} = \langle Q_2\rangle$ can be expressed by introducing the photon numbers n_R and n_L respectively in the right and left intermediate modes. We may rewrite the event $\{Q_2 = 0\}$ explicitly from conditions on photon numbers as $\big(\{n_L > 0\}\wedge\{n_R > 0\}\big)\vee\big(\{n_L = 0\}\wedge\{n_R = 0\}\big)$, and note that photon numbers in the two output modes are independent of one another. Hence from Eq. (39) it is established that $C_{12} = \mathbb{P}(Q_2 = +1) = 4e^{-\frac{3|\alpha|^2}{4}}\sinh\big(|\alpha|^2/4\big)$.

Next, $C_{13} = \langle Q_3\rangle = -1$ is straightforward as the output state when there is no intermediate measurement is $|0\rangle\otimes|-\alpha\rangle$, hence all the flux arrives at the right hand output detector.

Finally $C_{23} \propto \langle Q_3\rangle_L + \langle Q_3\rangle_R = 0$, because the beam splitters are 50:50. Since cases where possible interference may occur, and the vacuum, are assigned $Q_2 = 0$, the situations that contribute to C_{23} are those where photons impinge on the second beam splitter from only one side. Then the detection probabilities are equal in both output modes, and since Q_3 takes opposite values in those cases, the average value is null. This results in the following LG correlation:

$$K(\alpha) = 1 + 4e^{-\frac{3|\alpha|^2}{4}}\sinh\left(\frac{|\alpha|^2}{4}\right), \tag{40}$$

for which a plot is shown in Fig. 6.

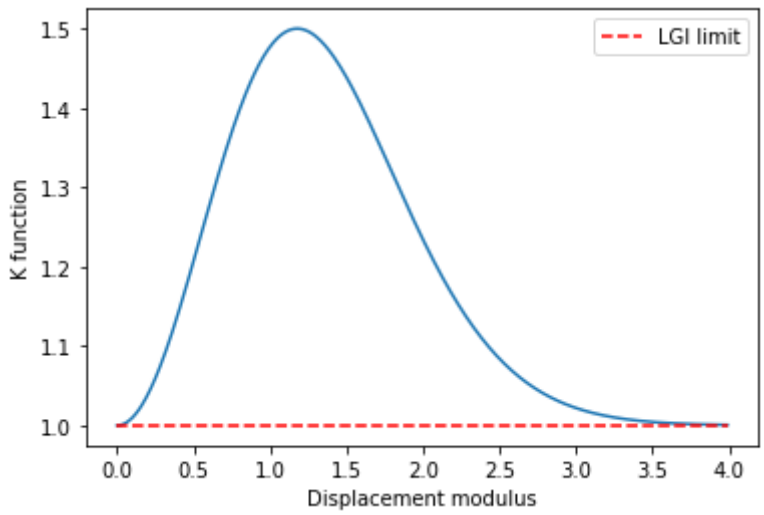


Figure 6: LG correlation function with respect to the modulus of the displacement. Plot obtained for a coherent state input in the Mach-Zehnder interferometer with appropriate observable value assignment.

We observe a violation of the LGI which becomes maximal when the average photon number $|\alpha|^2$ is just over 1. More precisely, the maximum is reached at $|\alpha|^2 = 2\ln(2)$, with a corresponding value of $K(\alpha_{\max}) = 1.5$. Let us note that this maximum is reached when the intermediate modes are equally balanced superpositions of the vacuum state and all other Fock states $2^{-1/2}(|0\rangle + |n > 0\rangle)$.

We also note that the K function decays for high laser intensities. This is due to our observable value assignment choice. Indeed, as the laser field becomes more intense, trials in which all photons end up in the same mode become less likely, so we should expect C_{12} to drop to 0.

3.2.3 *Violation with dephased states*

Using the same setup and observable assignment, we let go of any sort of phase reference in the input coherent state. That is to say, we now consider the input state $\rho_1(\alpha) = \sum_{n=0}^{+\infty} p_n(\alpha)\,|n,0\rangle\langle n,0|$, where $p_n(\alpha)$ is given by Eq. (39). The output state is formally given by $\rho_3 = BB\rho_1 B^\dagger B^\dagger$. By linearity of all performed operations, we may as well decompose our calculation step-by-step by considering Fock input states $\rho_1(n) = |n,0\rangle\langle n,0|$. The state after the first beam splitter reads $\rho_2(n) = \frac{1}{n!} B a_L^{\dagger\, n} B^\dagger\,|0,0\rangle\langle 0,0|\, B a_L^n B^\dagger$, and beam splitter transformations (26) yield

$$\rho_2(n) = \frac{1}{2^n} \sum_{k,\ell=0}^{n} \sqrt{\binom{n}{k}\binom{n}{\ell}} (-1)^{k+\ell}\,|k, n-k\rangle\langle \ell, n-\ell|\,.$$

Let us begin by computing $C_{12} = \langle Q_2 \rangle$ where

$$Q_2 = \sum_{n=1}^{+\infty} |0,n\rangle\langle 0,n| + |n,0\rangle\langle n,0| \,. \tag{41}$$

Since $Q_2 \in \{0,+1\}$ the expectation value is straightforwardly evaluated to $\langle Q_2 \rangle = \mathbb{P}(Q_2 = +1)$. Because we assume 50:50 beam splitters, we can write $\mathbb{P}(Q_2 = +1) = \sum_{n=1}^{+\infty} \frac{1}{2^{n-1}} p_n(\alpha) = 2e^{-|\alpha|^2}\left(e^{|\alpha|^2/2} - 1\right)$. This result, for which we shall show a more general and direct derivation in a later section, is identical to the previously established expression for C_{12}.

As previously argued $C_{23} = 0$, by virtue of the following inspection. If photons are in both modes or there are no photons, then $Q_2 = 0$, so those cases, regardless of the obtained value of Q_3, do not contribute to C_{23}. If photons are all in the same mode then $Q_2 = +1$ and because the beam splitter is 50:50 the assignment of Q_3 values results in an overall average value of 0.

Finally, to compute C_{13}, what we seek is $\langle Q_3 \rangle = \mathrm{Tr}(\rho_3 Q_3)$ where

$$Q_3 = \left(\sum_{n=1}^{+\infty} |n,0\rangle\langle n,0| - |0,n\rangle\langle 0,n|\right) - |0,0\rangle\langle 0,0| \,, \tag{42}$$

so we may project out all components of the density operator for which the product with Q_3 would give an off-diagonal element. The projected density matrices will be written with a tilde $\tilde{\rho}$. Applying the beam splitter transformations (26), one finds the projected output state $\tilde{\rho}_3(n) = |0,n\rangle\langle 0,n|$ (see Appendix C.1 for a detailed proof), so that $\tilde{\rho}_3(\alpha) = \sum_{n=0}^{+\infty} p_n(\alpha)\, |0,n\rangle\langle 0,n|$.

From this, one finds $C_{13} = \langle Q_3 \rangle = \mathrm{Tr}(Q_3 \tilde{\rho}_3(\alpha)) = -1$, which is identical to the previously established C_{13} for a coherent input state. Therefore the LG correlation function, which we note with a prime to indicate dephased input, takes the same form as Eq. (40):

$$K'(\alpha) = 1 + 4e^{-\frac{3|\alpha|^2}{4}} \sinh\left(\frac{|\alpha|^2}{4}\right). \tag{43}$$

This shows that the LGI is violated even if the input state is completely decohered, and underlines the fact that the LGI violation with a coherent state does not come the from quantum superposition involved in $|\alpha\rangle$ when represented in the Fock basis.

Interestingly, similar calculations with a different photon number probability distribution $q_n(\lambda)$ allow to compute K' for a thermal state. Consider a thermal state at the left input mode of the first beam splitter $\rho_1(\lambda) = \sum_{n=0}^{+\infty} q_n(\lambda)\, |n,0\rangle\langle n,0|$, where $q_n(\lambda) = e^{-n\lambda}(1 - e^{-\lambda})$ and $\lambda = \hbar\omega/k_B T \in]0,+\infty[$ defines the temperature through the photon energy $\hbar\omega$ and the Boltzmann constant k_B. As argued previously, $C_{13} = \langle Q_3 \rangle = \mathrm{Tr}(Q_3 \rho_3(\lambda)) = -\sum_{n=0}^{+\infty} q_n = -1$, and $C_{23} = 0$. We

also find $C_{12} = \sum_{n=1}^{+\infty} \frac{1}{2^{n-1}} q_n(\lambda) = 2(1-e^{-\lambda})\left(\frac{1}{2e^{\lambda}-1}\right)$ through a calculation that is similar to that previously presented. This yields

$$K'(\lambda) = 1 + 2(1-e^{-\lambda})\left(\frac{1}{2e^{\lambda}-1}\right). \tag{44}$$

The LG correlation function in this case reaches its maximum value $K_M = \frac{2}{(1+\sqrt{2})^2} + 1 \approx 1.343$ at $\lambda_M = \ln\left(1+1/\sqrt{2}\right)$, which shows LGI violations to be allowed, in theory, with thermal states.

3.2.4 *Violation with intermediate dephasing*

Let us now examine the effect of decoherence after the first beam splitter. To do so, we choose to write down the intermediate state after the first beam splitter when there is no intermediate measurement as $\rho_2(\gamma) = (\mathbb{1} \otimes \Delta_\gamma)\rho_2$, where Δ_γ is a dephasing channel which simply introduces a damping factor $\gamma \in [0,1]$ on the off-diagonal terms of the right intermediate mode, in the Fock basis. Formally, Δ_γ is a super-operator with operator-sum (or Kraus) representation $\{\sqrt{\gamma}\mathbb{1}, \sqrt{1-\gamma}\,|n\rangle\langle n|_{n\in\mathbb{N}}\}$ where γ is the damping factor. In particular, Δ_1 is the identity super-operator and Δ_0 completely decoheres a quantum state.

For an input Fock state $\rho_1(n)$ the intermediate state with decoherence reads

$$\rho_2(n,\gamma) = \frac{1}{2^n}\sum_{k,\ell=0}^{n}\sqrt{\binom{n}{k}\binom{n}{\ell}}(-1)^{k+\ell} \times (\gamma + (1-\gamma)\delta_{k,\ell})\,|k,n-k\rangle\langle \ell, n-\ell|\,,$$

where $\delta_{k,\ell}$ is a Kronecker symbol.

The C_{12} correlator is unaffected by decoherence, to show this we note that

$$\mathrm{Tr}(Q_2\rho_2(n,\gamma)) = \frac{1}{2^n}\sum_{k,\ell=0}^{n}\sqrt{\binom{n}{k}\binom{n}{\ell}}(-1)^{k+\ell} \times (\gamma + (1-\gamma)\delta_{k,\ell})\,\langle \ell, n-\ell|Q_2|k,n-k\rangle\,.$$

From Eq. (41) one finds $Q_2\,|k,n-k\rangle = (1-\delta_n)\,(|0,n\rangle\,\delta_k + |n,0\rangle\,\delta_{k,n})$, hence $\langle \ell, n-\ell|Q_2|k,n-k\rangle = (1-\delta_n)(\delta_\ell\delta_k + \delta_{\ell,n}\delta_{k,n})$. From this, one can deduce $\mathrm{Tr}(Q_2\rho_2(n,\gamma)) = \frac{1}{2^{n-1}}(1-\delta_n)$, and the announced result follows immediately. Note that the dephasing parameter γ does not affect this correlator. Decoherence does not affect C_{23} either, as the trials where $Q_2 = +1$ is measured negatively correspond to completely dephased states (all photons are in the same mode).

However, the decoherence does affect $C_{13} = \langle Q_3 \rangle$. With calculations similar to those laid out previously, the relevant submatrix for the trace reads

$$\tilde{\rho}_3(n,\gamma) = (\gamma - 1)\delta_{n,0}\,|0,0\rangle\langle 0,0| + \gamma\,|0,n\rangle\langle 0,n| + \frac{1}{4^n}\binom{2n}{n}(1-\gamma)\big(\,|n,0\rangle\langle n,0| + |0,n\rangle\langle 0,n|\,\big).$$

Thus $\mathrm{Tr}(Q_3\tilde{\rho}_3(n,\gamma)) = (1-\gamma)\delta_{n,0} - \gamma - 2\delta_{n,0}\frac{1}{4^n}\binom{2n}{n}(1-\gamma)$, and performing the weighted sum with the distribution given by Eq. (39) gives $\langle Q_3 \rangle = -e^{-|\alpha|^2} - \gamma(1 - e^{-|\alpha|^2})$. This results in a new LG correlation function of two variables, the plot of which is shown in Fig. 7 for a few values of the damping factor γ. Its expression reads

$$K'(\alpha,\gamma) = 4e^{-\frac{3|\alpha|^2}{4}}\sinh\left(\frac{|\alpha|^2}{4}\right) + (1-\gamma)e^{-|\alpha|^2} + \gamma. \tag{45}$$

If the input state is a coherent state $|\alpha\rangle$, it turns out all the correlators are identical. For completeness these correlators are derived explicitly in Appendix C.2.

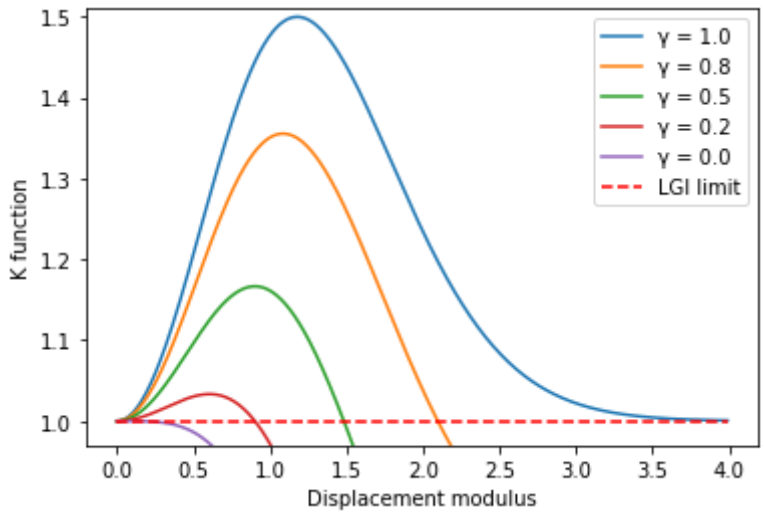


Figure 7: LG correlation function for coherent state or Poissonian Fock mixture input, with respect to the modulus of the corresponding displacement, for different values of the damping factor γ of the intermediate dephasing.

We observe that the LGIs are still violated even with strong decoherence. In fact, as long as the state after the first beam splitter is not completely decohered ($\gamma > 0$), an LGI violation remains possible, and the only way an LGI violation is realized for all non-zero laser intensity is if there is strictly no loss of coherence ($\gamma = 1$).

The maximum with respect to the damping factor is achieved at $|\alpha|^2 = 2\ln(1+\gamma)$. So we expect the maximal value to be reached at

lower and lower laser intensities with increasing decoherence. The corresponding maximum reads

$$K'(\alpha_{max}, \gamma) = 1 + \frac{\gamma}{1+\gamma}. \tag{46}$$

This final form is consistent with previous results, yielding no LGI violation for $\gamma = 0$ (complete decoherence) and a maximum of 1.5 when $\gamma = 1$ (no decoherence).

3.3 CONCLUSION

In this chapter, we have reviewed some fundamental aspects of the LGI, namely its relationship to macroscopic realism, and seen that the significance of its violation must be treated with much more care than in the case of Bell's inequalities.

Despite being much more subtle to manipulate, the LGI violation is commonly treated as a witness of non-classical behavior, almost on the same footing as Bell's inequalities. We have shown that by carefully thinking about observable assignments, it is possible to make use of negative measurements and achieve an LGI violation with even the most classical states of light.

In our presentation, we have progressively treated more and more classical inputs. We have begun from the highly non-classical Fock state, and proceeded to find a violation with the coherent state. We have shown that our results were not affected by the loss of initial phase reference, which allowed to contemplate, and indeed confirm violations with thermal states. We have also considered the effect of intermediate partial loss of phase reference, and demonstrated that LGI violations remained possible. In the end, we have shown that what pilots the LGI violation is the vacuum component of the state, but it does not carry as strong a consequence as a Bell inequality violation, which requires entanglement.

Should the proposed experiment with classical states of light be carried out successfully, this would show consistency with the fact that classical wave mechanics, being able to reproduce quantum random walk statistics [161], may simulate an LGI violation.

All in all, we have shown that what the LGIs really tests, both from a foundations of physics perspective, and from the operational quantum information theoretic perspective, is perhaps much weaker than one would think, from being first introduced to the LGIs as "temporal Bell inequalities".

4

WITNESSING NON-STANDARD QUANTUM DYNAMICS

Il n'est pas certain que tout soit incertain.[1]

— **Blaise Pascal** [162]

Among the most remarkable features of quantum mechanics is the Heisenberg uncertainty principle, which stems from the non-commutativity of position and momentum operators. In practice, it dictates that localizing a system more and more precisely comes with higher uncertainty on its conjugate momentum. However the inclusion of gravitational effects is predicted to result in the emergence of a fundamental limit to the localization scale, on the order of the Planck length $\ell_p = \sqrt{\hbar G/c^3} \approx 1.6 \times 10^{-35}$ m.

In this chapter, we present the so-called Generalized Uncertainty Principle (GUP), which is a modification of Heisenberg's uncertainty relations that is necessary in order to maintain consistency with our current knowledge of the gravitational interaction. We relate the GUP to a deformation of the canonical commutation relation, and explain the extent to which finding empirical evidence of the GUP is challenging. After introducing a novel approach, based on quantum control, we present a critical no-go theorem limiting such methods. We demonstrate how one can circumvent this no-go theorem by taking into account correlations in probes which are used to test the GUP.

4.1 THE GENERALIZED UNCERTAINTY PRINCIPLE

In this section, we set the scene with a short review around the GUP. We explain how it emerges, and mention some conceptual issues that it entails. We also present the algebraic formulation of the GUP, on which the experimental test of interest relies on.

4.1.1 *Origins of minimum localization scales*

Minimum localization scales are not predicted by quantum theory alone. Indeed, Heisenberg's uncertainty relations $\sigma_x \sigma_p \geqslant \frac{\hbar}{2}$ do not forbid arbitrarily fine squeezing of a quantum state in the position space, at the expense of high uncertainty in momentum space. This observation, though derived in a modern fashion from non-commutativity through Robertson's inequalities as shown in Sec. 2.2.3, can

1 Translation: *It is not certain that all is uncertain.*

be established directly through a very general thought experiment, owed to Heisenberg.

Consider the simple scenario where a quasi-monochromatic optical wave of wavelength λ scatters from an electron, into a detector. This process amounts to measuring the position of the electron, and the uncertainty is naturally expected to be proportional to the wavelength $\sigma_x \sim \lambda$. The scattering event has a lower bound momentum exchange, corresponding to the momentum of a single photon $p = \frac{h}{\lambda}$ which has been imparted to the electron. This yields the order of magnitude $\sigma_x \sim \frac{\hbar}{\sigma_p}$.

Although this thought experiment may seem perfectly valid at first sight, it shrouds an important assumption, according to which gravitational effects negligibly contribute to the dynamics which is essentially governed by quantum electrodynamics. In many different approaches, the inclusion of gravitational effects in the quantum dynamical description, assuming that the employed gravitational model holds at the given length or energy scale, results in a modification of Heisenberg's uncertainty relations. Before exploring some of those approaches, the very first hints of a fundamental minimum localization scales may already be found through rough estimates, using Newtonian gravity and by treating light as massive particle with an effective mass $m = \frac{E}{c^2}$.

Suppose that the characteristic distance over which the electron interacts gravitationally with the photon is ℓ, the characteristic gravitational acceleration of the electron is $\frac{GE}{c^2\ell^2}$ which takes places over a characteristic duration $\frac{\ell}{c}$, leading to a characteristic gravitational delocalization scale $\sigma_x^G \sim \frac{GE}{c^2\ell^2}(\frac{\ell}{c})^2 \sim \frac{GE}{c^4}$. Since the photon momentum $p = \frac{E}{c}$ is roughly the momentum uncertainty of the electron σ_p, one arrives at $\sigma_x^G \sim \frac{G\sigma_p}{c^3} \sim \frac{G\hbar}{c^3}\frac{\sigma_p}{\hbar} = \ell_p^2\frac{\sigma_p}{\hbar}$. Roughly adding the uncertainties, one arrives at $\sigma_x \sim \frac{\hbar}{\sigma_p} + \ell_p^2\frac{\sigma_p}{\hbar}$, which constitutes the GUP. It turns out that the full general relativistic treatment agrees with this back-of-the-envelope estimation, as shown in Ref. [163].

A somewhat more formal approach to arrive at the minimum localization scale, is the argument of light ranging. Recall that in flat Minkowski spacetime, assuming a $(+,-,-,-)$ metric signature, the line elements are given by $ds^2 = (cdt)^2 - dx^2$. In the Newtonian limit and denoting $\phi = \frac{Gm}{r}$ the Newtonian gravitational potential sourced by an effective mass m, the Schwarzschild metric takes the form $ds^2 = (1 + \frac{2\phi}{c^2})(cdt)^2 - (1 - \frac{2\phi}{c^2})dx^2$. For weak fields[2] one sees that for two events separated by a coordinate space interval dx, the corresponding proper space interval with the gravitational field is $dx^G = dx(1 - \frac{2\phi}{c^2})^{1/2} \approx dx(1 - \frac{\phi}{c^2})$, to first order. This means that any given length ℓ in flat spacetime undergoes a gravitational distortion $\sigma_\ell^G = \ell\frac{\phi}{c^2}$. Let us now suppose that we would like to measure

2 Note that at the surface of the Sun where the acceleration of gravity is 28g, one has $\phi/c^2 \approx 10^{-6}$. This illustrates why the weak field limit is valid in many cases.

the space interval between two points separated by ℓ in flat spacetime, using light ranging. The lowest mass-energy introduced in the interval by injecting an optical signal with associated wavelength λ is the energy content of a single photon $E = \frac{h}{\lambda c}$. The effective gravitational field sourced by the weakest possible signal is then $\phi \sim \frac{Gh}{\ell \lambda c}$ inducing a gravitational distortion $\sigma_\ell^G \sim \frac{Gh}{\lambda c^3} = \ell_p^2/\lambda$. The total length uncertainty is then $\sigma_\ell = \lambda + \ell_p^2/\lambda$, and as we see, extremely long wavelengths may not resolve the distance properly, while extremely short wavelength come with strong gravitational distortions. Somewhere in the middle, for $\lambda = \ell_p$ one reaches the minimum uncertainty, which is manifestly nonzero.

In addition to the simple light ranging thought experiment, there are many other elementary arguments leading to this minimal length scale as shown in Ref. [164]. One can establish the Planck limit from the equalization of the Compton wavelength and the Schwarzschild radius, by the analysis of the energy density of the gravitational field, by investigating the minimal energy required to probe a small volume, to name a few. While these are many instructive heuristic arguments for the existence of a minimum length scale, the earliest formal indications of such a phenomenon originated from gravitational instabilities arising in ultra-high-energy scattering in string theory [165–167]. Interestingly, minimum spacetime intervals can also be arrived at in loop quantum gravity, even though contrary to string theory which relies on a fixed background metric, loop quantum gravity identifies metric perturbations and gravitational field as the same entity. More precisely, loop quantum gravity features discrete spacetime [168] in the sense of Wheeler's quantum foam [169].

This preamble on minimum length scales and the GUP cannot be closed without the mention of an important issue arising in light of those observations, first considered in Ref. [170], pertaining to the non-compactness of the Lorentz transformation group. On the one hand, it seems that most approaches to quantum gravity, formal or heuristic, agree on the existence of a fundamental minimum length. On the other hand, special relativity dictates that all spacetime intervals are reference frame dependent. How can one then make the claim that physics does not change under passive transformations, if there is to exist a fundamental length? To put it bluntly, how can there be length-scale (or momentum scale) dependent effects and events if any length interval (or system momentum) can be increased or decreased when viewed from a Lorentz-boosted frame?

Understanding how loop quantum gravity and string theory avoid this violation of Lorentz invariance is well beyond the scope of this thesis. However, it is possible to explore the consequences of such a violation in a formalism that was in fact established to address this very issue, called Doubly Special Relativity (DSR). At its core, DSR introduces a new invariant $\kappa \propto \ell_p^{-1}$ in addition to c, ensuring invari-

ance of the Planck length [171], the Planck mass [172] or the Planck energy [173]. Assuming this extra invariant comes with some interesting consequences. For instance, under a boost in the z direction with reduced velocity β, the usual Lorentz transformations for momentum $p_0' = \gamma(p_0 - \beta p_z); p_z = \gamma(p_z - \beta p_0)$ take the modified form

$$\begin{cases} p_0' &= \frac{\gamma(p_0 - \beta p_z)}{f(p_0, p_z)} \\ p_x' &= \frac{p_x}{f(p_0, p_z)} \\ p_y' &= \frac{p_y}{f(p_0, p_z)} \\ p_z' &= \frac{\gamma(p_z - \beta p_0)}{f(p_0, p_z)} \end{cases},$$

where $f(p_0, p_z) = 1 + \ell_p((\gamma - 1)p_0 - \gamma\beta p_z)$ gives a non-linear correction which vanishes as $\ell_p \to 0$. We note that intervals orthogonal to the boost direction are modified. Algebraically, DSR changes the action of the Lorentz group on the momentum space. Depending on which version of DSR one is dealing with, other effects may include a modification of the dispersion relation $E^2 = p^2c^2 + m^2c^4$, implying an energy dependent speed of light. In turn, this raises the issue of large scale locality violation [174].

Another issue that is worth mentioning with DSR, is that for the sake of preserving observer-independence (of length or energy scale effects), non-linear modifications to the Lorentz action on momentum space are introduced. However, these non-linear modifications spoil the compatibility of reference frame change with the additivity of momenta in composite systems. Under a modified Lorentz transformation $\tilde{\Lambda}$, the relationship between the total momentum of a bipartite system and the momenta of its composites becomes frame-dependent $\tilde{\Lambda}(p_1 + p_2) \neq \tilde{\Lambda}(p_1) + \tilde{\Lambda}(p_2)$. This paradox is termed *soccer ball problem* [175], and remains an open problem. Among proposed solutions, one *ad-hoc* approach is to consider a rescaling of Planckian non-linear effects so that $f(p_0, p_z) = 1 + \frac{\ell_p}{N}((\gamma - 1)p_0 - \gamma\beta p_z)$, where N is the number of composites [173]. Such modifications of Planck scale corrections, namely its implications for GUP phenomenology, will be the central object of this chapter, as we shall see in Sec. 4.3.

To close this short overview of minimum length scales and discrete spacetime, it is worth mentioning the possibility to preserve Lorentz invariance while having a discrete spacetime in the framework of causal sets [176]. In this theory, the causal structure of spacetime subsumes the background manifold given by special relativity, and instead simply consists of a partially ordered set of points. The main assumption of causal set theory is that a causal set unequivocally determines the macroscopic (coarse-grained) spacetime manifold. A proof of such assumption has yet to be established, however some edge cases have been addressed [177]. It was shown that despite having a discrete spacetime, forming causal sets with randomized sets of

spacetime points may preserve Lorentz invariance. It was shown in Ref. [178], that a Poisson process fulfills the desired property.

4.1.2 *Algebraic formulation*

As we have seen, heuristic arguments as well as formal candidate theories of quantum gravity predict a fundamental lower bound for the localization scale of physical systems. One way to bridge this observation with the Heisenberg uncertainty relations consists in viewing Planck scale corrections as arising from a modification of the canonical commutation relations.

The algebraic structure underlying the GUP stems from the assumptions that the momenta in different directions commute, so as to leave the translation group invariant, that the 3 dimensional rotation group is not deformed, and that $[x, x]$, $[x, p]$ commutators are deformed. Under those assumptions, the required forms of the commutators read $[x_i, x_j] = (\frac{\hbar}{\kappa c})^2 a(p) i\varepsilon_{ijk} J_k$ and $[x_i, p_j] = i\hbar\delta_{ij} f(p)$, where J_k is a rotation generator, ε is the Levi-Civita symbol, $a(p)$ and $f(p)$ are arbitrary functions which depend only on the norm of the momentum, and κ is a deformation parameter ($\kappa \to +\infty$ restores standard physics). Further imposing compatibility with the Jacobi identities, one arrives at the conditions $\frac{da(p)}{dp} p.J = 0$ and $p^{-1} f(p) \frac{df(p)}{dp} = -\frac{a(p)}{\kappa^2 c^2}$. Identifying J with the orbital angular momentum, the first condition is always satisfied, so that one may freely choose $f(p)$, which is chosen to read $f(p) = 1 + \beta p^2$ in Ref. [179]. Thus one can capture the GUP through the modified commutation relation $[x, p] = i\hbar(1 + \beta p^2)$. This quadratic dependence on the momentum is in accordance with predictions from string theory [166, 167], and black hole physics [180, 181].

With this modified commutation relation at hand, the Heisenberg uncertainty relation Eq. (14) then yields

$$\sigma_x \sigma_p \geqslant \frac{\hbar}{2}(1 + \beta\sigma_p^2 + \beta \langle p^2 \rangle) \geqslant \frac{\hbar}{2}(1 + \beta\sigma_p^2). \tag{47}$$

As a result an absolute lower bound for σ_x as a function of σ_p becomes apparent, and reads $\sigma_x^{\min} = \hbar\sqrt{\beta}$, as shown in Fig. 8. If one introduces the dimensionless scalar $\beta_0 = \beta m_p c^2$ where $m_p = \sqrt{\frac{\hbar c}{G}}$ is the Planck mass, then minimum localization scales on the order of ℓ_p amounts to having $\beta_0 \sim 1$. It is worth mentioning that although this deformation is the most widely studied, another form which reads $[x, p] = i\hbar(1 + \frac{p^2}{\kappa^2 c^2})^{1/2}$ was posited by having imposed $da/dp = 0$ when the angular momentum is not identified with the orbital angular momentum [182, 183]. The inclusion of a linear term was also considered in Ref. [184] in accordance with DSR. Finally, it should be noted that the GUP can be arrived at by maintaining the standard

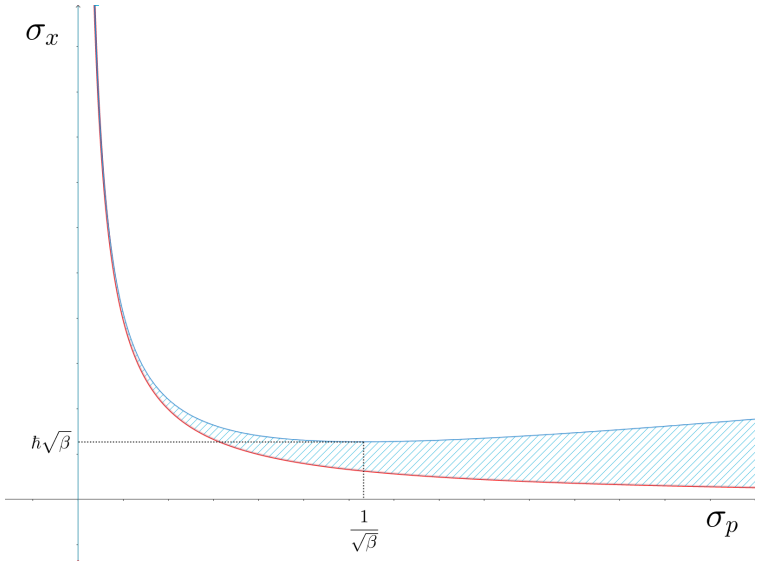


Figure 8: Minimum localization scale with respect to the momentum uncertainty for the standard uncertainty principle (shown in red) and the GUP (shown in blue). The hatched area corresponds to regimes that would be ruled out by empirical manifestations of GUP.

commutation relations, and instead defining a modified momentum with high energy corrections, as shown in Ref. [184].

4.2 TESTING THE GENERALIZED UNCERTAINTY PRINCIPLE

In this section, we touch upon the difficulty in observing evidence supporting the GUP. We present a quantum optomechanical protocol to test the GUP and we derive an observable non-standard signature from first principles. We close this section with the presentation a critical no-go theorem, which may put into question the relevance of all tests of GUP relying on macroscopic probes.

4.2.1 *Experimental approaches*

The physics community has yet to establish a consistent framework unifying gravitational and quantum effects. Despite the theoretical hints towards Planck scale effects such as the GUP, for lack of empirical evidence, the Planckian landscape has remained essentially opaque and the different paths to quantum gravity difficult ones to tread on. In hopes to gather some experimental data, in recent years more and more investigations around the GUP have turned to phenomenological aspects. Let us briefly review some notable attempts in this direction, involving either microscopic experimental probes, cosmic events or macroscopic experimental probes. On the grounds that all quantum mechanical Hamiltonians are affected by the modifications of the commutation relations (or equivalently by the defor-

mation of the momentum operator), those proposals aim to test GUP deviations to standard predictions.

In Ref. [185], the authors suggest to investigate deviations to well known quantum effects such as the Lamb shift and the tunneling current of a scanning tunneling microscope. If we consider the non standard commutator $[x, p] = i\hbar(1 + \beta p^2)$, where $\beta = \frac{\beta_0}{m_p c^2}$, then the Lamb shift for the ground state is shown to be perturbed from its standard form by $\frac{\Delta E_0^{GUP}}{\Delta E_0} = 10\beta_0 \frac{m}{m_p} \frac{E_0}{m_p c^2} \approx 4.7 \times 10^{-49}\beta_0$. With current data indicating an agreement in the Lamb shift with standard predictions up to 12 decimal places, this implies $\beta_0 \lesssim 10^{36}$. The tunneling current for realistic microscope parameters would deviate from standard predictions by the relative amount $\frac{\delta I}{I_0} \approx 10^{-48}\beta_0$, meaning that for the excess non-standard current to induce an excess charge of one electron, the wait time is $\tau = 10^{29}\beta_0^{-1}$s. With a readout time of 1 year, the lack of deviations to standard theory would yield the constraint $\beta_0 \lesssim 10^{21}$.

On the other end of the macroscopicity spectrum, in Ref. [186], the authors instead investigate non-standard deviations to the mass-temperature relation for a Schwarzschild black hole of mass M. Considering the GUP form Eq.(47) $\sigma_x \sigma_p \geqslant \frac{\hbar}{2}(1 + \beta\sigma_p^2)$, the relative deviation to the Hawking temperature is found to be $\frac{\Delta T}{T_H} \approx \frac{\beta_0 m_p^2}{4\pi^2 M}$, to first order in β_0. For a Solar mass black hole, agreement with the Hawking temperature would suggest $\beta_0 \lesssim 10^{78}$. This temperature correction in turn induces an additional perturbation in the Schwarzschild metric. By characterizing the non-standard corrections to the Schwarzschild metric of the form $F(r) = 1 - \frac{2GM}{r} + \varepsilon\frac{G^2M^2}{r^2}$, with the relationship $\beta_0 = -\frac{\pi^2 M^2}{4m_p^2}\varepsilon^2$, the authors derive GUP effects on Mercury's perihelion precession, which after one revolution is found to take the form $\Delta\phi \approx \frac{6\pi GM}{(1-e^2)a}(1 - \frac{\varepsilon}{6})$, where e is the orbit eccentricity, a is the semi-major axis, and the general relativistic prediction is recovered when $\varepsilon \to 0$. Comparing with current observational data, one has the constraint $\varepsilon \lesssim 10^{-4}$ yielding $\beta_0 \lesssim 10^{69}$. Measurements of periastron shifts were also considered for quasars, but do not yield tighter bounds for β_0.

Let us finally turn to some experiments of particular interest for the present thesis, which find themselves to be somewhere between the cosmological scale and the atomic scale. In Ref. [187], an ultracold ton-scale gravitational wave detector's is analysed. Assuming again the GUP form Eq.(47), the effect on the ground energy of the large metallic bars reads $E_0 = \frac{\hbar\omega_0}{2}((1 + \frac{\beta}{4})^{1/2} + \frac{\beta}{2})$, where ω_0 is the mechanical mode frequency. A bound on β_0 can then be related to the experimentally measured energy, this reads $\beta_0 < 2\frac{E_{measured}}{\hbar\omega_0}\frac{m_p}{m}\frac{m_p c^2}{\hbar\omega_0}$. The reported measurements yield $\beta_0 \lesssim 10^{33}$. It was proposed in Ref. [188], to test the non-standard deformations to commutation relations through their predicted effect on the motion of macroscopic har-

monic oscillators, namely an anharmonic contribution. By inspecting the amplitude dependent frequency shift $\tilde{\omega} = (1 + \frac{\beta}{2} a_0^2)\omega_0$ of a range of mechanical oscillators, a relatively tight upper bound $\beta_0 \lesssim 10^7$ is established. Using bulk acoustic wave quartz oscillators, an even tighter bound of $\beta_0 \lesssim 10^4$ was more recently established in Ref. [189]. Another proposal relying on a mesoscopic optomechanical setup to probe deformations of the commutation relations was also put forward, and will be the object of the next section.

4.2.2 *The generalized optomechanical protocol*

In this section, we revisit a toy model inspired from a proposal that we term "optomechanical protocol" [190]. The optomechanical protocol suggests that one can gain information on the type of evolution undergone by a mechanical oscillator by inspecting the non-linear phase that the light picks up after having interacted with the oscillator.

A sequence of light pulses drives a mechanical oscillator around a closed phase space trajectory, returning the oscillator to its initial state (in the absence of commutator deformations), while imparting a (mechanical state-independent) non-linear optical phase. This phase is of interest as it may carry non-standard signatures and, as we shall show from first principles, is quartic in the photon number if GUP corrections exist, and is quadratic otherwise. In the remainder of this section, we re-derive results of the optomechanical protocol in a more general fashion, in the sense that we defer specifying a given form of optomechanical coupling to the final steps of our derivation.

Let us consider a single particle of mass m that is harmonically trapped with angular frequency Ω, interacting with a single mode optical field with annihilation operator a and angular frequency Ω_F. In standard quantum mechanics, the optomechanical Hamiltonian reads

$$H^s = \frac{p^2}{2m} + \frac{1}{2} m\Omega^2 x^2 + \hbar\Omega_F \left(a^\dagger a + \frac{1}{2}\right) + g(t) a^\dagger a x,$$

where x is the position of the particle with respect to its rest position, p is its conjugate momentum, the s superscript stands for "standard", and where $g(t)$ is the coupling function. Note that in our approach we keep $g(t)$ general. By rescaling the variables as $q = \sqrt{m\Omega} x$ and $p \to \frac{1}{\sqrt{m\Omega}} p$ we rewrite the previous equation as

$$H^s = \frac{\Omega}{2}\left(p^2 + q^2\right) + \hbar\Omega_F \left(a^\dagger a + \frac{1}{2}\right) + \frac{1}{\sqrt{m\Omega}} g(t) a^\dagger a q.$$

We shall define $H_1^s(t) = \frac{1}{\sqrt{m\Omega}} g(t) a^\dagger a q$ as the interaction part, and the free part as $H_0 = \frac{\Omega}{2}\left(p^2 + q^2\right) + \hbar\Omega_F \left(a^\dagger a + \frac{1}{2}\right)$.

We seek to express the resulting oscillator-state-independent phase accumulated by the light field at the end of the interaction. The fact

that this phase term does not depend on the oscillator state is important as we seek to test modifications to the commutation relations. With no knowledge of the true commutation relations, the initial (ground) state of the mechanical oscillator is ill-defined. We will work in the interaction picture, where operators A are transformed as $\tilde{A}(t) = e^{iH_0 t/\hbar} A e^{-iH_0 t/\hbar}$. The unitary evolution of the system can be written as $\tilde{\rho}(t) = \tilde{U}(t)\tilde{\rho}(0)\tilde{U}^\dagger(t)$, and since its time derivative must be consistent with the Liouville equation $\frac{d}{dt}\tilde{\rho}(t) = -\frac{i}{\hbar}[\tilde{H}_1(t), \tilde{\rho}(t)]$, this requires the unitary propagator to satisfy $\frac{d}{dt}\tilde{U}(t) = \frac{-i}{\hbar}\tilde{H}_1(t)\tilde{U}(t)$. Since the interaction Hamiltonians do not necessarily commute at different times, the propagator solving the equation takes the form $\tilde{U}(t) = \exp(\Theta(t))$ where $\Theta(t) = \sum_{k=1}^{+\infty} \Theta_k(t)$ is given by a Magnus series (see Sec. 2.1.3 for details).

Because the first order unequal time commutators are scalars, only the two first terms in the Magnus expansion are non-vanishing. Explicitly these terms are

$$\Theta_1(t) = -\frac{i}{\hbar}\int_0^t dt_1 \tilde{H}_1(t_1)$$
$$\Theta_2(t) = \frac{1}{2}\left(\frac{-i}{\hbar}\right)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 [\tilde{H}_1(t_1), \tilde{H}_1(t_2)].$$

With those two terms we have exactly solved the dynamics, as the interaction Hamiltonian at any time commutes with the commutator, all following terms of the Magnus expansion are zero. To lighten the notations, let us define $g'(t) = g(t)\cos(\Omega t)$ and $g''(t) = g(t)\sin(\Omega t)$, (note that the primes *do not* represent derivatives) so that one may rewrite the interaction term as $\tilde{H}_1^s(t) = a^\dagger a(g'(t)q + g''(t)p)/\sqrt{m\Omega}$. The first term in the Magnus expansion then reads

$$\Theta_1(t) = -\frac{i}{\hbar}\frac{1}{\sqrt{m\Omega}} a^\dagger a(G'(t)q + G''(t)p),$$

where $G' = \int_0^t g'(t_1)dt_1$, $G'' = \int_0^t g''(t_1)dt_1$, and the second term reads

$$\Theta_2(t) = -\frac{i(a^\dagger a)^2}{2\hbar m\Omega}\int_0^t dt_1 (g'(t_1)G''(t_1) - g''(t_1)G'(t_1)),$$

where we have applied the standard commutation relation $[q, p] = i\hbar$. Hence we find that the propagator takes the form

$$\tilde{U}(t) = \exp\left(-\frac{i}{\hbar}\frac{(a^\dagger a)^2}{m\Omega}F(t)\right)\exp\left(-\frac{i}{\hbar}\frac{a^\dagger a}{\sqrt{m\Omega}}(G'(t)q + G''(t)p)\right), \tag{48}$$

where $F(t) = \frac{1}{2}\int_0^t dt_1 (g'(t_1)G''(t_1) - g''(t_1)G'(t_1))$ gives a phase term which is independent of the mechanical oscillator's state and is quadratic in the photon number.

We now introduce the GUP modification to the commutation relations. While it is possible[3] to analytically work out the dynamics of the system by imposing $[x, p] = i\hbar(1 + \beta p^2)$, we instead work with the usual commutation relations but redefine the momentum as $p \to p(1 + \frac{\beta}{3}p^2)$, as in Refs. [185, 191], which yields the modified commutation relations. The Hamiltonian, with reduced variables, now takes the form

$$H = \frac{\Omega}{2}\left(p^2 + q^2\right) + \hbar\Omega_F\left(a^\dagger a + \frac{1}{2}\right) + \frac{1}{\sqrt{m\Omega}}g(t)a^\dagger a q + \frac{1}{3}m\Omega^2\beta p^4 + O(\beta^2).$$

We will not carry out any perturbative treatment of the coupling term $g(t)$, we simply expand the Hamiltonian in orders of β and keep the order 1 correction, assuming that higher order terms are negligible[4]. We furthermore neglect possible corrections to the optical Hamiltonian. Let us also note that the extra interaction term due to the GUP correction changes the ground state, which is why we will focus on a state-independent non-standard signature.

We shall now define

$$H_1(t) = \frac{1}{\sqrt{m\Omega}}g(t)a^\dagger a q + \frac{1}{3}m\Omega^2\beta p^4,$$

as the interaction term. In the same manner as the standard phase was found, we work in the interaction picture where the propagator satisfies the differential equation $\frac{d}{dt}\tilde{U}(t) = -\frac{i}{\hbar}\tilde{H}_1(t)\tilde{U}(t)$. In order to compute the Magnus terms, one needs to express the different commutators between $\tilde{H}_1$ at different times, and while the p^4 term does give rise to many non-vanishing higher-order commutators, to first order in the GUP correction β, the Magnus expansion only has 5 non-vanishing terms. We have explicitly:

$$\tilde{H}_1(t) = \frac{1}{\sqrt{m\Omega}}g(t)a^\dagger a\tilde{q}(t) + \frac{1}{3}m\Omega^2\beta\tilde{p}^4(t), \tag{49}$$

where $\tilde{q}(t) = \cos(\Omega t)q + \sin(\Omega t)p$ and $\tilde{p}(t) = \cos(\Omega t)p - \sin(\Omega t)q$ is given by well-known commutator dynamics. Using standard commutation relations, one establishes the following commutator expressions:

$$\begin{aligned} [\tilde{q}(t_1), \tilde{q}(t_2)] &= i\hbar\sin(\Omega(t_2 - t_1)), \\ \forall n \in \mathbb{N}^*,\ [\tilde{q}(t_1), \tilde{p}^n(t_2)] &= ni\hbar\tilde{p}^{n-1}(t_2)\cos(\Omega(t_2 - t_1)). \end{aligned} \tag{50}$$

To order 1 in β, it is clear that the first commutator $[\tilde{H}_1(t_1), \tilde{H}_1(t_2)]$ will take the form $C + \beta\tilde{p}^3 + O(\beta^2)$, where C commutes with the

3 But prohibitively complicated.

4 Higher order terms in β come with higher powers of the operators. The assumption that higher order corrections are negligible assume some reasonably localized state in the (q, p) phase space, which is the case for low energy states.

interaction Hamiltonian. So the next order nested commutators are all at least of order 1 in β. After some calculations (see Appendix D.1 for details) the fifth order commutator is found to be:

$$[\tilde{H}_1(t_1),[\tilde{H}_1(t_2),[\tilde{H}_1(t_3),[\tilde{H}_1(t_4),\tilde{H}_1(t_5)]]]] = \frac{4!}{3}(a^\dagger a)^4(i\hbar)^4\beta\frac{1}{m}\prod_{j=1}^{4} g(t_j)\cos\big(\Omega(t_5-t_j)\big) - (t_4 \leftrightarrow t_5), \quad (51)$$

where $(t_4 \leftrightarrow t_5)$ signifies that there is an extra term that is identical up to a swap between two time arguments.

The fifth order Magnus term, which is an integral of such fifth order nested commutators (up to some permutations of time indices), is particularly interesting as it is independent of the mechanical-oscillator operators $\tilde{q}(t)$ and $\tilde{p}(t)$. In order to further work out its form, we note that it is a quintuple nested integral of 22 nested commutators [192]. Using the shorthand $\tilde{H}_i := \tilde{H}_1(t_i)$ and defining the nested integral operator

$$\int_{(5,t)} dt^5 := \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \int_0^{t_3} dt_4 \int_0^{t_4} dt_5,$$

this term takes the explicit form given in Eq. (52).

$$\begin{aligned}
\Theta_5(t) = \left(\frac{-i}{\hbar}\right)^5 \int_{(5,t)} dt^5 \Big(& \\
& -\frac{1}{30}[\tilde{H}_5,[\tilde{H}_4,[\tilde{H}_3,[\tilde{H}_2,\tilde{H}_1]]]] + \frac{2}{15}[\tilde{H}_1,[\tilde{H}_5,[\tilde{H}_4,[\tilde{H}_2,\tilde{H}_3]]]] \\
& -\frac{1}{30}[\tilde{H}_1,[\tilde{H}_4,[\tilde{H}_3,[\tilde{H}_2,\tilde{H}_5]]]] - \frac{1}{30}[\tilde{H}_1,[\tilde{H}_5,[\tilde{H}_3,[\tilde{H}_2,\tilde{H}_4]]]] \\
& +\frac{1}{15}[[\tilde{H}_5,\tilde{H}_1],[\tilde{H}_4,[\tilde{H}_2,\tilde{H}_3]]] + \frac{1}{15}[[\tilde{H}_4,\tilde{H}_1],[\tilde{H}_5,[\tilde{H}_2,\tilde{H}_3]]] \\
& -\frac{1}{60}[[\tilde{H}_2,\tilde{H}_3],[\tilde{H}_5,[\tilde{H}_4,\tilde{H}_1]]] + \frac{1}{15}[[\tilde{H}_3,\tilde{H}_1],[\tilde{H}_5,[\tilde{H}_2,\tilde{H}_4]]] \\
& -\frac{1}{60}[[\tilde{H}_2,\tilde{H}_4],[\tilde{H}_5,[\tilde{H}_3,\tilde{H}_1]]] - \frac{1}{60}[[\tilde{H}_2,\tilde{H}_5],[\tilde{H}_4,[\tilde{H}_3,\tilde{H}_1]]] \\
& -\frac{1}{60}[[\tilde{H}_3,\tilde{H}_4],[\tilde{H}_5,[\tilde{H}_2,\tilde{H}_1]]] - \frac{1}{60}[[\tilde{H}_3,\tilde{H}_4],[\tilde{H}_1,[\tilde{H}_2,\tilde{H}_5]]] \\
& -\frac{1}{60}[[\tilde{H}_5,\tilde{H}_1],[\tilde{H}_3,[\tilde{H}_2,\tilde{H}_4]]] - \frac{1}{60}[[\tilde{H}_4,\tilde{H}_1],[\tilde{H}_3,[\tilde{H}_2,\tilde{H}_5]]] \\
& -\frac{1}{60}[[\tilde{H}_3,\tilde{H}_5],[\tilde{H}_4,[\tilde{H}_2,\tilde{H}_1]]] - \frac{1}{60}[[\tilde{H}_3,\tilde{H}_5],[\tilde{H}_1,[\tilde{H}_2,\tilde{H}_4]]] \\
& -\frac{1}{60}[[\tilde{H}_4,\tilde{H}_5],[\tilde{H}_1,[\tilde{H}_2,\tilde{H}_3]]] - \frac{1}{60}[[\tilde{H}_2,\tilde{H}_3],[\tilde{H}_1,[\tilde{H}_4,\tilde{H}_5]]] \\
& -\frac{1}{60}[[\tilde{H}_2,\tilde{H}_4],[\tilde{H}_1,[\tilde{H}_3,\tilde{H}_5]]] - \frac{1}{60}[[\tilde{H}_2,\tilde{H}_1],[\tilde{H}_4,[\tilde{H}_3,\tilde{H}_5]]] \\
& -\frac{1}{60}[[\tilde{H}_4,\tilde{H}_5],[\tilde{H}_3,[\tilde{H}_2,\tilde{H}_1]]] - \frac{1}{60}[[\tilde{H}_3,\tilde{H}_1],[\tilde{H}_4,[\tilde{H}_2,\tilde{H}_5]]]\Big).
\end{aligned} \quad (52)$$

Fortunately, simplifications are possible, as 18 of those nested commutators are of the form $[[\tilde{H}_1(t_i), \tilde{H}_1(t_j)], [\tilde{H}_1(t_k), [\tilde{H}_1(t_l), \tilde{H}_1(t_m)]]]$. Looking at Eqs. (74) and (75), we see that they are at least quadratic in β. To first order in β we are thus left with the four terms

$$\Theta_5(t) = \left(\frac{-i}{\hbar}\right)^5 \sum_{\sigma\in S} \int_{(5,t)} dt^5 \lambda_\sigma \\ \times [\tilde{H}_1(t_{\sigma(1)}), [\tilde{H}_1(t_{\sigma(2)}), [\tilde{H}_1(t_{\sigma(3)}), [\tilde{H}_1(t_{\sigma(4)}), \tilde{H}_1(t_{\sigma(5)})]]]], \quad (53)$$

where we have defined the set S the elements of which are the permutations $(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = ((54321), (15423), (14325), (15324))$ and their associated coefficients $\lambda_{\sigma_1} = \lambda_{\sigma_3} = \lambda_{\sigma_4} = -\frac{1}{30}$ and $\lambda_{\sigma_2} = \frac{2}{15}$. Combining the previous equation with Eq. (51) one arrives at the following expression which holds for arbitrary coupling functions $g(t)$, to first order in β:

$$\Theta_5(t) = -\frac{i}{\hbar}\frac{4!}{3}(a^\dagger a)^4 \frac{\beta}{m} \sum_{\sigma\in S} \int_{(5,t)} dt^5 \lambda_\sigma \\ \left(\prod_{j=1}^{4} g(t_{\sigma(j)}) \cos\big(\Omega(t_{\sigma(5)} - t_{\sigma(j)})\big) - (t_{\sigma(4)} \leftrightarrow t_{\sigma(5)})\right). \quad (54)$$

Similar to the pulsed regime considered in Ref. [190], this fifth Magnus term, which is proportional to the GUP correction β, contributes to the propagator as a highly non-linear phase factor depending on the fourth power of the photon number.

This is to compare with the standard case of unmodified commutation relations, where the analogous oscillator-state-independent phase factor $\exp\big(-\frac{i}{\hbar} m (a^\dagger a)^2 F(t)\big)$ in Eq. (48), is quadratic in the photon number. Our formula is valid for any optomechanical coupling function $g(t)$. In the next section we shall analytically apply it to the case where the coupling function consists of four pulses, as was considered in Ref. [190].

4.2.3 *The four pulse case*

We now make use of our general formula for a single particle, with a specific and relatively simple coupling function. To do so, it is useful to first define $f(t_1, ..., t_5) = \prod_{j=1}^{4} \cos\big(\Omega(t_5 - t_j)\big)$. In the context of pulsed interaction, the coupling term is well approximated by a sum of Dirac distributions $g(t) = \lambda \sum_{i=0}^{3} \delta(t - \tau_i)$. The Dirac delta interaction leaves the mechanical oscillator's state fixed over the duration of the pulse which is identical to the approximation used for pulsed optomechanics (up to a global phase on the light). Here a succession of four Dirac pulses at instants $(\tau_i)_{0\leqslant i\leqslant 3}$ is considered, where $\lambda \geqslant 0$ is a coupling strength.

After some calculations shown in Appendix D.2, the fifth order Magnus term can be found to read

$$\begin{aligned}\Theta_5(t) = -\frac{i}{\hbar}\frac{4!}{3}(a^\dagger a)^4 \frac{\beta}{m}\frac{\lambda^4}{30} \sum_{i_1 i_2 i_3 i_4=0}^{3} \Bigg\{ & \\ H(t,\tau_{i_4},\tau_{i_3},\tau_{i_2},\tau_{i_1}) & \left(\int_{\tau_{i_3}}^{\tau_{i_4}} ds - \int_{\tau_{i_4}}^{t} ds\right) \\ + H(t,\tau_{i_1},\tau_{i_4},\tau_{i_3},\tau_{i_2}) & \left(4\int_{\tau_{i_3}}^{\tau_{i_4}} ds - 4\int_{\tau_{i_4}}^{\tau_{i_1}} ds - \int_{0}^{\tau_{i_3}} ds\right) \\ + H(t,\tau_{i_1},\tau_{i_3},\tau_{i_2},\tau_{i_4}) & \left(\int_{\tau_{i_3}}^{\tau_{i_1}} ds\right) \\ + H(t,\tau_{i_1},\tau_{i_3},\tau_{i_4},\tau_{i_2}) & \left(\int_{\tau_{i_3}}^{\tau_{i_1}} ds\right) \Bigg\} f(\tau_{i_1},\tau_{i_2},\tau_{i_3},\tau_{i_4},s).\end{aligned} \tag{55}$$

In the particular case where the interaction instants are $\tau_k = t_0 + k\theta = t_0 + k\frac{\pi}{2\Omega}$, where θ is a quarter of the oscillator period, and for times $t > t_0 + 3\theta$ after which all four matter-field interactions have taken place, one finds a closed form result

$$\Theta_5(t) = \left(\frac{-i}{\hbar}\right)\frac{4!}{3}(a^\dagger a)^4 \frac{\beta}{m}\frac{\lambda^4}{30\Omega}\frac{5(9\pi-16)}{32}.$$

All higher order Magnus terms vanish, hence the solution obtained from the $\Theta_i, 1 \leqslant i \leqslant 5$ is exact, to order 1 in β. We observe that this fifth-Magnus term is a constant of time for $t > t_0 + 3\theta$, which is expected as the full system undergoes free evolution. Similar to what was found in Ref. [190], this mechanical-state-independent phase factor increases as the fourth power of the optical intensity $(a^\dagger a)$ and the interaction strength λ.

4.2.4 *A no-go theorem for macroscopic probes*

We have seen in Sec. 4.1.1 that the existence of a fundamental minimum length scale is at odds with Lorentz invariance, and that this issue, should it be addressed through doubly special relativity, leads to the soccer ball problem for composite systems. It turns out that, beyond doubly special relativity, fundamental issues when dealing with many-body systems are already apparent as soon as a modification of commutation relations is assumed. Such issues are of concern for quantum gravity phenomenology: the optomechanical protocol [190] focuses on detecting non-standard effects on the motion of the center of mass of an optically driven mechanical oscillator, while in Ref. [187], Planckian effects are sought in the energy of a longitudinal normal mode of a 2 ton aluminum bar.

Whereas heuristic arguments presented in Sec. 4.1.1 do lead to Planck scale effects in single high energy physical systems, one may

object that the center of mass is merely a geometrical construct, rather than a real physical object, and as such achieving Planck scale localization of a center of mass of a macroscopic probe may be irrelevant.

Such experimental proposals to probe Planck scale effects with macroscopic systems have led to upper-bound constraints on β_0, and it is taken for granted that Planck scale regimes should become observable when experiments unravel deviations to standard predictions around $\beta_0 \sim 1$. However, as argued in Ref. [193], while modifications to commutation relations $[x, p] = i\hbar(1 + \beta p^2)$ may have amplitude β for the position and momentum of a fundamental particle, there is no evidence suggesting that those modifications may be extrapolated to center of mass coordinates and total momentum of a many-body system. This can be clarified in a straightforward calculation. If one considers the center of mass coordinates of a composite system of N equally massive subsystems $X = \frac{1}{N}\sum_{k=1}^{N} x_k$ and $P = \sum_{k=1}^{N} p_k$ with a deformed commutator $[x_i, p_j] = i\hbar(1 + \beta p_j^2)\delta_{ij}$ then

$$[X, P] = i\hbar\left(1 + \frac{\beta}{N^2}P^2 + \frac{\beta}{N}\sum_{k=1}^{N}\left(p_k^2 - \frac{P^2}{N^2}\right)\right), \tag{56}$$

where we have expanded and simplified the center of mass variables commutator $\frac{1}{N}\sum_{i,j}[x_i, p_j]$. In the quasi-rigid limit ($\forall i,\ p_i \approx P/N$), which justifies the center of mass variable description of a composite system, the variance of the momentum distribution over the subsystems vanishes, so that $[X, P] \approx i\hbar\left(1 + \frac{\beta}{N^2}P^2\right)$, thus deformations to the center of mass commutator are suppressed by the (potentially macroscopic) number of constituent particles. In other words, having experimental evidence which set the upper bound $\beta_0 < 1$ does not necessarily invalidate GUP corrections, as they may simply not be detectable in such regimes. If experiments on electrons have GUP correction amplitudes of order $\beta \sim 1$, Eq. (56) suggests that the relevant Planckian regime may have much lower corrections. For the coherent control of a picogram mass [194], assuming GUP corrections $\beta_0 \sim 1$ for a nucleon, Planck scale corrections may range anywhere within the interval $10^{-32} \lesssim \beta_0 \lesssim 10^{-16}$. This leads to an important question: are many-body macroscopic systems relevant probes for Planck scale behaviour?

To phrase the problem in other words, while microscopic systems require energy levels far out of reach to test $\beta_0 \sim 1$ GUP corrections, macroscopic systems have become an interesting avenue to attempt reaching the $\beta_0 \sim 1$ regime, however the expected non-standard corrections may become attenuated by the very number of constituents of the probe thus displacing the relevant regime to probe considerably below $\beta_0 \sim 1$.

Another fundamental question, that we shall not attempt to tackle in this thesis but worth mention, arises at the sight of Eq.(56): which physical systems are "fundamental enough" to be affected by the full

magnitude of the GUP correction $\beta_0 \sim 1$? In the next section, we will discuss at length how to circumvent the no-go theorem by relinquishing the quasi-rigid limit, and attempt to answer the first question positively. Specifically, we will show how macroscopic probes may still very well be relevant probes for Planckian effects.

4.3 GOING BEYOND THE NO-GO THEOREM

In this section, we show how an accurate description of macroscopic probes to test the GUP may constitute a way out of the no-go theorem.

4.3.1 *Underlying principle*

As we have seen, the GUP correction amplitude β_0 may be suppressed when working with center of mass coordinates of a many-body system. Although the scaling of the suppression is unknown in general [195], from Eq. (56) one can expect a scaling somewhere between $1/N$ (for uncorrelated systems) and $1/N^2$ (for rigid systems). However, in specially correlated fine-tuned systems, it may be that some Planck scale effects could become amplified: this would be the case if some signature of the GUP correction is found to have a superquadratic scaling with the number of elementary constituents, overcoming the suppression of the GUP correction itself.

In what follows, we carry out this investigation in the context of the optomechanical protocol, which we extend to the case of a non-rigid many-body probe. In the optomechanical protocol, the non-standard signature arising from the interaction between a single mode optical field with a many-body system will be taken to be a phase term Φ that is quartic in the photon number and is independent of the state of the many-body mechanical system. To be clear, the goal of the presented study is not to determine an absolute GUP correction amplitude β_0. Rather, regardless of β_0, in the hypothesis where the correction scales in $\beta_N = O(\frac{1}{N^2})$, proving that the non-standard signature Φ_N scales superquadratically will result in an overall amplification $\Phi_N(\beta_N)$ of Planckian effects.

In order to observe superquadratic scaling, one must first be able to fully characterize the dynamics of many-body systems in a sufficiently general manner to allow for a broad type of interaction patterns and couplings between subsystems. This accurate description is what has motivated the generalization of the optomechanical protocol. In the next sections, we derive closed form formulas for the dynamics of the many-body optomechanical probe, and show numerical evidence of superquadratic scaling.

4.3.2 *General dynamics of the many-body probe*

Let us extend our analysis to the case of $N \in \mathbb{N}^*$ harmonically coupled identical trapped particles. The total Hamiltonian to first order in β can be written as $H(t) = H_0 + H_1(t)$ where the free Hamiltonian is

$$H_0 = \hbar\Omega_F\left(a^\dagger a + \frac{1}{2}\right) + \sum_{i=1}^{N}\left(\frac{1}{2m}p_i^2 + \frac{1}{2}m\Omega^2 x_i^2\right) + \frac{1}{2}m\Omega_c^2\sum_{i=1}^{N-1}(x_{i+1}-x_i)^2,$$

however our approach does not require a specific potential term, and holds for general potentials of the form $\frac{m}{2}x^T h x$ where h is a symmetric matrix (Hessian of the potential). The interaction Hamiltonian is

$$H_1(t) = \sum_{i=1}^{N} g_i(t)x_i(a^\dagger a) + \left(\frac{\beta}{3m}\right)\sum_{i=1}^{N} p_i^4, \tag{57}$$

where Ω_c is the coupling frequency between neighboring oscillators. In the same way as before, the time propagator in the interaction picture satisfies the differential equation $\frac{d}{dt}\tilde{U}(t) = -\frac{i}{\hbar}\tilde{H}_1(t)\tilde{U}(t)$. Thus the propagator satisfies $\tilde{U}(t) = \exp\left(\sum_{k=1}^{+\infty}\Theta_k(t)\right)$, as it is given by a Magnus series. We are led to expressing nested self-commutators of the interaction Hamiltonian. Expressing the interaction Hamiltonian (57) in the interaction picture, one arrives at an expression similar to Eq. (53) for the fifth order Magnus term:

$$\Theta_5(t) = \left(\frac{-i}{\hbar}\right)^5\int_{(5,t)}\sum_{\sigma\in S}\lambda_\sigma F_\sigma,$$

where to first order in β one has

$$\begin{aligned} F_\sigma = \frac{\beta}{3m}(a^\dagger a)^4 \sum_{i_1,i_2,i_3,i_4,i_5=1}^{N} & g_{i_1}(t_{\sigma(1)})g_{i_2}(t_{\sigma(2)})g_{i_3}(t_{\sigma(3)})g_{i_4}(t_{\sigma(4)}) \\ \times [\tilde{x}_{i_1}(t_{\sigma(1)}), [\tilde{x}_{i_2}(t_{\sigma(2)}), [\tilde{x}_{i_3}(t_{\sigma(3)}), [\tilde{x}_{i_4}(t_{\sigma(4)}), \tilde{p}_{i_5}^4(t_{\sigma(5)})]]]] & \\ - (t_{\sigma(4)} \leftrightarrow t_{\sigma(5)} \wedge i_4 \leftrightarrow i_5). & \end{aligned} \tag{58}$$

In order to express the nested commutator in general, we claim that $[\tilde{x}_i(t_1), \tilde{p}_j(t_2)] := C_{ij}(t_1 - t_2)$ is a c-number. Indeed, one can write the free Hamiltonian H_0 as

$$H_0 = \hbar\Omega_F\left(a^\dagger a + \frac{1}{2}\right) + \frac{1}{2m}p^T p + \frac{1}{2}m x^T h x,$$

where h is a symmetric matrix characterising the potential term. One can define the normal variables as $(\phi, \pi) = (\omega^{\frac{1}{2}}P^T\sqrt{m}x, \omega^{-\frac{1}{2}}P^T\frac{1}{\sqrt{m}}p)$,

where $\omega^2 = P^T h P = \mathrm{diag}(\omega_i^2)$ is the diagonal form of the h matrix, consisting of the squares of the normal frequencies, and where P is the orthogonal transformation matrix. Let us stress that m is a scalar and ω is a diagonal matrix. With those normal variables, the free Hamiltonian takes the simple form

$$H_0 = \hbar\Omega_F \left(a^\dagger a + \frac{1}{2}\right) + \frac{1}{2}\sum_{i=1}^{N} \omega_i(\pi_i^2 + \phi_i^2).$$

We furthermore note that because $P^T P = I_N$, the transformation is canonical $[\phi_i, \pi_j] = i\hbar\sqrt{\omega_i/\omega_j}\sum_{k,l=1}^{N} P_{ki}P_{lj}\delta_{k,l} = i\hbar\delta_{ij}$. For simplicity we will rewrite the variable transformations as $x = O\phi$ and $p = O'\pi$ where O and O' are orthogonal matrices. Using the shorthand notation for the free propagator $U_0(t) := e^{-iH_0 t/\hbar}$ one can now establish that

$$\begin{aligned}
[\tilde{x}_i(t_1), \tilde{p}_j(t_2)] &= [U_0^\dagger(t_1)x_i U_0(t_1), U_0^\dagger(t_2)p_j U_0(t_2)] \\
&= [U_0^\dagger(t_1)(O\phi)_i U_0(t_1), U_0^\dagger(t_2)(O'\pi)_j U_0(t_2)] \\
&= \sum_{k,\ell=1}^{N} O_{ik}O'_{j\ell}[\tilde{\phi}_k(t_1), \tilde{\pi}_\ell(t_2)].
\end{aligned}$$

In the rotating frame, we have $\tilde{\phi}_k(t_1) = \cos(\omega_k t_1)\phi_k + \sin(\omega_k t_1)\pi_k$ and $\tilde{\pi}_\ell(t_2) = \cos(\omega_\ell t_2)\pi_\ell - \sin(\omega_\ell t_2)\phi_\ell$, from which it follows that

$$[\tilde{x}_i(t_1), \tilde{p}_j(t_2)] = i\hbar\sum_{k=1}^{N} O_{ik}O'_{jk}\cos(\omega_k(t_2 - t_1)),$$

which proves that $C_{ij}(t_1 - t_2)$ is a c-number. Thus the commutators take the form $C_{ij}(t_1 - t_2) = i\hbar\sum_{k=1}^{N} O_{ik}O'_{jk}\cos(\omega_k(t_2 - t_1))$ where O and O' are some scaled normal mode transformation matrices defined by $O = \frac{1}{\sqrt{m}}P\omega^{-1/2}$ and $O' = \sqrt{m}P\omega^{1/2}$.

One can now express the nested commutators as

$$\begin{aligned}
&[\tilde{x}_{i_1}(t_{\sigma(1)}), [\tilde{x}_{i_2}(t_{\sigma(2)}), [\tilde{x}_{i_3}(t_{\sigma(3)}), [\tilde{x}_{i_4}(t_{\sigma(4)}), \tilde{p}_{i_5}^4(t_{\sigma(5)})]]]] \\
&\qquad = 4!\prod_{s=1}^{4} C_{i_s i_5}(t_{\sigma(s)} - t_{\sigma(5)}),
\end{aligned}$$

and Eq. (58) can be cast as

$$F_\sigma = \frac{\beta}{m}\frac{4!}{3}(a^\dagger a)^4 \sum_{j=1}^{N}\left[\prod_{s=1}^{4}\left(D_j(t_{\sigma(s)}, t_{\sigma(5)})\right) - (t_{\sigma(4)} \leftrightarrow t_{\sigma(5)})\right],$$

where $D_j(t, t') = \sum_{i=1}^{N} g_i(t)C_{ij}(t - t')$. Hence the fifth Magnus term is found to read

$$\begin{aligned}
\Theta_5(t) = \left(\frac{-i}{\hbar}\right)^5 \frac{4!}{3}\frac{\beta}{m}(a^\dagger a)^4 \sum_{\sigma\in S}\lambda_\sigma \int_{(5,t)} dt^5 \\
\sum_{j=1}^{N}\left[\left(\prod_{s=1}^{4} D_j(t_{\sigma(s)}, t_{\sigma(5)})\right) - (t_{\sigma(4)} \leftrightarrow t_{\sigma(5)})\right]. \quad (59)
\end{aligned}$$

At this stage, it becomes apparent that the problem reduces to the knowledge of the normal modes and frequencies through the explicit formula $D_j(t,t') = i\hbar \sum_{i=1}^{N} g_i(t) \sum_{k=1}^{N} O_{ik} O'_{jk} \cos(\omega_k(t-t'))$.

We have thus found an analytical form for the mechanical-state-independent phase factor. As in the single oscillator case, this factor depends on the fourth power of the optical intensity, however the expression now involves the mechanical properties of the body described by its normal mode transformations and associated frequencies. To no surprise, if the potential terms correspond to coupled trapped particles, one recovers Eq. (54) by setting $N = 1$, for which the normal mode transformations are trivial.

Finding how $\Theta_5(t)$ should scale with the number of particles N generally is not evident. In what follows, we will consider once again a pulsed regime where four pulses of light interact with the system, which will consist of many copies of a mechanical oscillator which are coupled to the neighboring oscillators, and show numerically that there can be superquadratic scaling.

4.3.3 *Scaling of the non-standard signature*

We seek to use our general formula given by Eq. (59) in the case where four pulses of light are sent through a lattice of N coupled oscillators (or sites). That is, we consider coupling functions of the form $g_k(t) = \lambda \sum_{i=0}^{3} \delta(t - (t_0 + iT + (k-1)\tau))$ where λ is a coupling strength, T is the time separating two pulses for a given site, and τ the time taken by the pulse to travel from one site to the next one. We shall work under the assumption that $T \geqslant N\tau$, which means that the pulse is re-injected only once it has finished interacting with all the lattice sites. The setup and the interaction functions are illustrated in Fig. 9.

After some calculations similar to those previously undertaken for the single oscillator driven by pulsed light (see Appendix D.3 for details), one arrives at the following expression for the fifth order Magnus term:

$$\Theta_5(t) = -\frac{i}{\hbar}\frac{4!}{3}\frac{\beta}{m}(a^\dagger a)^4 \sum_{i_1 i_2 i_3 i_4 j=1}^{N} \sum_{\nu_1\nu_2\nu_3\nu_4=1}^{N} \left(\prod_{s=1}^{4} O_{i_s\nu_s} O'_{j\nu_s}\right) \frac{\lambda^4}{30} \times$$
$$\sum_{\alpha_1\alpha_2\alpha_3\alpha_4=0}^{3} \Bigg\{ H(t,\theta_4,\theta_3,\theta_2,\theta_1)\left(\int_{\theta_3}^{\theta_4} ds - \int_{\theta_4}^{t} ds\right)$$
$$+ H(t,\theta_1,\theta_4,\theta_3,\theta_2)\left(4\int_{\theta_3}^{\theta_4} ds - 4\int_{\theta_4}^{\theta_1} ds - \int_{0}^{\theta_3} ds\right)$$
$$+ H(t,\theta_1,\theta_3,\theta_2,\theta_4)\left(\int_{\theta_3}^{\theta_1} ds\right) + H(t,\theta_1,\theta_3,\theta_4,\theta_2)\left(\int_{\theta_3}^{\theta_1} ds\right)\Bigg\}$$
$$\varphi_{\nu_1\nu_2\nu_3\nu_4}(\theta_1,\theta_2,\theta_3,\theta_4,s),$$

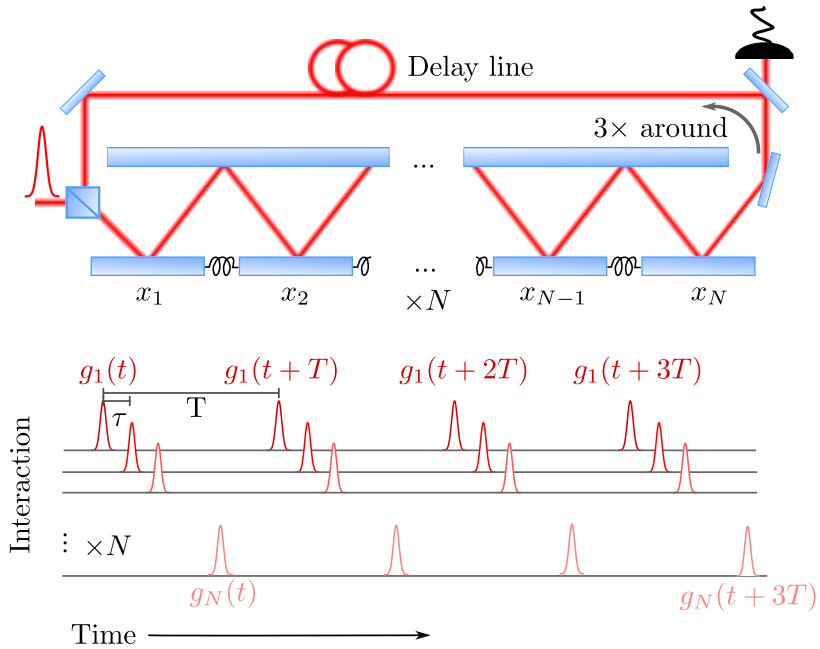


Figure 9: Generalization of the optomechanical protocol where the single trapped particle is replaced with a lattice of coupled oscillators. Each lattice site is affected 4 times by a light pulse, with time separation T. The time taken for the pulse to go from a site to the next is noted τ. The pulse is re-injected only once it has interacted with the whole lattice i.e. $T \geqslant n\tau$.

where we have defined $\varphi_{\nu_1\nu_2\nu_3\nu_4}(t_1, ..., t_5) = \prod_{s=1}^{4} \cos(\omega_{\nu_s}(t_s - t_5))$ and $\forall r \in \{1, 2, 3, 4\}$, $\theta_r := t_0 + \alpha_r T + (i_r - 1)\tau$.

Note that if the oscillators are uncoupled, the normal mode transformations are trivial and one has $O_{i_s\nu_s} O'_{j\nu_s} = \delta_{i_s,\nu_s}\delta_{j,\nu_s}$. In this case the fifth Magnus term reads

$$\begin{aligned}\Theta_5(t) = &-\frac{i}{\hbar}\frac{4!}{3}\frac{\beta}{m}(a^\dagger a)^4 \sum_{j=1}^{N} \frac{\lambda^4}{30} \\ &\sum_{\alpha_1\alpha_2\alpha_3\alpha_4=0}^{3} \Bigg\{ H(t,\theta_4,\theta_3,\theta_2,\theta_1)\left(\int_{\theta_3}^{\theta_4} ds - \int_{\theta_4}^{t} ds\right) \\ &+ H(t,\theta_1,\theta_4,\theta_3,\theta_2)\left(4\int_{\theta_3}^{\theta_4} ds - 4\int_{\theta_4}^{\theta_1} ds - \int_{0}^{\theta_3} ds\right) \\ &+ H(t,\theta_1,\theta_3,\theta_2,\theta_4)\left(\int_{\theta_3}^{\theta_1} ds\right) + H(t,\theta_1,\theta_3,\theta_4,\theta_2)\left(\int_{\theta_3}^{\theta_1} ds\right)\Bigg\} \\ &\varphi_{jjjj}(\theta_1,\theta_2,\theta_3,\theta_4,s).\end{aligned}$$

The vector of normal frequencies is simply $\omega^T = \Omega(1, 1..., 1)$ and we have $\theta_k = t_0 + \alpha_k T + (j-1)\tau$ so the Heaviside functions only depend on the α dummy variables. The functions φ_{jjjj} are thus identical and the sum over j simply gives a multiplication by the number of lat-

tice sites N. That is, one obtains N times the Magnus term given by Eq. (77). The absence of coupling between the oscillators is equivalent to repeating the single oscillator experiment a number of times, from which one does expect a linear increase of the non-standard signature picked-up by the light. By fixing $N = 1$ one naturally recovers Eq. (77).

As shown in Fig. 10a, numerics reveal the presence of superquadratic scaling, at least up to $N = 5$, for coupling frequencies Ω_c equal to a tenth or a half of the trap frequency that we chose to be $\Omega = 2\pi \times 10^5$Hz to facilitate comparison with Ref. [190]. The plotted quantity is an absolute phase factor $|\Phi(N)|$ for $N \in \{1, 2, 3, 4, 5\}$ defined by $\Theta_5(t) = \frac{-i}{\hbar}\frac{4!}{3}\frac{\beta}{m}(a^\dagger a)^4 \frac{\lambda^4}{30}\Phi(N)$. In general this is a complicated factor, depending on the coupling $g(t)$, the trapping frequencies of each lattice sites, and the coupling frequencies between them. We have assumed the form given by the last equation, i.e. we work in pulsed regime, and the pulses are separated by a quarter trapping period which is assumed to be the same for all sites, and we have further assumed $\tau = T/(2N)$.

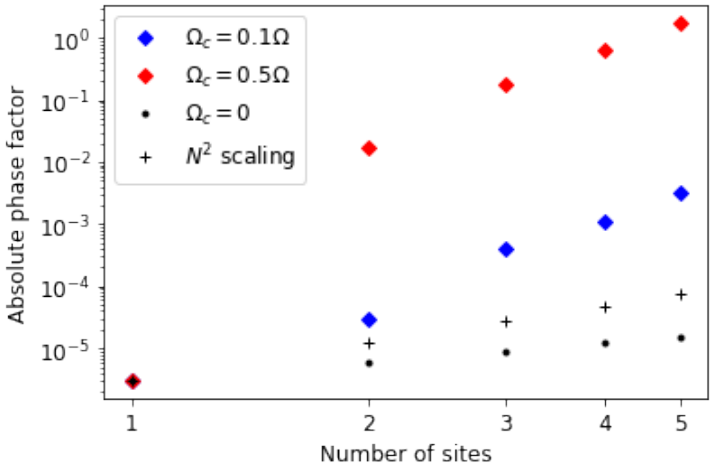
For coupling frequencies that are comparable or greater than the trap frequency, we see in Fig. 10b that there remains an advantage, however for the considered coupling frequencies, the absolute phase factor is not an increasing function of the number of sites.

4.4 CONCLUSION

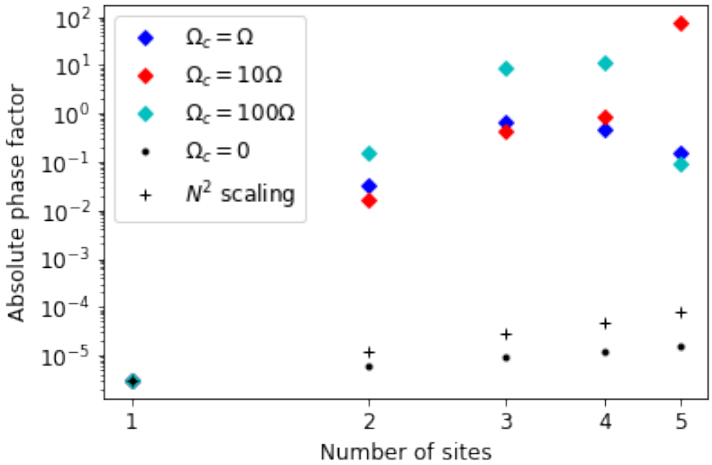
In this chapter, we have introduced the GUP as possible gravitational signature that should affect quantum mechanical motion, from heuristic arguments, and presented its important algebraic formulation, before reviewing some traditional and modern approaches to gather empirical evidence supporting the GUP.

In particular, we have revisited a proposal to indirectly test non-standard deviations to quantum dynamics: an optomechanical protocol that aims to detect highly nonlinear phase terms that should arise in the optical field driving a mechanical oscillator, as a result of modifications of commutation relations. Although rigid macroscopic systems are not viable probes for Planck scale effects, as the GUP corrections to the commutation relations of center of mass variables of such systems are expected to scale as the squared inverse of the number of constituents, the more general case of correlated many-body systems was left unexplored.

In the presented work, we have considered the motion of such systems in general and, to first order in the GUP corrections, we have derived the full dynamics for completely general light-matter coupling functions. We have provided a derivation of explicit forms for the fifth order Magnus term which consists of a phase factor that is independent of the mechanical oscillator's state. Many parameters



(a) Case $\Omega_c < \Omega$.



(b) Case $\Omega_c \geqslant \Omega$.

Figure 10: Log-log representation of the absolute phase factor as a function of the number of lattice sites, for different coupling frequencies Ω_c. Trap frequency $\Omega = 2\pi \times 10^5$Hz. Delay time $T = \pi/(2\Omega)$ and $\tau = T/(2N)$. The uncoupled case is represented by black dots and scales linearly with the number of lattice sites, while quadratic scaling is represented by black crosses. The absolute phase factor under nonzero coupling is represented with diamonds, and dominates the quadratic scaling, however the scaling with N is not always increasing.

of correlated many-body systems could be tuned, such as the retardation time taken by the optical signal between two lattice sites, or the spatial width of the optical pulse. Limiting ourselves to a pulsed regime, we have demonstrated that superquadratic scaling was already possible up to $N = 5$ subsystems by tuning only the coupling frequency between lattice sites.

The work presented in this chapter offers new perspectives for controlled many-body quantum dynamics, and may help to re-affirm finely tuned macroscopic probes as potential amplifiers for testing quantum gravitational effects. In addition to showing how macroscopic probes may be relevant to test Planck scale physics, the general calculations laid out in this work may benefit further investigations and tests of fundamental physics using optomechanical systems.

5 WITNESSING NON-CLASSICAL GRAVITY

Rien n'est beau comme la pesanteur dans les plis fugitifs des ondulations de la mer ou les plis presques éternels des montagnes.[1]

— **Simone Weil** [196]

Gravitation is quite paradoxically the earliest of physical interactions to have been studied by mankind, through the movement of planets, falling objects, and ballistics, yet it is to date the only known interaction that physicists fail to describe in a way that is consistent with all other forces. The quest for a unified theory, loosely referred to as quantum gravity, is still in its infancy, largely because catching sight of empirical data either supporting or rejecting hypotheses about the quantum nature of gravity is extremely demanding.

In this chapter, we recapitulate the quantum gravity problem, and present some of the challenges in finding evidence for quantum gravity. Having set the context, we introduce some modern and game-changing strategies for quantum gravity phenomenology based on quantum information and quantum control. We go into some detail in refining a widely acclaimed proposal, which consists in testing the entangling capacity of gravitation, and we show how it may yield results even in the presence of unwanted, and ill-characterized interactions. Finally, we consider a variant of such a protocol, which at first glance may seem less reasonable than its original version, as it involves probing gravitational properties sourced by light. We present some arguments explaining why such a variant should not be dismissed too hastily.

5.1 NON-CLASSICALITY OF GRAVITY

In this section, we review the main challenges that lie on the path to a quantum theory of gravity. We present traditional and modern approaches to obtain empirical clues towards quantum gravity, and focus on a particular proposal which has attracted much attention.

5.1.1 *The odyssean quest for quantum gravity*

Contemporary physics is in a peculiar state: it seems to have given a clear description of phenomena ranging from the inner workings

1 Translation: *Nothing is as beautiful as gravity in the fugacious crests of the undulating sea or the near eternal ones of the mountains.*

of the atomic nuclei, all the way up to planetary and stellar dynamics. However, as it stands today, our understanding of the universe could be considered somewhat two-faced. On the one hand Einstein's theory of General Relativity (GR) has provided undisputed predictions of the dynamics of systems governed by gravity. On the other hand quantum field theories, such as the standard model of particle physics, have been able to describe with extreme accuracy the behavior of systems governed by all other known interactions.

Taken separately, these two spearheads of modern physics are nothing short of theoretical marvels in their own domains of validity. However, contrary to other classical field theories that were superseded and unified into a quantum field theoretic framework, called the standard model, GR has so far been particularly resistant to all quantization attempts and up to this day remains a completely classical field theory. The methods that were successful when dealing with the interactions of the standard model simply do not work with GR. To be more precise, it is not so much that GR cannot be quantized, but rather that its quantized version is non-renormalizable [197, 198].

While it may look like the quest for quantizing gravity is just another human fantasy, this endeavour is not merely motivated by mathematical aesthetics. On top of all the issues arising when considering gravitational corrections to the uncertainty principle, as discussed in Chapter 4, GR on its own suffers from internal issues, such as the apparition of singularities in black holes. Furthermore, the current juxtaposition of GR and quantum field theory, referred to as quantum field theory in curved spacetime, implies that black holes emit thermal radiation and thus may destroy information, which is in contradiction with quantum theory [199]. Another motivation for a unified framework is the fact that mass-energy distributions exist in quantum superpositions, however GR simply cannot provide a description of the gravitational field sourced by such a quantum distribution.

Besides the herculean mathematical issues arising in attempts to quantize gravity, the quest for such a unified framework has been hampered by the downright lack of empirical evidence of any quantum gravitational effects. Such an obstacle was unfortunately baked into the very nature of the two theories: because of the sheer weakness of the gravitational interaction compared to the known quantum forces, the quantum effects of gravity, should they exist, are expected to become appreciable only at the Planck scale. As such, the direct observation of a graviton is an almost unfathomably distant dream. To give a figure of merit, even with a Jupiter-mass[2] noiseless graviton detector placed in close orbit around a neutron star, the frequency of graviton detections is expected in the most optimistic case to be on the order of once per century [200].

2 A matter system much more massive than Jupiter would collapse under its own weight to superatomic densities.

Faced with the next-to-impossible direct detection of the graviton, many phenomenological models have been put forward in the hopes to find some clues towards quantum gravity. Phenomenological models do not aim to provide a fundamental description of quantum gravity, but rather aim to extend what is already known in a specific direction so as to formulate deviations from standard theory. Instead of seeking the direct detection of a graviton, one may hope to observe some other types of quantum gravitational effects. Most of those efforts have been traditionally directed towards high energy processes.

For instance, evidence for quantum gravity in colliders may take the form of modifications of standard model cross sections, or the production of black holes. In astrophysics, one can seek excess supernovae cooling [201], a diffuse cosmic gamma-ray background [202], or re-heating of supernovae remnants [203]. As mentioned in Sec. 4.1.1, DSR predicts an energy-dependent speed of light, and this may be picked-up by the observation of energy-dependent arrival times of high energy photons from gamma ray bursts [204]. Lorentz invariance violations or objective collapse models [130] may also be tested by studying the flux-ratio of cosmogenic neutrinos species [205].

So far we have mainly talked about the conceptual and empirical hardship one faces in attempts to quantize gravity or to find evidence of quantum gravitational effects. It should be noted that quantum theory itself is riddled with foundational and interpretation issues, namely regarding the measurement problem [114]. Because of this, some work has been done towards an opposite approach, in which it is not gravity that is to be quantized, but rather quantum theory that should be "gravitized" [132, 206].

This reflection must give us pause: with no current empirical deviations to standard GR and quantum theory, it is unclear what it sought after or what is designated by "quantum gravity". In fact, quantum gravity may not imply the quantization of gravity. To make room for the possibility that gravity may be an emergent phenomenon, rather than a fundamental interaction, one must contemplate the possibility that quantizing gravitational degrees of freedom may be of no avail [207]. With this in mind, the quest for quantum gravity[3] may more conservatively be defined as any approach that aims to solve the problem of describing gravitational interactions sourced by quantum distributions of mass-energy.

5.1.2 *Quantum control based proposals*

Looking back at the long history of quantum gravity phenomenology, one may regret that finding empirical hints may hinge on our capacity to characterize physical systems in extremely high energy settings, be it in the uninviting neighborhood of a black hole singular-

3 One may opt for the less committing terminology of "non-classical gravity".

ity, in the hardly accessible fossilized early universe, or in extremely expensive yet inadequately energetic accelerators sheltered beneath the landscapes of Geneva. Although table-top tests of quantum gravity have long been considered to be impossible, recent years have seen a series of experimental and engineering breakthroughs in the fine coherent control of larger and larger quantum systems, which in conjunction with the immense progress of quantum information theory, have opened up new avenues to tackle quantum gravity phenomenology from the comfort of a laboratory.

One such table-top proposal was studied in Sec. 4.2.2 to test the generalized uncertainty principle [190]. Many table-top proposals using low-velocity, high-mass, long coherence time systems, have been put forward to test quantum gravitational features. In Ref. [208] Bose-Einstein condensates are proposed to test the non-gaussianity of the dynamics induced by non-classical gravity. Bose-Einstein condensates are also put forward in Ref. [209], where the authors claim that gravitational decoherence may be probed in the gravitational self-energies of condensates with different geometries. In Refs. [210, 211] optomechanical systems are suggested as a platform to detect the minute gravitational fields sourced by positional cat states of massive systems. This being said, one particular kind of approach to table-top tests of quantum gravity that has recently received much attention, is based on quantum entanglement.

We have mentioned in our closing of Sec. 5.1.1 that a primary challenge to establishing a quantum theory of gravity, is the very clarification of what is meant by quantum, as opposed to classical. Many features described by quantum mechanics and absent from classical physics may include quantum tunneling, Heisenberg's uncertainty relations, or coherent superpositions of states. What the advent of quantum information theory has brought to the table, are proper, model-independent and operational notions of non-classicality, essentially classes of correlations. Among those operational notions, quantum entanglement has been at the center of attention. This non-classical correlation that we have presented at length in Sec. 2.4 cannot be increased through local operations and classical communication, by definition. Because of this unambiguous and model-agnostic definition, many modern proposals to test gravitational non-classicality have been centered around the detection of entanglement generated by the gravitational coupling between two or more systems [212–214]. We shall refer to these as Gravity Mediated Entanglement (GME) protocols.

The foundational bedrock of such experiments is the quantum information theoretic fact that entanglement cannot be generated under LOCC operations. As such, any experimental manifestation of entanglement between systems the dynamics of which can be proven to be mainly gravitational, is proof that one cannot model the gravitational

interaction as the action of a classical channel. As it stands, this result has also been derived from locality and the interoperability of information in broader frameworks such as constructor theory [215], which does not assume quantum theory nor general relativity, and does not commit to any kind of dynamics for the mediator. Investigations from the basic framework of generalized probabilistic theories (a subset of which is quantum theory) have led to a similar conclusion [216]. Namely, it was shown using the diagrammatic language of quantum process theory (see Ref. [59] for a thorough and pedagogical introduction) that one cannot have the conjunction of the following three hypotheses

1. Gravity has the capacity to generate entanglement.
2. Gravity mediates the interaction between two systems.
3. Gravity is classical.

While this holds true for entanglement, it is of course no longer the case when one considers a weaker quantum correlation such as discord, which can increase through LOCC operations. It was recently shown that a fully classical model treating gravitation as a weak continuous measurement of position [217] may not generate entanglement, but may generate discord between two systems [218].

While the aforementioned protocols to test GME seem more promising than the presumed dead-end of direct graviton detection, they suffer from the weakness of the gravitational coupling. By relying on the entanglement of the motional states, these proposals essentially try to pick up contributions from the quadratic term in the Newtonian gravitational potential expansion

$$H_G = -\frac{Gm^2}{d}\left(1 + \frac{(x_1 - x_2)}{d} + \frac{(x_1 - x_2)^2}{d^2} + O\left(\left(\frac{x_1 - x_2}{d}\right)^3\right)\right),$$

where x_1 and x_2 label the two system's positions with respect to their respective trap centers, and it is assumed $(x_2 - x_1) \ll d$. The order 0 term is an offset, the linear term is local and as such does not entangle the motional states. It is only at the quadratic order that cross terms between operators of the two systems appear, effectively inducing a two-mode squeezing. As a figure of merit, for micro-particles of mass 10^{-7}kg trapped with a frequency $\omega = 10^5$Hz and a trap separation distance $d = 10^{-4}$m, the ratio between consecutive terms in the expansion is 10^{-12}.

There exists a very different flavour of GME protocol, that we shall *very appropriately* refer to as Doubly Interferometric Gravity Mediated Entanglement (DIGME) protocol, which was proposed by Bose et al. [219] and Marletto and Vedral [220]. Instead of relying on motional states, the DIGME protocol relies on a phase entanglement in a doubly interferometric setup. At the cost of requiring massive cat-states,

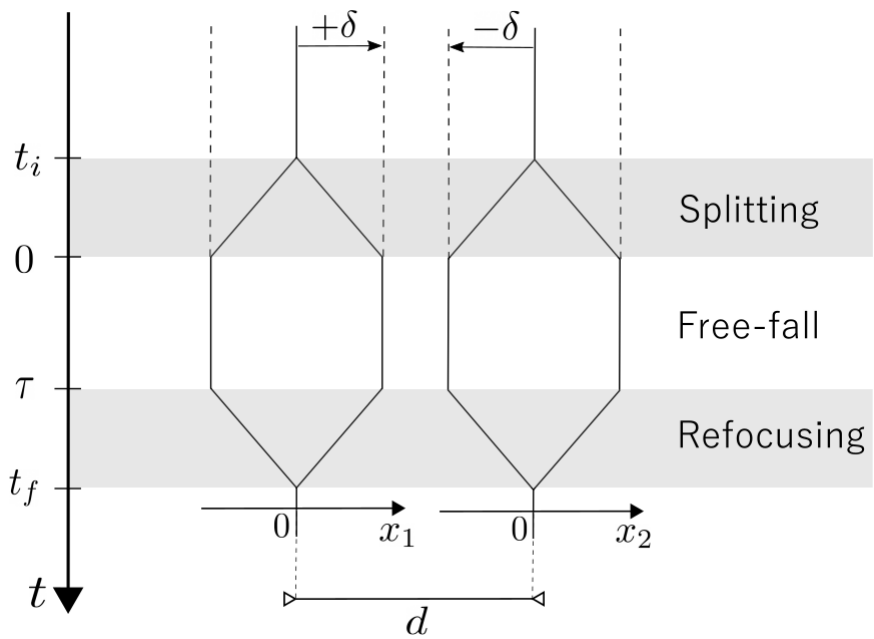


Figure 11: The three steps of the DIGME protocol.

this approach has two salient advantages compared to the direct analysis of motional states. The first one, is to have an entanglement signal that is amplified by the minuteness of the Planck constant. The second, is that this entanglement is driven by the much stronger linear term of the gravitational potential expansion, instead of the quadratic term. Let us dedicate the next section to a more detailed overview of the DIGME setup. Throughout the remainder of this thesis, we shall refer to the admittedly more fleshed out proposal by Bose et al., upon which most of the work presented here was based.

5.1.3 *The massive DIGME protocol: first pass*

Let us present in a nutshell the Bose et al. DIGME proposal, as originally exposed. Essentially, this proposal consists in splitting two localized systems by entangling their spatial positions to their spin degree of freedom, through a Stern-Gerlach type process. Under some assumptions that we shall discuss in further details, the phase accumulated by each pair of position states will differ, and will depend on $H_G/\hbar$. This phase information can then be stored into the spin degree of freedom by refocusing the massive systems, and thus entanglement may be read off from bipartite spin measurements.

Explicitly, the DIGME proposal breaks down in three steps: a spin-dependent spatial splitting, a free-fall, and a refocusing, as shown in Fig. 11. Let us introduce the respective states $|L\rangle, |C\rangle, |R\rangle$ for left, center and right position eigenstates for each system, of identical effective mass m. The center state $|C\rangle_{1,2}$ of each system is taken to be

the eigenstate corresponding to the origin of each system's position coordinate $x_{1,2} = 0$. We further denote $d > 0$ the separation between the two central states. Under the assumption that the massive system is always in a (superposition of) position eigenstate(s), that we shall refer to as Position Eigenstate Approximation (PEA), the initial state of the bipartite system is written as $|\psi(t_i)\rangle = |C, s_+\rangle |C, s_+\rangle$, where $|s_+\rangle = \frac{1}{\sqrt{2}}(|s_L\rangle + |s_R\rangle)$. After the spin dependent spatial splitting, the state reads

$$|\psi(0)\rangle = \frac{1}{2}(|L, s_L\rangle + |R, s_R\rangle)(|L, s_L\rangle + |R, s_R\rangle) = \frac{1}{2} \sum_{ij\in\{L,R\}} |i, s_i\rangle \left|j, s_j\right\rangle .$$

With a Newtonian gravitational potential, assuming that the positional drift between the systems evolving under their mutual gravitational influences is negligible, the noiseless state after a free-fall of duration τ is given by

$$|\psi(\tau)\rangle = \frac{1}{2} \sum_{ij\in\{L,R\}} e^{-i\phi_{ij}(\tau)} |i, s_i\rangle \left|j, s_j\right\rangle , \tag{60}$$

where $\phi_{ij}(t_f) = \phi_{ij}(\tau) = -\frac{Gm^2\tau}{\hbar d_{ij}}$ and d_{ij} is the distance between the two systems in the positional state $|ij\rangle$. By refocusing the two systems, one can discard the position dependence and find a final bipartite spin state $|\psi_s(\tau)\rangle = \frac{1}{2}\sum_{ij\in\{L,R\}} e^{-i\phi_{ij}(\tau)} \left|s_i, s_j\right\rangle$. In the ideal scenario that is considered here, the refocusing disentangles the positions from the spins in a very short time compared to the free-fall duration, and as such one can trace out the position degree of freedom without introducing noise in the spins. In Sec. 5.2.1, we will turn back to this assumption, in particular in combination with the PEA.

Assuming that the splitting and refocusing shift the positions of both systems by the same amount δ, we have $d_{RR} = d_{LL} = d$ so that one can instead look at the relative phases $\Delta\phi_{ij}(\tau) = \phi_{ij}(\tau) - \phi$ where $\phi = -Gm^2\tau/\hbar d$, which is non-vanishing only for $i \neq j$. Up to a global phase, it is then established that the final spin state reads

$$|\psi_s(\tau)\rangle = \frac{1}{2}(|s_L\rangle \otimes (|s_L\rangle + e^{i\Delta\phi_{LR}} |s_R\rangle) + |s_R\rangle \otimes (|s_R\rangle + e^{i\Delta\phi_{RL}} |s_L\rangle)).$$

An elementary entanglement condition for this state can be derived from the very definition of non-separability. Indeed, one can rewrite the state as $|\psi_s\rangle = \frac{1}{\sqrt{2}}(|s_L\rangle \otimes |a\rangle + |s_R\rangle \otimes |b\rangle)$ where we have the linear dependence equivalence

$$|a\rangle \propto |b\rangle \iff \exists\alpha \in \mathbb{R},\ e^{i\alpha} |s_L\rangle + e^{i\alpha+\Delta\phi_{LR}} |s_R\rangle = e^{i\Delta\phi_{RL}} |s_L\rangle + |s_R\rangle .$$

From this, it becomes apparent that the state may be factorized if and only if $(\alpha - \Delta\phi_{RL}, \alpha + \Delta\phi_{LR}) \in (2\pi\mathbb{Z})^2$. That is, a necessary and sufficient condition for entanglement reads $\Delta\phi_{RL} + \Delta\phi_{LR} \notin 2\pi\mathbb{Z}$.

Associating the $|s_{L,R}\rangle$ spin states with the eigenbasis of the Pauli Z operator, explicitly $Z|s_L\rangle = |s_L\rangle$ and $Z|s_R\rangle = -|s_R\rangle$, one can easily establish the following expectation values[4] on the state $|\psi_s\rangle$

$$\begin{cases} \langle X \otimes Z\rangle &= \frac{1}{2}(\cos(\Delta\phi_{RL}) - \cos(\Delta\phi_{LR})) \\ \langle Y \otimes Y\rangle &= \frac{1}{2}(\cos(\Delta\phi_{RL} - \Delta\phi_{LR}) - 1) \end{cases},$$

where X, Y are the two other Pauli operators as defined in Eq. (28). Under the separability condition, $\Delta\phi_{LR} + \Delta\phi_{RL} \in 2\pi\mathbb{Z}$ it becomes apparent that one necessarily has $\langle X \otimes Z\rangle = 0$ and $\langle Y \otimes Y\rangle = -\sin^2(\Delta\phi_{RL})$. In light of this observation, Bose et al. define the simple criterion $|\langle X \otimes Z\rangle + \langle Y \otimes Y\rangle| > 1$ as a sufficient condition for entanglement.

As a figure of merit, let us consider the following set of parameter values: $d = 400\ \mu m, \delta = 125\ \mu m, m = 10^{-14}$ kg. Then the sufficient condition is met after a free fall duration of around 8 seconds. As we can see, by having turned the weakness of the Planck constant into an advantage that helps compete against the weak Gm^2 factor, the DIGME approach yields much more promising (or much less inauspicious) prospects for the test of quantum gravitational effects. While the DIGME protocol has impressively allowed to even consider probing quantum gravitational effects in a laboratory, the required effective masses and interaction durations remain well beyond what is currently achievable.

As presented at this stage, there are some challenges the DIGME protocol is faced with, which do not fall under engineering capabilities, but are more intrinsic to the platform and the model itself. The main physical limitation to GME revelation is the presence of unwanted quantum forces whenever one makes use of matter. Even with the elimination of residual electrostatic or dipole-dipole interactions, there is no circumventing the Casimir interaction, a macroscopic force first predicted by Hendrick Casimir [221] during his study of the Van der Waal's forces between a pair of polarizable molecules, arising from the vacuum fluctuations of the electromagnetic field.

In the original proposal by Bose et al., this effect is not omitted, but rather taken care of by having a voluntarily coarse entanglement criterion. That is, the entanglement condition may require much more phase signal than actually needed to have an entangled state. While this increases the required interaction time τ, in return one can be confident that in regimes where the gravitational coupling is much stronger than the Casimir coupling (which entails a closest approach distance), any data satisfying the entanglement condition may not have appeared through the Casimir interaction alone.

Clarifying this statement about empirical data supporting GME will be the center of our focus in the next sections. We will spend time to extend and formalize the DIGME proposal, to include mixed states and decoherence, devise a way to overcome the Casimir closest

4 It is understood that $|\psi_s\rangle$ and the relative phases $\Delta\phi$ are functions of τ.

approach limit, establish an optimal entanglement witness, and touch upon a loophole in certifying GME in the presence of ill-determined entangling forces. The following analysis will serve to illustrate the robustness of DIGME approaches.

5.2 THE MASSIVE DIGME PROTOCOL: SECOND PASS

In this section, we go over the DIGME protocol, present a new entanglement witness, and show how to account for noisy states and decoherence. We show how one can conclusively infer GME from empirical data.

5.2.1 *The position eigenstate approximation*

In our first pass of the DIGME protocol, we have presented two theoretical simplifications: using position eigenstates, and assuming that tracing out the motional degree of freedom after refocusing does not completely decohere the spin state. Although these simplifications help focus on the key ideas, it should be noted that they are contradictory. Should the states be rigorously δ-distributed in position-space, then drift can absolutely not be neglected. Let us re-derive and formalize the dynamics without relying on the PEA, and by considering the possibility of having mixed initial trapped motional states, particularly initial thermal states, for their ubiquity in experiments. We will find that the resulting corrections to the PEA are negligible for a reasonable range of trapping frequencies and temperatures.

Let us now represent the initial state of the system with the density operator ρ^i which is a product of two motional states in a superposition of spin states, separated by distance d. At the end of the splitting operation, which is a spin-controlled spatial displacement by $\pm\delta$, the system is in state $\rho(0)$ which is two spatial superpositions. The free-fall duration is labelled by τ, after which the state is $\rho(\tau)$. The non-adaptive refocusing merges the positional superpositions without taking into account drift during free-fall, and results in a final state that depends on the free-fall duration $\rho^f(\tau)$.

As in the original proposal, we assume that the splitting and refocusing operations can be carried out in a short time compared to the free-fall duration, and use a Newtonian potential for gravity. Since $d/c \ll \tau$, this is a completely valid static limit to the fully general relativistic description [222], which formulates the same predictions in the case of superposition of geometries [223].

Consider two identical particles of mass m that are initially in a product of two arbitrary motional states and in a superposition of spin states $\rho^i = (\pi_1 \otimes \rho_+) \otimes (\pi_2 \otimes \rho_+)$, where we have denoted the spin state $\rho_+ := \frac{1}{2}(|s_L\rangle + |s_R\rangle)(\langle s_L| + \langle s_R|)$, which will provide labels for the displacements. As in the original proposal, the spin-controlled

spatial splitting is assumed to simply shift the positions, such that the momentum expectation values at the beginning of the free fall vanishes. The splitting operation reads $(D_L \otimes |s_L\rangle\langle s_L| + D_R \otimes |s_R\rangle\langle s_R|)^{\otimes 2}$, where $D_\mu = D(\kappa_\mu) = e^{\kappa_\mu a^\dagger - \kappa_\mu^* a}$ is the displacement operator as defined in Eq. (18), and $\kappa_R = -\kappa_L = \kappa \in \mathbb{R}_+$. We denote δ the physical distance by which the state is displaced, so $\kappa = \delta\sqrt{m\omega/2\hbar}$ where ω is some initial trap frequency.

In the noiseless case, the final state obtained at the end of the free-fall after the refocusing operation, which is the Hermitian conjugate of the splitting, reads

$$\rho^f(\tau) = \frac{1}{4}\sum_{\alpha\beta\mu\nu}(D_\alpha^\dagger \otimes D_\beta^\dagger)U_d(D_\alpha \otimes D_\beta)\rho^i(D_\mu \otimes D_\nu)U_d(D_\mu^\dagger \otimes D_\nu^\dagger),$$

where the sum is carried out over $(\alpha, \beta, \mu, \nu) \in \{L, R\}$, U_d is the unitary propagator generated by the Newtonian gravitational Hamiltonian $H_d = (p_1^2 + p_2^2)/2m - Gm^2/(d + x_2 - x_1)$ for a duration τ, and G is the gravitational constant. One can view the action of the displacement operators as an origin shift of the positions, which can be absorbed in the separating distance d. Explicitly, this amounts to defining distinct propagators through $(D_\mu^\dagger \otimes D_\nu^\dagger)U_d(D_\mu \otimes D_\nu) := U_{d_{\mu\nu}}$ where $d_{\mu\nu} = d - \delta_\mu + \delta_\nu \in \{d - 2\delta, d, d + 2\delta\}$. Thus, we have transposed the situation where we had three distinct relative displacements, to one where we have three distinct separations and propagators acting on the same initial state. Then, by pulling out the potential offset term $-Gm^2/d_{\mu\nu}$ from the Hamiltonian, the matrix elements $s_{\alpha\beta\mu\nu}$ of the reduced spin state $\mathrm{Tr}_{\mathrm{motion}}[\rho^f(\tau)] = \sum_{\alpha\beta\mu\nu} s_{\alpha\beta\mu\nu}\,|s_\alpha s_\beta\rangle\langle s_\mu s_\nu|$ read

$$s_{\alpha\beta\mu\nu} = \frac{1}{4}\exp\left[\frac{-iGm^2\tau}{\hbar}Q^{(1)}_{\alpha\beta\mu\nu}\right]\mathrm{Tr}\left[\mathcal{U}_{\alpha\beta}{}^\dagger\mathcal{U}_{\mu\nu}(\pi_1 \otimes \pi_2)\right], \tag{61}$$

where we have introduced $\forall n \in \mathbb{N}$, $Q^{(n)}_{\alpha\beta\mu\nu} = \frac{1}{d^n_{\alpha\beta}} - \frac{1}{d^n_{\mu\nu}}$, and where $\mathcal{U}_{\alpha\beta}$ are propagators generated by the Hamiltonians with vanishing potential offset. In doing so, we have represented the propagation of the full system up to a shift of position operator origins, as a sum of four pairwise evolutions, three of which are distinct. The result obtained with the PEA approximation can be arrived at by discarding the remaining trace.

Up to now, what we have done was valid for position coordinates in the open disc of convergence of the analytic expansion of the potential term. Let us restrict ourselves to the case where $|x_2 - x_1| \ll d - 2\delta$ and inspect some results we might infer with a truncated potential. With an order 1 truncation the BCH identity gives

$$\mathcal{U}^\dagger_{\alpha\beta}\mathcal{U}_{\mu\nu} = e^{-i\tau^3 G^2 m^3 Q^{(4)}_{\alpha\beta\mu\nu}/6\hbar} D\left(\theta_{\alpha\beta\mu\nu}\right) \otimes D\left(-\theta_{\alpha\beta\mu\nu}\right), \tag{62}$$

where $\theta_{\alpha\beta\mu\nu} = \frac{GmQ^{(2)}_{\alpha\beta\mu\nu}\tau}{\sqrt{2}}\left[\frac{\tau}{2}\sqrt{\frac{m\omega}{\hbar}} - i\sqrt{\frac{m}{\hbar\omega}}\right]$. As classical intuition would suggest, the two particles are displaced towards one another and acquire opposite momenta.

By further restricting ourselves to the case of two initially identical motional states $\pi_1 = \pi_2 = \pi$, we obtain

$$\mathrm{Tr}\left[\mathcal{U}_{\alpha\beta}{}^{\dagger}\mathcal{U}_{\mu\nu}\pi^{\otimes 2}\right] = e^{-i\tau^3 G^2 m^3 Q^{(4)}_{\alpha\beta\mu\nu}/6\hbar} e^{-|\theta_{\alpha\beta\mu\nu}|^2}\left(C_N\left(\frac{\theta_{\alpha\beta\mu\nu}}{2}\right)\right)^2, \tag{63}$$

where $C_N : \lambda \longmapsto \mathrm{Tr}\left[\pi e^{\lambda a^\dagger} e^{-\lambda^* a}\right]$ is the normally ordered characteristic function of π [73]. From Eq. (24), the spin density matrix elements for an initial thermal state with $\langle N\rangle = \overline{n}$ is deduced to obey

$$s_{\alpha\beta\mu\nu} = \frac{1}{4} e^{-iGm^2\tau Q^{(1)}_{\alpha\beta\mu\nu}/\hbar} e^{-iG^2 m^3\tau^3 Q^{(4)}_{\alpha\beta\mu\nu}/6\hbar} e^{-(\frac{\overline{n}}{2}+1)|\theta_{\alpha\beta\mu\nu}|^2}. \tag{64}$$

The first phase factor was the only term accounted for in our first pass of the DIGME protocol. The second phase factor comes in as a first order phase correction. The third factor corresponds to a first order decoherence effect due to the drift of the particles. Detailed derivations of Eqs. (63) and (64) can be found in Appendix E.1.

Let us now evaluate the validity of the PEA approximation. To facilitate comparison, we work with the parameters of the original proposal, ($d = 400$ μm, $\delta = 125$ μm, $m = 10^{-14}$ kg) and with a sensible trapping frequency $\omega = 10^3$ Hz [224]. For the fastest oscillating terms ($\alpha\beta\mu\nu = \mathrm{LRRL}$) we have $|Q^{(1)}| \sim 3.6 \times 10^3$ m^{-1} and $|Q^{(4)}| \sim 6.2 \times 10^{14}$ m^{-4}. The first phase reaches unit radian after a characteristic free-fall duration $\tau \sim 4.4$ s. After 10 seconds of free-fall, the phase correction is approximately 4×10^{-12} rad and the decoherence factors are $\exp(-2.8 \times 10^{-8})$ and $\exp(-0.014)$ respectively for zero temperature and $T = 7.6$ mK ($\overline{n} = 10^6$). This shows the PEA to be perfectly valid for the purpose of this proposal.

In the PEA, the reduced spin state can be considered pure and reads $|\psi_s(\tau)\rangle = \frac{1}{2}(|00\rangle + e^{i\Delta\phi_{LR}}|01\rangle + e^{i\Delta\phi_{RL}}|10\rangle + |11\rangle)$ up to a global phase, where $\Delta\phi_{\mu\nu} = Gm^2\tau(\frac{1}{d} - \frac{1}{d_{\mu\nu}})$. This is the form that was directly posited in the original proposal, and we shall take it as our noiseless state.

It was furthermore argued that the original parameters constitute a regime in which Casimir-Polder (CP) interactions may be neglected. The CP potential [225] reads $V^C_{\mu\nu} = -\alpha(R,\epsilon)/(d_{\mu\nu} + x_2 - x_1)^7$, where the coupling constant $\alpha(R,\epsilon) = \left(\frac{\epsilon-1}{\epsilon+2}\right)^2 \frac{23\hbar c R^6}{4\pi}$ depends on the radius R of the microspheres and their relative permittivity ϵ. Inclusion of the CP interaction leads to the following form for the spin density matrix elements:

$$s_{\alpha\beta\mu\nu} = \frac{1}{4}\exp\left(\frac{-i\tau}{\hbar}\left(Gm^2 Q^{(1)}_{\alpha\beta\mu\nu} + \alpha Q^{(7)}_{\alpha\beta\mu\nu}\right)\right) \times \mathrm{Tr}\left[\mathcal{U}_{\alpha\beta}{}^{\dagger}\mathcal{U}_{\mu\nu}(\pi_1 \otimes \pi_2)\right]. \tag{65}$$

With $R \approx 10^{-4}$ m, which roughly corresponds to a diamond microsphere of mass 10^{-14} kg and $\epsilon \approx 5.7$, the most rapidly evolving terms

have a gravity frequency of 0.226 Hz and a CP frequency 0.016 Hz. This confirms that the dynamics is dominated by the gravitational coupling for closest approach kept above roughly 200 μm.

Because we will shortly demonstrate how to overcome this CP closest approach limit, it is worth showing that the PEA is still valid in a smaller setup separation. If we decrease the separation distance d from 450 μm to 350 μm, the closest approach distance is reduced to 100 μm such that for the $|RL\rangle$ pair the dynamics is dominated by CP coupling. Specifically, the CP potential becomes roughly 4 times as strong as the gravitational potential. While this will require more caution in interpreting the entanglement as arising from gravity, working in this tighter setup lowers the required free-fall duration for an appreciable phase to $\tau \approx 54$ ms. In this regime, after 1 second of free-fall, the phase correction is approximately 7.03×10^{-14} rad and the decoherence factors are $\exp(-5 \times 10^{-11})$ and $\exp(-2.5 \times 10^{-6})$ respectively for zero temperature and $T = 7.6$ mK ($\overline{n} = 10^6$). This warrants our unreserved use of the PEA in the remainder of this chapter.

5.2.2 *An optimal entanglement witness*

Let us now cast the entanglement condition shown in Sec. 5.1.3 into the formal language of entanglement witnessing. We will also use the tools presented in Sec. 2.4.4 to build another witness which will pick up entanglement immediately as the free-fall stage begins, and consider a decoherence effect.

From the pure spin state resulting from the PEA, one can read off $\Delta\phi_{LR} + \Delta\phi_{RL} \in \{2n\pi \mid n \in \mathbb{Z}\}$ as a necessary and sufficient condition for separability. We have seen that $|\langle X \otimes Z\rangle + \langle Y \otimes Y\rangle| > 1$ is a sufficient condition for entanglement, where X, Y, Z denote Pauli operators. Formally, this amounts to choosing

$$W_0 = I \otimes I + X \otimes Z + Y \otimes Y,$$

as an entanglement witness [226], as for any separable two qubit state ρ, $\mathrm{Tr}(W_0\rho) \geqslant 0$. In the noiseless case, entanglement is revealed after roughly 8 seconds of free-fall, as shown in Fig. 12.

Although the order of magnitude for the required free-fall time is promising, it would still correspond to a falling distance of a few 10^2 meters on Earth, and is still 3 orders of magnitude above the coherence times observed in cutting edge matter-wave interferometry with much less massive particles [227]. Let us investigate how to shorten this characteristic duration, which would help make the protocol more robust to decoherence.

To illustrate the effect of decoherence, we choose a scattering term that induces an exponential dephasing of local motional states [228]. With no further knowledge of the practical implementation of this experiment, this model may only serve as an example, but is repre-

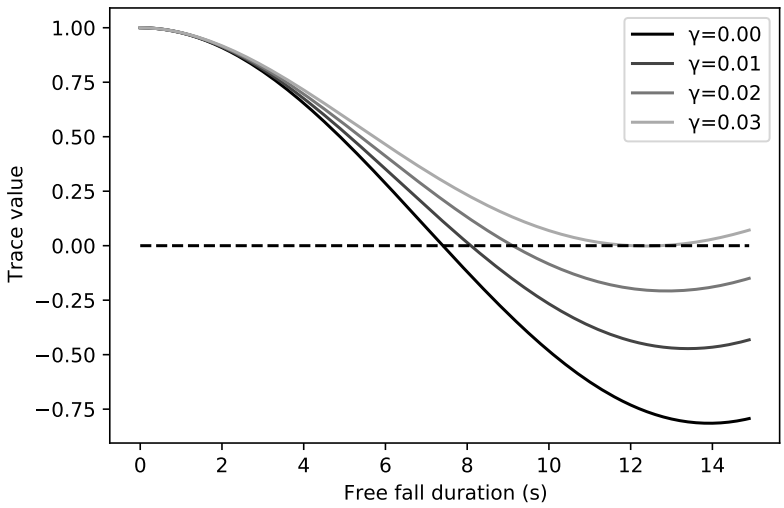


Figure 12: $\mathrm{Tr}(W_0 |\psi_s\rangle\langle\psi_s|)$, where W_0 is the entanglement witness put forward in [219], as a function of free-fall time under decoherence rates γ. Lighter lines represent stronger decoherence, and the dashed line is the negativity limit. At $\gamma = 0.03$ the witness can no longer reveal entanglement.

sentative of what would *a priori* affect any real implementation [229], and it is a relevant one to examine as it affects the coherence that matters most for any interference to take place. We shall denote the off-diagonal damping rate γ. Explicitly in the local position eigenstate basis $\{|L\rangle, |R\rangle\}$, the decoherence after duration τ acts as a dephasing channel $\pi \longmapsto (1-p)\pi + pZ\pi Z$ where $p = (1-e^{-\gamma\tau})/2$. Numerics show that the original witness W_0 fails to detect any entanglement for $\gamma \geqslant 0.03\ s^{-1}$. In an ideal zero-temperature noiseless scenario, it requires over 8 seconds of free-fall time for entanglement revelation when in fact state negativity [230] $\mathcal{N}(\rho_s) = \sum_{\lambda \in \mathrm{Sp}(\rho_s)\cap\mathbb{R}_-} |\lambda|$ is achieved immediately, as shown in Fig. 13. For this reason, relatively low decoherence rates will result in failure of entanglement witnessing.

To build another entanglement witness with a few local Pauli measurements in the spirit of [231], we use the PPT-criterion [99]. We assume $\phi = \Delta\phi_{LR} \gg \Delta\phi_{RL}, \Delta\phi$, which amounts to neglecting all but the phase induced by the strongest interacting pair of states. The final spin state reads $|\psi_s(\phi)\rangle = \frac{1}{2}(|00\rangle + |01\rangle + e^{i\phi}|10\rangle + |11\rangle)$ under the PEA, with corresponding density operator $\rho_s(\phi) := |\psi_s(\phi)\rangle\langle\psi_s(\phi)|$. The eigenstate associated with the negative eigenvalue of the partially transposed spin state $\rho_s^{\Gamma_2}(\phi)$ takes the following expression: $|\chi_-(\phi)\rangle = \frac{1}{2}(|00\rangle + ie^{-i\phi/2}|01\rangle - ie^{i\phi/2}|10\rangle - e^{-i\phi}|11\rangle)$. At $\phi = 0$

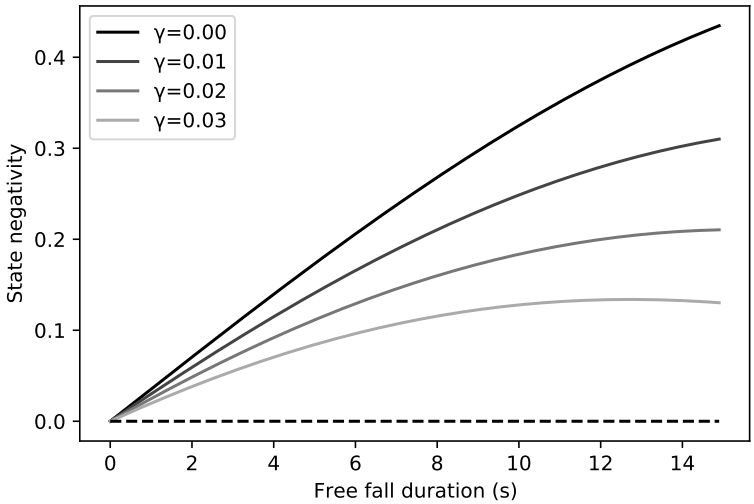


Figure 13: Negativity of the spin state with respect to free-fall time under decoherence rates γ. Lighter lines represent stronger decoherence, and the dashed line is the negativity limit. Negativity is an entanglement monotone, and the state is entangled when the negativity is positive.

one has $4\,|\chi_-\rangle\langle\chi_-| = I \otimes I - X \otimes X + Z \otimes Y - Y \otimes Z$, therefore the following operator defines a witness:

$$W_1 = 4\,|\chi_-\rangle\langle\chi_-|^{\Gamma_2} = I \otimes I - X \otimes X - Z \otimes Y - Y \otimes Z.$$

This witness reveals entanglement immediately after the start of the free-fall, as shown in Fig. 14, as long as the decoherence rate γ satisfies $\gamma < (\omega_{RL} + \omega_{LR})/2$ where the ω are respective coupling strengths $\omega_{\mu\nu} t = \Delta\phi_{\mu\nu}$, see Appendix E.2. With the original parameter settings, the witness works in principle for $\gamma < 0.0627\ s^{-1}$. Numerics show that the state is in fact not entangled for any higher decoherence rates, hence our witness is in this sense optimal.

While having a witness that detects entanglement with arbitrarily small phase signal may be advantageous, one must now imperatively take into account other entangling forces, such as the CP interaction, which will necessarily contribute to the entanglement detection. In the following section, we will discuss how to rigorously formulate statistical statements on the influence of non-gravitational interactions in the observed data.

5.2.3 *GME in the presence of unknown interactions*

In order to ensure that the final entangled spin state was induced by a gravitational propagator in the presence of other interactions, such as CP, that we for now assume we have good knowledge of, we adapt the

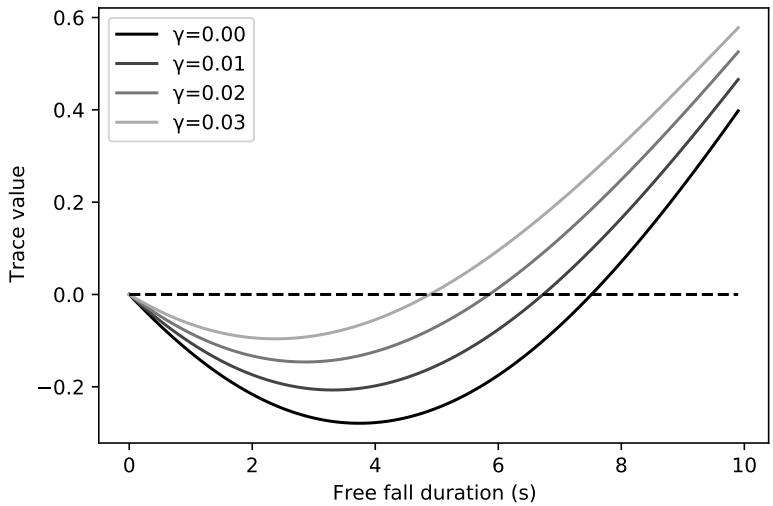


Figure 14: $\mathrm{Tr}(W_1 |\psi_s\rangle\langle\psi_s|)$ as a function of free-fall time under decoherence rates γ. Lighter lines represent stronger decoherence, and the dashed line is the negativity limit. The witness in theory can reveal entanglement even for relatively strong decoherence rates if the free-fall time is kept short. This comes at the expense of expectation values that are closer to zero.

approach developed in [232] for entanglement verification. In using such statistical methods, we assume the experiment can be repeated, for instance with particle recycling as outlined in [211]. The likelihood ratio test being the most powerful test for a given confidence level, according to the Neyman-Pearson lemma [233], we look at likelihood ratios between

- The null hypothesis H_0: *"The observed state is entangled state and results from CP interactions without gravity."*
- The alternative hypothesis H_a: *"The observed state is entangled and results not only from CP coupling but also from a gravitational interaction."*

It should be noted that ruling out H_0 in favor of H_a is essentially making two statements. The first one is that the observed empirical data is highly unlikely to have occurred without gravitational coupling. The second, is that the data corresponds to an entangled state. We begin by focusing on ruling out the absence of gravitational contribution.

To obtain the likelihood ratios, in general one can choose to measure a list of bipartite Pauli observables $\underline{\sigma} = [\sigma_1, ..., \sigma_l]$, $N \in \mathbb{N}^*$ times each. Each bipartite observable has 4 eigenstates which can

be listed as $\underline{e} = [|e_{11}\rangle, ..., |e_{14}\rangle, |e_{21}\rangle, ..., |e_{l4}\rangle]$. This list defines a $4l$-dimensional probability vector

$$\underline{p} = [p_{ij}]_{1\leqslant i\leqslant l, 1\leqslant j\leqslant 4} = [\mathrm{Tr}(\rho\,|e_{ij}\rangle\langle e_{ij}|)].$$

The data $\underline{n} = [n_{11}, ..., n_{14}, n_{21}, ..., n_{l4}]$ is a list of number of occurrences of measurement outcomes, each corresponding to an obtained eigenstate. The probability of obtaining the empirical data vector $\underline{n}$ from state ρ is given by the joint probability distribution

$$\mathbb{P}(\underline{n}|\rho) = \prod_{ij} p_{ij}^{n_{ij}} \stackrel{\text{def.}}{=} \mathcal{L}(\rho|\underline{n}),$$

and defines the likelihood $\mathcal{L}(\rho|\underline{n})$ of the state ρ given the empirical data vector $\underline{n}$.

The likelihood ratio, assuming the alternative state is obtained at the end of the experiment, reads

$$\Lambda_a = \frac{\mathcal{L}(\rho_0(\gamma, t)|\underline{n}_a)}{\mathcal{L}(\rho_a(\gamma, t)|\underline{n}_a)},$$

where ρ_0 is the spin state obtained at the end of the experiment under an exclusively CP induced evolution (null hypothesis state), ρ_a is the spin state obtained under the full CP and gravitational propagator (alternative hypothesis state), and $\underline{n}_a$ is an empirical vector obtained from measurements on ρ_a. The free-fall duration τ is chosen as the minimizing argument for the witness expectation value in the alternative hypothesis, so as to maximize the probability of certifying entanglement. Let us note that this makes τ dependent on the decoherence rate γ.

In order to have numbers suitable for numeric encoding, we shall use the logarithmic likelihood ratio $\lambda_a = -2\log(\Lambda_a)$, which reduces to the scalar product $\lambda_a = 2\underline{n}_a.(\log(\underline{p}_a) - \log(\underline{p}_0))$ in the alternative hypothesis, where the subscripts for the probability vectors indicate to the state (ρ_0 or ρ_a) they correspond to. For the W_1 witness measurement, we have $l = 3$ and the data $\underline{n}_a$ is a vector which encodes $3N$ empirical measurement outcomes (N for each of the bipartite Pauli observable $X \otimes X, Y \otimes Z, Z \otimes Y$) on ρ_a. High values of λ_a strongly support the alternative hypothesis.

To determine what value of λ_a is sufficiently high, what we would aim to achieve in the DIGME protocol is to minimize false positives, that is, to have a small significance level α or equivalently a high confidence level $1 - \alpha$. For a desired significance level α we define a minimum $\lambda_{\min}$ by

$$\mathbb{P}(\lambda_0 \geqslant \lambda_{\min}) = \alpha,$$

where λ_0 is the likelihood ratio λ_a assuming the null hypothesis is true. That is, the lower the significance level, the lower the probability that the likelihood ratio λ_a exceeds the threshold $\lambda_{\min}$ under the

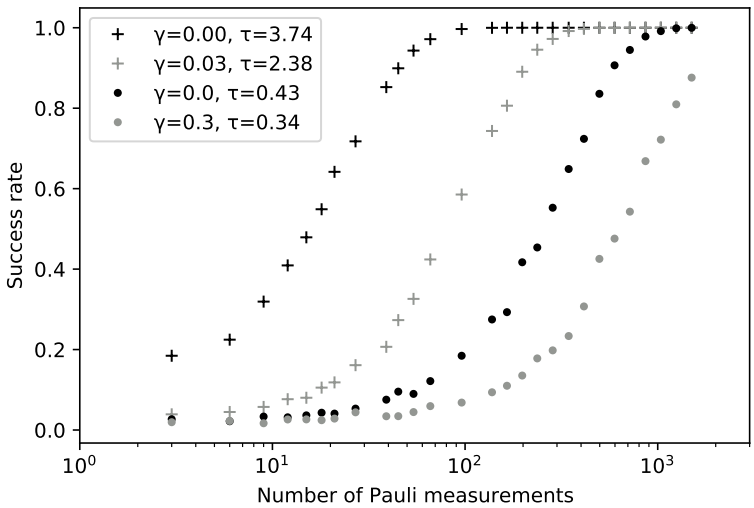


Figure 15: W_1 measurement state distinction success rates for a 99% confidence threshold, with respect to the number of bipartite Pauli measurements, for noiseless (black) and noisy scenarios (gray). The crosses correspond to the original setting with separation distance $d = 450$ μm while the dots correspond to $d = 350$ μm.

null hypothesis, i.e. the lower chance of a false positive (erroneous rejection of the null hypothesis).

In practice, we generate multiple data vectors $\underline{n}_0$ assuming the null hypothesis is true, and use the distribution of the resulting λ_0 for different values of N. For $\alpha = 1\%$, $\lambda_{\min}$ is then the 99-th percentile of the obtained λ_0. Once the $\lambda_{\min}(N, \gamma, \tau(\gamma))$ are determined, one can generate the λ_a from data where the alternative hypothesis is assumed true and inspect the frequency of $\lambda_a \geqslant \lambda_{\min}$. This frequency is termed state distinction success rate, and is what has been plotted in Fig. 15 for a confidence level of 99%, for the original parameter settings, and for a closer separation $d = 350$ μm. For the original separation $d = 450$ μm, in the noiseless case as well as with decoherence rate $\gamma = 0.03$ s^{-1}, 10^2 measurements of W_1, obtained with 3×10^2 repetitions of the experiment is enough to consistently rule out ρ_0. In the closer separation setting $d = 350$ μm certifying the alternative state reliably, requires around 10^3 repetitions.

As stated previously, one must also be able to certify entanglement from the empirical data. We see from Fig. 17 that even if, with $d = 450$ μm, 10^2 and $\gamma = 0.03$ s^{-1}, a number of 10^2 witness measurements is sufficient to rule out H_0, there is only a 70% chance for entanglement to be certified. Conversely, in the closer separation setup $d = 350$ μm the resulting state is more entangled, which makes the entanglement certification more likely to succeed, but ruling out H_0 becomes more demanding. In any case, with this approach, the

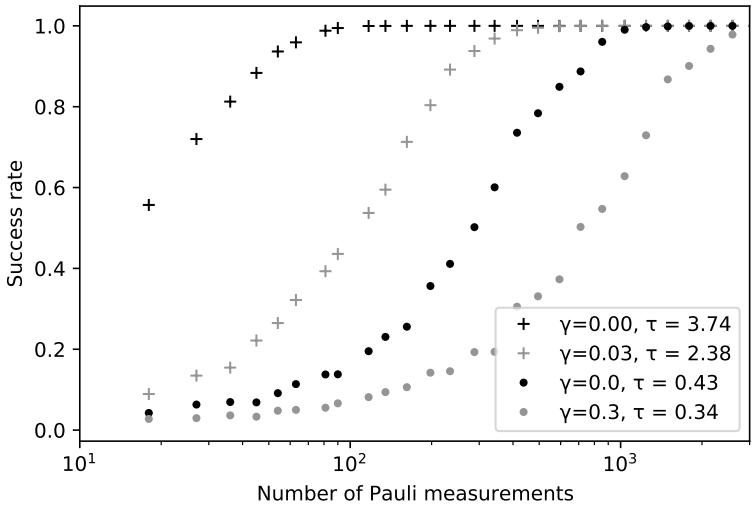


Figure 16: Tomographic state distinction success rates, for a 99% confidence threshold, with respect to the number of bipartite Pauli measurements, for noiseless (black) and noisy (gray) scenarios. The crosses correspond to the original separation distance $d = 450$ μm while the dots correspond to $d = 350$ μm.

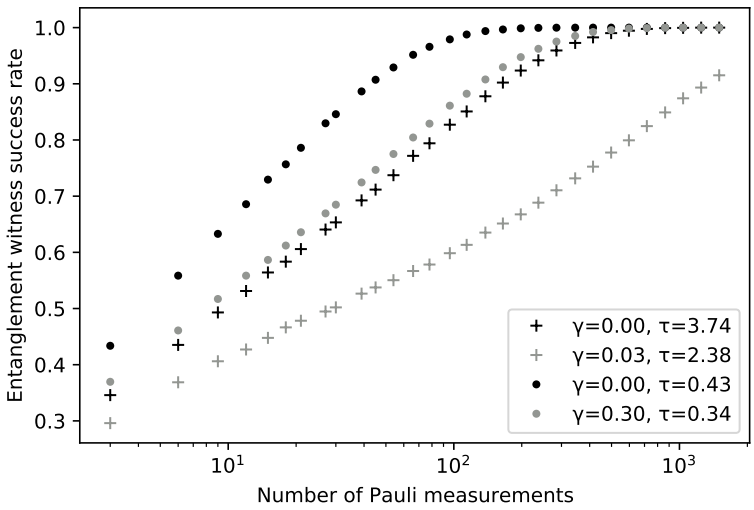


Figure 17: Probability of observing a negative empirical W_1 witness average, with respect to the number of bipartite Pauli measurements, for noiseless (black) and noisy (gray) scenarios. The crosses correspond to the original separation distance $d = 450$ μm while the dots correspond to $d = 350$ μm.

DIGME protocol no longer requires working in a regime where CP coupling is negligible.

Hence, from the repeated measurement of a single entanglement witness, provided good enough knowledge of non-gravitational interactions, one can confirm the presence of an entangled state that could not have been obtained without a gravitational contribution. The statistical approach shown here in the case of CP coupling may very well be applied to rule out many other versions of the null hypothesis. One could for instance choose to include a dipole-dipole interaction term, or test some modified versions of gravity such as derived in [234].

One may wonder whether quantum state tomography could be more reliable for our hypothesis testing. In fact, to rule out H_0, the witness measurement and the state tomography are equivalently efficient even in a regime dominated by CP interactions, that is, with the separation d brought down to 350 μm, as shown by the dotted plots in Fig. 15 and Fig. 16. In both tomographic and witness measurement cases, the CP limit can be overcome, and distinguishing the two states reliably requires around 10^3 bipartite Pauli measurements, that is, around 3×10^2 witness measurements, or 10^2 state tomographies. While it seems that witness measurement and full tomography may be equivalent, we will shortly see why the latter method allows to draw more ironclad conclusions on GME from the observed data.

Before we move on to the non-monotonicity loophole, one may object that in order to carry out our hypothesis testing, we have assumed good knowledge of the non-gravitational interactions. What if there are uncertainties in the non-gravitational couplings? It happens that the CP coupling constant $\alpha(R, \epsilon)$ is a perfect example of a quantity that cannot be precisely known, as it depends on the geometry of the never strictly spherical microdiamonds. At first glance from Eq. (65) it seems that an uncertainty in the CP coupling strength could potentially generate a wide range of null hypotheses, some of which may account for the observed data assuming H_a. The task we are faced with is now to rule out all modified but plausible versions of H_0, in which α is modified from its predicted value, in favor of H_a. The reason why this may look like a dead-end is that the witness expectation values $\langle W_1 \rangle_0$ and $\langle W_1 \rangle_a$ measured on the two possible states after a fixed free-fall duration τ may very well coincide if α is modified. Let us show a precise example.

For the original separation distance $d = 450$ μm, where the CP coupling is negligible compared to the gravitational coupling, it is quite unlikely that any uncertainty on the CP would account for any observed data (this would require over 500% uncertainty on the coupling α). However, the whole point of our analysis is to explore the possibility of overcoming the CP closest approach limit. In the tighter setup with $d = 350$ μm, not having precise knowledge of α becomes

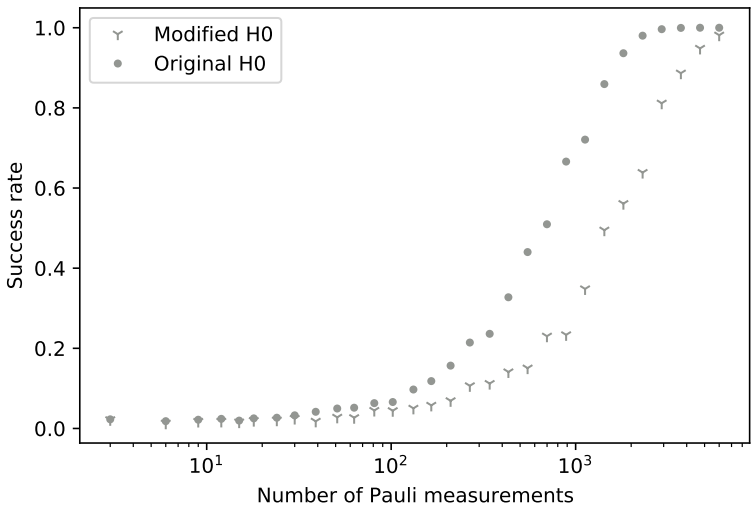


Figure 18: Witness measurement success rates with $d = 350\ \mu m, \gamma = 0.3\ s^{-1}$ of ruling out H_0 (dots) or the modified H_0 (tri markers) in favor of H_a, with respect to the number of bipartite Pauli measurements.

more problematic. With this closer separation setting and a decoherence rate of $\gamma = 0.3\ s^{-1}$ the proposed optimal free-fall duration for witnessing entanglement is $\tau = 0.34$ s. Numerics show that for this free-fall duration, a modified null hypothesis state where $\alpha' = 1.087\alpha$ will yield the same witness expectation value. In other words, a 9% uncertainty on α is enough for witness measurement values on the null-hypothesis state to converge to the same value as in the alternative hypothesis.

To solve this type of issue, a well known method exists and is sometimes referred to as a differential measurement. It consists is exploiting the fact that the CP potential follows a $1/r^7$ law, whereas the gravitational follows $1/r$, which would incur a discrepancy in the data as soon as the experiment is repeated with a new separation distance. Some reflection reveals that in fact, no such manipulation is necessary, as the DIGME protocol happens to already be differential, and so is intrinsically robust to this type of uncertainties. Let us clarify this observation.

Although one can imagine a modified α that could make the null and alternative witness expectation values coincide, in fact discrepancies will still appear in the individual Pauli observables constituting the witness measurement. This is corroborated by the plot shown in Fig. 18 where we observe that the state distinction success rate still increases with the number of measurements, despite having performed $\alpha \to 1.087\alpha$ for the null hypothesis state. This modification of α in the null hypothesis does increase the required number of repetitions to rule out H_0, but does not make this task impossible. The number

of bipartite Pauli measurements for a good state distinction success rate goes from a few 10^3 to a little less than 10^4.

Looking back at the spin density matrices in the null and alternative hypotheses, one notices that they can never be made equal by any amplification or damping of the coupling constants. This is because in Eq. (65) the $Q^{(1)}$ and $Q^{(7)}$ quantities are non-proportional tensors, they are differences between several proximities to different powers. From this general observation, one even obtains for free the robustness against any unwanted effects the potentials of which are not $1/r$, such as dipole-dipole interactions, which would involve a $Q^{(3)}$ quantity that is linearly independent of $Q^{(1)}$ and $Q^{(7)}$.

5.2.4 *Closing the non-monotonicity loophole*

Finally, we address a potential loophole to which a witness measurement approach is exposed. We describe how full tomography can provide a solution. We present results from tomographic simulations which provide an order of magnitude for the number of measurements required.

We have shown that by analyzing the witness Pauli measurements, it was possible to consistently state with a high degree of statistical confidence not only that the state is entangled but also that the state was produced by a gravitational interaction as opposed to merely a CP interaction. On its own, this would already constitute a highly significant observation, but there remains a critical loophole. Since entanglement witnesses are not entanglement monotones, one could argue that we have not explicitly shown that gravity has *increased* the entanglement. Indeed, the null hypothesis state is already entangled, with negativity $\mathcal{N}(\rho_0) > 0$, and there may well exist other valid quantum states ρ'_a that are indistinguishable from ρ_a by only looking at the witness statistics, and that may have negativities satisfying $\mathcal{N}(\rho_0) > \mathcal{N}(\rho'_a) > 0$. One such loophole state is shown and its construction explained in Appendix E.3. No matter how such a state may arise, a way forward to eliminate this loophole can be provided by using full tomography to calculate an entanglement monotone, as we shall demonstrate.

Quantum state tomography is a method to estimate quantum states from a complete set of measurements on many copies of the same state. It has been widely studied in general [1, 235] as well as in its application to entanglement verification [236]. Tomographic data allows one to reconstruct states, and in turn make statistical statements regarding entanglement monotones. To construct our state estimators, we use the popular method of maximum likelihood estimation [237]. While it was pointed out that this may not always be the most accurate estimation method [238], it is sufficient for our purpose, and has been extensively used in experiments [239–241].

Setting \ Repetitions		9	90	9×10^2	9×10^3
$d = 450\mu m$	$\gamma = 0$	1.8%	40.7%	$> 99.9\%$	$> 99.9\%$
	$\gamma = 0.03$	2.6%	2.8%	66.3%	$> 99.9\%$
$d = 350\mu m$	$\gamma = 0$	1.2%	7.5%	53.2%	$> 99.9\%$
	$\gamma = 0.3$	1.7%	4.1%	10.2%	88.7%

Table 4: Probability for the reconstructed alternative hypothesis state to have a higher negativity than the 99-th percentile most entangled reconstructed null hypothesis state, with respect to the number of Pauli measurements. Results shown for the original and shorter separation distances, and for the noiseless and strongest decoherence rate cases.

We seek to predict how reliably the experiment with tomographic data can certify gravitationally induced entanglement growth. To this end, we simulate a series of full tomographies on ρ_0 and ρ_a, and reconstruct their corresponding maximum likelihood states ρ_{ML} following a fixed-point iterative method [242]. Explicitly, the maximum likelihood state can be obtained from the empirical data vector $\underline{n} = [n_i]$ containing the number of occurrences of the Pauli-measurement outcome $|e_i\rangle\langle e_i|$ as it solves $\rho_{ML} = R(\rho_{ML})\rho_{ML}$, where

$$R : \rho \longmapsto \frac{1}{\|\underline{n}\|_1} \sum_i \frac{n_i}{\mathrm{Tr}(\rho\,|e_i\rangle\langle e_i|)}\,|e_i\rangle\langle e_i|\,.$$

Then the constructed sequence of two-qubit density matrices defined by $\rho_0 = I_4/4$ and $\forall k \in \mathbb{N}, \rho_{k+1} = \mathcal{N}_{\mathrm{Tr}}\left(R(\rho_k)\rho_k R(\rho_k)\right)$ where $\mathcal{N}_{\mathrm{Tr}}$ designates trace normalization, converges heuristically to the maximum likelihood state. We end the algorithm at the 100th iteration. Among 10^3 state reconstructions using 9×10 measurements, the fidelity [243] $\mathcal{F}(\rho_{100}, \rho) = \left(\mathrm{Tr}\left(\sqrt{\sqrt{\rho_{100}}\rho\sqrt{\rho_{100}}}\right)\right)^2$ between the simulated states is at least 90% and on average 95%. Among 10^3 state reconstructions using 9×10^3 measurements, the fidelity is always over 99%.

From the maximum likelihood reconstructed states, we find different negativity distributions in the two hypotheses. The results are summed up in Table 4, and show that in the original separation $d = 450$ μm a few 10^3 Pauli measurements is enough to consistently reject the null hypothesis and loophole states when $\gamma = 0.03\ s^{-1}$, and for the closer setup $d = 350$ μm where the CP interaction becomes significant, 10^4 Pauli measurements is sufficient to reject the null hypothesis and loophole sates around 90% of the time when $\gamma = 0.3\ s^{-1}$.

It should therefore be possible, by reconstructing the state from tomographic data on a relatively large but not unreasonable number of measurements, to obtain reliable proof of entanglement growth by gravitational interaction even in the presence of other stronger and possibly ill-known couplings, and decoherence.

5.3 THE PHOTONIC DIGME PROTOCOL

In this section, we present a variant of the DIGME protocol, which uses light instead of matter. We motivate this investigation in light of our previous analysis, having established that repeatability is crucial for a conclusive GME certification. We give a figure of merit for the required light pulses in order to have an appreciable phase.

5.3.1 *Motivations for a photonic protocol*

As innovative as it is, the massive DIGME protocol's implementation faces several experimental challenges and limitations, some of which pertain to engineering and experimental capabilities, while others are intrinsic to the protocol. From the point of view of experimental implementation, among the most critical obstacles, we may mention the coherent control of a microdiamond of mass on the order of 10^{-14} kg, which is several orders of magnitude beyond current cutting-edge quantum control [227, 244, 245]. What's more, the mismatch between nitrogen vacancy centers and centers of mass will induce a torque, the absence of which anyhow does not eliminate the issue of free-rotation [246]. Another concern as we have seen in the previous section, is the importance of repeatability in order to build up statistics. Ideally, one may achieve repeatability by recycling the particles, but the amount of trials one may run over a fixed time span may be limited by overheating issues [247–251]. Finally, we have discussed at length the effect of the CP interaction, which may only be accounted for with even greater repeatability.

From the theoretical perspective, the massive DIGME may only test the non-relativistic Newtonian regime of gravity, but may not capture features of gravity as a relativistic quantum field [252].

To resolve, or rather circumvent, some of the hurdles the massive DIGME proposal has to overcome, we present in this section an alternate approach, where we consider light beams as our gravitational split source. General relativity predicts that radiation, as much as matter, sources a gravitational field, the properties of which have been extensively studied [253–258]. We will chose the polarization-dependent beam-splitting as an optical equivalent to the Stern-Gerlach operation which performs a spin-dependent spatial splitting. While in the massive DIGME one measures a spin entanglement witness, we now consider the measurement of a polarization entanglement witness.

An immediate advantage of the photonic DIGME protocol is the absence of any unwanted interactions other than gravity. The effect of the direct short-range photon-photon scattering [259] can be safely neglected as long as the beams are not overlapping, and for low-energy photons. Thus, in the photonic DIGME protocol, the challenge to overcome is no longer the discrimination between different competitive

sources that may generate entanglement, but the certification of entanglement with a weak signal.

It is not hard, however, to imagine why such a variant may be prohibitively challenging, and perhaps why it has not been considered in the literature: the phase signal due to the gravitational coupling of light is expected to be extremely small. Furthermore, as we shall see, contrary to the massive DIGME protocol, one cannot have light beams interact along the whole interferometer length, further reducing the phase signal. Far from claiming to have found a revolutionary near term implementation of DIGME, the analysis presented here rather serves as a first attempt to quantify *how challenging* this approach may be. As previously stated, even if the entanglement generation may be weaker than in the massive DIGME - which as should be noted requires unreasonably large masses for appreciable signal- there is certainly a case for such an investigation in light of near-future experimental and technological advances. Modern laser technology [260, 261] allow for great tuneability and control of high-intensity light beams, as well as practical repeatability. While a single photon may only have a negligibly small effect on gravity mediated entanglement due to its small coupling to gravity, the collective effect and reliability of light as a source of entanglement generation may outscore any massive counterpart as a platform for witnessing GME.

Another advantage of the photonic DIGME, beyond experimental considerations, is its relevance in the investigation of both relativistic and quantum effects. Due to the easier tuneability of frequency - as opposed to mass - finer features of gravity and other deviations from classicality may be more easily probed. Furthermore, light may be viewed as a more convincing candidate, insofar as some gravitational degrees of freedom can be claimed to be quantized when DIGME experiments are performed within light-crossing times between spatial branches [262].

Incidentally, the investigation presented here may also be seen as way to practically demonstrate the gravitational coupling of light beams for the first time, regardless of entanglement. Various aspects of detecting the gravitational field of light beams were considered in Ref. [263]. Very recently, investigations around light have gained in popularity in regards to relativistic tests of GME, as shown by the recent study of photon-matter entanglement in Ref. [264], and photon self-interactions in Ref. [265].

Our presentation is structured as follows. We begin by describing the setup and introducing basic notions and approximations. We give a brief overview of the path integral description of the experiment, and how one extracts a phase signal. We also present some instructive and well-established calculations on the metric perturbations sourced by a single circularly polarized light pulse and introduce further helpful notations. Building on this basic situation, we construct the

metric perturbation for two counter-propagating pulses and derive the action for two circularly polarized counter-propagating, spatially separated light pulses. After showing some numerical estimations of the gravitationally generated phase, we discuss some further directions worth examining, such as improvements, further challenges, and more sophisticated models to describe the photonic DIGME protocol.

5.3.2 *Setup and assumptions*

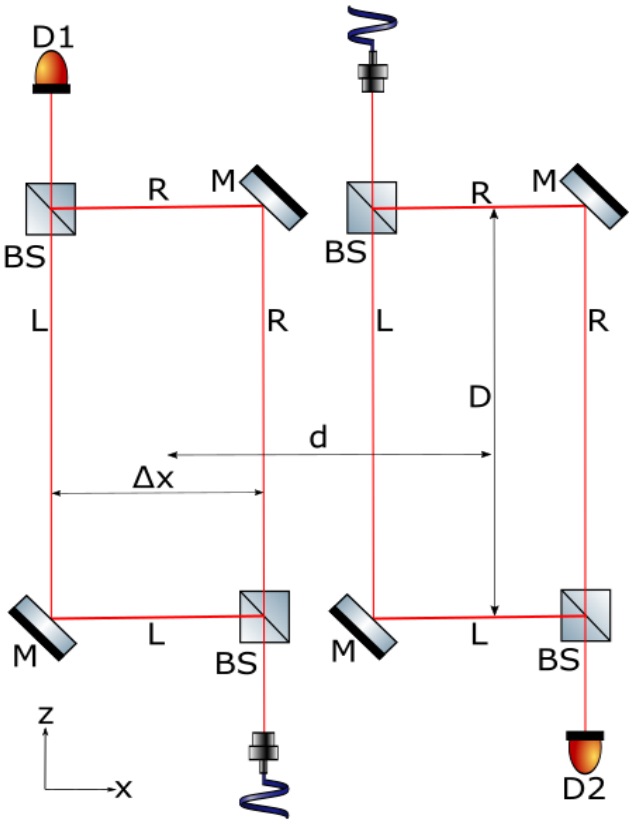


Figure 19: The double Mach-Zehnder interferometer setup of the photonic DIGME protocol. Two pulses of length L impinge on polarizing beam splitters, as they enter interferometer arms of length D which, for certain states, entangles their polarization degree of freedom with their output mode. With the use of waveplates, each beam splits into left and right circular polarization. Each pair of counter-propagating pulses interact gravitationally. Upon recombination, entanglement is witnessed through local polarization measurements.

Let us consider a setup consisting of two Mach-Zehnder interferometers, as shown in Fig. 19, that receive two counter-propagating light pulses as inputs. The length of each interferometer is D and the transverse separation of the two centers is d. Each input pulse

enters through a polarizing beam splitter. The reason why we chose two counter-propagating light pulses is that co-propagating pulses in vacuum do not interact [255, 266].

In general, the DIGME protocol consists of systems Q_a, $a \in \{1, 2\}$, that are both described by a spatial state $\vec{x}_a^{s_a}(t)$, which is made to depend on an internal degree of freedom s_a. In the massive case, this internal degree of freedom was taken to be the spin of a particle whereas for light, we shall take it to correspond to its polarization state. The internal configuration between two of the four different branches is then described by a state $|\sigma\rangle = \bigotimes_a |s_a\rangle$. After passing the light pulses through the beam splitter, separating light into horizontal or vertical polarization, a quarter-waveplate may be used to correspondingly have right-handed and left-handed circular components in output modes. At the end of the gravitational phase induction, the light pulses pass again through quarter-waveplates before passing through a beam splitter to detect the entanglement. Each beam splitter is assumed to be lossless 50:50.

Similar to the massive DIGME, once each of the two light pulses are in a spatial superposition entangled to their polarization degree of freedom, each branch will pick up a gravitationally generated phase. Even though light beams in coherent states [267–270] may contain a high expected photon number which may source an appreciable metric perturbation, let us note right away that they cannot be used for the DIGME protocol. Un-squeezed coherent states do not become entangled under beam splitting [271]. Because of this, in the remainder of this analysis, we focus on states for which the beam splitter is entangling, and we defer to a later section a discussion of such states. At the end of the gravitational interaction stage, the total position-polarization state will have evolved to have an identical expression to Eq.(60)

$$|\psi(\tau)\rangle = \frac{1}{2} \sum_{ij \in \{L,R\}} e^{-i\phi_{ij}(\tau)} |i, s_i\rangle \left|j, s_j\right\rangle,$$

from which one can read the final bipartite polarization state after refocusing

$$|\psi_s\rangle = \frac{1}{2}(|s_L\rangle \otimes (|s_L\rangle + e^{i\Delta\phi_{LR}} |s_R\rangle) + |s_R\rangle \otimes (|s_R\rangle + e^{i\Delta\phi_{RL}} |s_L\rangle)),$$

where exactly like in Sec. 5.1.3 we have left unspecified a global phase, and defined $\Delta\phi_{LR} := \phi_{LR} - \phi; \Delta\phi_{RL} := \phi_{RL} - \phi$ and $\phi_{RR} = \phi_{LL} = \phi$.

The gravitational interaction before the light pulses impinge on the first mirror is discarded, as we assume that the splitting and refocusing durations in the transverse direction are negligible compared to the travel time in the longitudinal direction, where the interaction takes place. Furthermore, by using appropriate waveplates one can always ensure that the four different branches are all described by either left or right-handed circular polarization states [272]. The reason why we assume circular polarization in the longitudinal stage

is not fundamental, but will simplify calculations as the associated the stress-energy density is constant. One may very-well relinquish this assumption, however longitudinally polarized pulses have stress-energy densities which are modulated along the propagation direction [273].

Given our setup and assumptions, the photonic DIGME considered here is operationally equivalent to the massive DIGME. Contrary to the massive DIGME, where the entangling phases are easily expressed under the Newtonian approximation and a Schrödinger propagator, there are no such simple toy models in the photonic case. In the following sections, we will take on the calculation of the entangling phases, which constitutes the main task of this investigation.

5.3.3 *Metric perturbation of a light pulse*

In the massive DIGME protocol as we have presented it, we have assumed a Newtonian gravitational action-at-a-distance. In order to enforce the locality of the gravitational field, a Lorentz-covariant description of the DIGME setup using path integrals was recently proposed [274]. We adopt this approach due to its freedom of choice in inserting the desired quantities which couple to each other gravitationally through the action.

Let us briefly go over the path integral description of the DIGME protocol. Given that the internal degree of freedom is entangled with the spatial mode, the time evolution operators can be expressed as $U_{i\to f} = \sum_\sigma |\sigma\rangle\langle\sigma| \otimes U^\sigma_{i\to f}$ where $U^\sigma_{i\to f}$ is defined from the initial and final total states $\left|\Psi^{i,f}\right\rangle$ of the system and fields. We assume that the field and the systems are not entangled with each other at the beginning and end of the protocol. Let us state the assumptions in Ref. [274], adapted for the purpose of our analysis:

1. Gravity is assumed to be weak ($\phi/c^2 \ll 1$ where ϕ can be taken to be an effective Newtonian potential).

2. The beam splitter does not couple to the gravitational field, and its action is only correlated with the spatial motion of the polarization state.

3. Loop corrections are assumed to be negligible, that is, we work in the stationary phase approximation.

4. The spatial modes of the different branches are assumed to be mutually orthogonal.

Under these approximations, the unitary time evolution operator for a polarization configuration σ reads $U^\sigma_{i\to f} \propto \exp\left\{\left(\frac{iS^\sigma}{\hbar}\right)\right\}\left|\Psi^f\right\rangle\left\langle\Psi^i\right|$, where S^σ is the joint on-shell action. There exists a decomposition of the action into $S = S_0 + S_{\mathcal{F}}$ with S_0 serving as a global phase that is

independent of σ and a phase which captures the field mediation $S_{\mathcal{F}}$. The phase can then be expressed as

$$\phi_\sigma = \frac{S^\sigma_{\mathcal{F}}[x^{s_a}_a, \mathcal{F}[x^{s_a}_a]]}{\hbar}.$$

The gravitational field sourced by systems considered in the DIGME protocol can be described as a perturbation of the Minkowski background metric $\eta_{\mu\nu}$. The action for such a linearized theory of gravity may be derived using standard general relativity [275]. We express the gravitational field $\mathcal{F}$ sourced by light as $g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}$ where $|h_{\mu\nu}| \ll 1$. We will work with the signature $(-,+,+,+)$. The on-shell action, after integration by parts, takes the form

$$S^\sigma_{\mathcal{F}} = \frac{1}{4}\int d^4x h_{\mu\nu} T^{\mu\nu}, \tag{66}$$

where $T_{\mu\nu}$ is the energy-momentum tensor. Here we work in the Lorentz gauge $\partial^\nu \bar{h}_{\mu\nu} = 0$, where we denote the trace reversal of a tensor $h_{\mu\nu}$ by $\bar{h}_{\mu\nu} = h_{\mu\nu} - \frac{1}{2}\eta_{\mu\nu}h$ and $h = \eta_{\mu\nu}h^{\mu\nu}$ as the trace of $h_{\mu\nu}$. The retarded solution of the linearized Einstein field equations [266, 274] is

$$h_{\mu\nu}(t,\vec{x}) = \frac{4G}{c^4}\int dx'^3 \eta_{\mu\alpha}\eta_{\nu\beta}\frac{\bar{T}^{\alpha\beta}(\vec{x}', t_r)}{|\vec{x}-\vec{x}'|}, \tag{67}$$

where $t_r := t - |\vec{x}-\vec{x}'|/c$ defines the retarded time.

In order to determine the action in the photonic DIGME protocol, we need to establish the form of the stress energy tensor, and the metric perturbation. To do so, let us start by inspecting a simpler situation: the stress energy components and metric perturbations associated with the propagation of a single light pulse over a distance D, as was carried out in Ref. [273].

The energy-momentum tensor of a single pulse $T^{\mu\nu}_0$ needs to account for contributions from the emitter and the absorber, to satisfy energy-momentum conservation. In free space and flat spacetime [276] we can express $T^{\mu\nu}$ using the field strength tensor $F_{\mu\nu}$ as $T^{\mu\nu}_0 = \frac{1}{\mu_0}\left(F^{\mu\alpha}F^\nu_\alpha - \frac{1}{4}\eta^{\mu\nu}F_{\alpha\beta}F^{\alpha\beta}\right)$, where $\mu_0 = 4\pi\cdot 10^{-7}\,\mathrm{H}\cdot\mathrm{m}^{-1}$ is the vacuum permeability. Considering an electromagnetic plane wave propagating in vacuum in the z-direction, the corresponding energy-momentum tensor depends only on $ct - z$. The energy density is given by $u = \frac{1}{2}(\varepsilon_0|\vec{E}_0|^2 + \frac{1}{\mu_0}|\vec{B}_0|^2) = \varepsilon_0|\vec{E}_0|^2$, where the vacuum permittivity is $\varepsilon_0 = 8.85\cdot 10^{-12}\,\mathrm{F}\cdot\mathrm{m}^{-1}$.

Thus the only non-vanishing components of the stress-energy tensor are given by $T^{00}_0 = T^{0z}_0 = T^{z0}_0 = T^{zz}_0 = u$, and it follows that the only non-vanishing components of the metric perturbation for a single pulse are $h_{00} = h_{zz} = -h_{0z} = -h_{z0} = h^p_0$. All in all, the energy density for a pulse propagating in the $+z$ direction is a function of the combination $ct - z$ only. We consider a pulse model in which

${T_0}^{\mu\nu} = Au(ct-z)\delta(x)\delta(y)$, where A is the effective area of the pulse in the xy-plane.

Consequently, evaluating the 00-component of Eq. (67) yields

$$h_0^p = \frac{4GA}{c^4}\int dz' \frac{u(ct_r(x,y,z,t,z')-z')}{\sqrt{\rho(x,y)^2+(z'-z)^2}}, \tag{68}$$

where $t_r = t - \sqrt{\rho(x,y)^2+(z-z')^2}/c$ is the retarded time, and we define $\rho(x,y) = \sqrt{x^2+y^2}$. To work out the integral, we perform the variable substitution $\zeta(x,y,z,z') = (z'-z) + \sqrt{\rho(x,y)^2+(z'-z)^2}$ in Eq. (68) and arrive at

$$h_0^p = \frac{4GA}{c^4}\int_{\zeta(x,y,z,a)}^{\zeta(x,y,z,b)} d\zeta \frac{u(ct-\zeta-z)}{\zeta}. \tag{69}$$

The integration boundaries a, b of each pulse contribution are chosen from the intersection of the world sheet boundaries of each pulse with the past light cone J^- of an observer located at spacetime position $x^\mu = (x,y,z,t)$. By denoting the pulse length L, one may define the auxiliary integration boundaries $\bar{a}, \bar{b}$ as solutions of $t_r(z') = \frac{z'+L}{c}$ and $t_r(z') = \frac{z'}{c}$. Explicitly:

$$\begin{cases} \bar{a}(x,y,z,t) &= z + \frac{(ct-L-z)^2-\rho(x,y)^2}{2(ct-L-z)} \\ \bar{b}(x,y,z,t) &= z + \frac{(ct-z)^2-\rho(x,y)^2}{2(ct-z)} \end{cases}.$$

Using these auxiliary boundaries, one can rewrite the integration boundaries a, b as

$$[a,b] = \begin{cases} \emptyset, & \bar{a} < \bar{b} < 0 < D & \text{(Zone I}_-\text{)} \\ \emptyset, & 0 < D < \bar{a} < \bar{b} & \text{(Zone I}_+\text{)} \\ [0,\bar{b}], & \bar{a} < 0 < \bar{b} < D & \text{(Zone II)} \\ [\bar{a},\bar{b}], & 0 < \bar{a} < \bar{b} < D & \text{(Zone III)} \\ [\bar{a},D], & 0 < \bar{a} < D < \bar{b} & \text{(Zone IV)} \\ [0,D], & \bar{a} < 0 < D < \bar{b} & \text{(Zone V)} \end{cases}$$

The different zones are shown in Fig. 20. Zones $I_\pm$ are causally disconnected from the pulse emission and thus correspond to vanishing metric perturbations. Zone II is defined by the pulse emission from the mirror, zone III only describes the free propagation of the pulse (excluding emission and absorption), zone IV describes pulse absorption only, while zone V describes both emission and absorption.

For circularly polarized pulses, the energy density is constant along the propagation axis $u(ct-z) = u_0$, and so Eq. (69) takes the simple form

$$h_0^p[x,y,z,t] = \frac{4GA}{c^4}u_0 \ln\left(\frac{\zeta(x,y,z,b_{x,y,z,t})}{\zeta(x,y,z,a_{x,y,z,t})}\right), \tag{70}$$

where we use an index notation for legibility $a_{x,y,z,t} := a(x,y,z,t)$ and similarly for b.

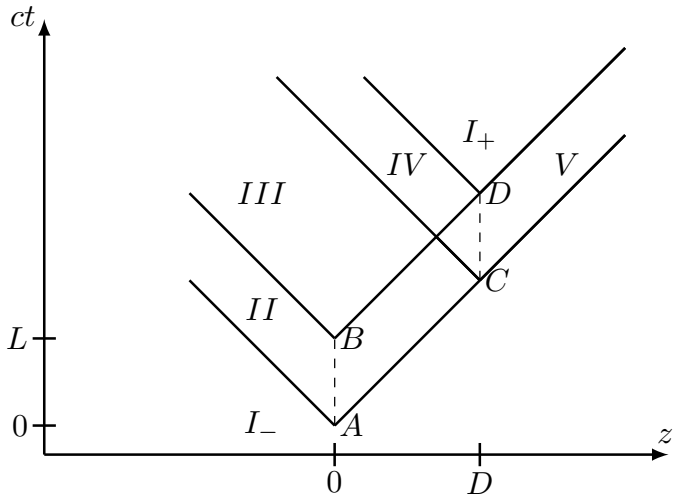


Figure 20: Sketch of the spacetime diagram of a single pulse propagating in the z direction. The various zones define different metric perturbations and arise from the intersection of the pulse's world sheet with the past light cone J^- of a spacetime event x^μ. The world sheet of the single pulse is spanned by A, B, C, D. The pulse begins to be emitted at event A, and its emission ends at B. Its absorption starts at C and ends at D. Figure adapted from Ref. [266].

5.3.4 *Estimation of the entangling phase*

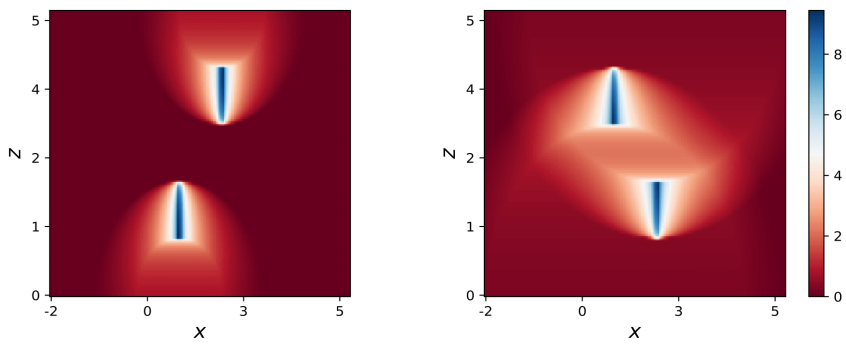
With this preliminary investigation, we are now ready to discuss the case of interest for DIGME. We consider two counter-propagating identical laser pulses, each with stress-energy tensor $T_a^{\mu\nu}$. We assume that the effective size of the two pulses is much smaller than their separation, so that diffraction effects are not a concern. The total stress-energy tensor takes the form

$$T^{\mu\nu}(t,\vec{x}) = \sum_{a=1}^{2} T_a^{\mu\nu} = Au_0 \sum_{a=1}^{2} \delta(x-x_a)\delta(y-y_a), \tag{71}$$

where A is the effective area of each pulse in the transverse plane and (x_a, y_a) are the respective positions of the pulses in the xy-plane. The two counter-propagating light pulses evolving parallel to the z-axis are initially separated by a distance approximately equal to D, with a sufficient separation along the x-axis $D \ll x_2 - x_1 \neq 0$. We also set $y_1 = y_2 = \mathrm{const}$.

In the framework of linearized gravity, we obtain the total metric perturbation for two pulses by adding the separate contributions of each single pulse. For two counter-propagating pulses along the z-direction that have respective transverse x coordinates $x_{1,2}$, we obtain:

$$\begin{aligned} h^p[x,y,z,t] &= h_1^p[x,y-y_1,z,t] + h_2^p[x,y-y_2,z,t] \\ &= h_0^p[x-x_1,y-y_1,z,t] + h_0^p[x-x_2,y-y_2,-z+D,t]. \end{aligned} \tag{72}$$



(a) Time $t = 2$. (b) Time $t = 4$.

Figure 21: Plots of the total metric perturbation h^p sourced by two counter-propagating pulses located at $x_1 = 1, x_2 = 2$ in the xz-plane. Parameter values $D = 5, L = 1$ and $\frac{4GA}{c^4}u_0 = c = 1$. Lengths are in units of ct.

The total metric perturbation h^p for two counter-propagating light pulses in the xz-plane is represented in Fig. 21.

We are now in good position to express the action associated with the process of interest. By substituting Eq. (71) into Eq. (66), one can establish

$$\begin{aligned} S^{\sigma}_{\mathcal{F}} = \kappa \int_{z=-\infty}^{\infty} dz \int_{t=0}^{\tau} dt \Bigg\{ & \ln\left(\frac{\zeta(0,0,z,b_{0,0,z,t})}{\zeta(0,0,z,a_{0,0,z,t})}\right) \\ & + \ln\left(\frac{\zeta(x_1-x_2,0,-z+D,b_{x_1-x_2,0,-z+D,t})}{\zeta(x_1-x_2,0,-z+D,a_{x_1-x_2,0,-z+D,t})}\right) \\ & + \ln\left(\frac{\zeta(x_2-x_1,0,z,b_{x_2-x_1,0,-z,t})}{\zeta(x_2-x_1,0,z,a_{x_2-x_1,0,z,t})}\right) \\ & + \ln\left(\frac{\zeta(0,0,-z+D,b_{0,0,-z+D,t})}{\zeta(0,0,-z+D,a_{0,0,-z+D,t})}\right)\Bigg\}, \end{aligned} \tag{73}$$

where τ is the interaction time and $\kappa := 4GA^2u_0^2/c^4$. The values for $x_{1,2}$ used for the different spatial branches are shown in Table 5.

Mode pair \ x-coordinate	x_1	x_2
LL	0	d
LR	0	$d+\Delta x$
RL	Δx	d
RR	Δx	$d+\Delta x$

Table 5: The values for $x_{1,2}$ in Eq. (73) are shown for the different spatial branches LL, LR, RL, RR.

From the expression of the action, we can now proceed to find the phase evolution associated with the counter-propagation of light pulses in each pair of modes. Given that $h_0^p[x,\cdot] = h_0^p[-x,\cdot]$, we consider the relative phase factor $e^{i\Delta\phi_{RL}}$ for the pair of modes $|RL\rangle$ that are the closest to one another:

$$\Delta\phi_{RL} = \frac{Au_0}{\hbar}\int_{z=-\infty}^{\infty} dz \int_{t=0}^{\tau} dt \Big\{ h_0^p[d-\Delta x, 0, -z+D, t] + h_0^p[d-\Delta x, 0, z, t] - h_0^p[d, 0, -z+D, t] - h_0^p[d, 0, z, t] \Big\}.$$

To numerically integrate $h_0^p[x,y,z,t]$ with sufficient accuracy, the z-integration limits increase with the interaction time τ. As we can see from Fig. 22 showing the integrand of the relative phase, this relative phase $\Delta\phi_{RL} = \phi_{RL} - \phi_{LL}$ is computed by taking those z values that are still causally connected to the emission of the two light pulses up to interaction time τ into account. Entanglement is not generated for events that are spacelike separated, in accordance with previous findings [274]. As one can notice from Fig. 22, the integrand of the relative phase converges as the interaction time τ is increased. This is due to the finite length of the interferometer D.

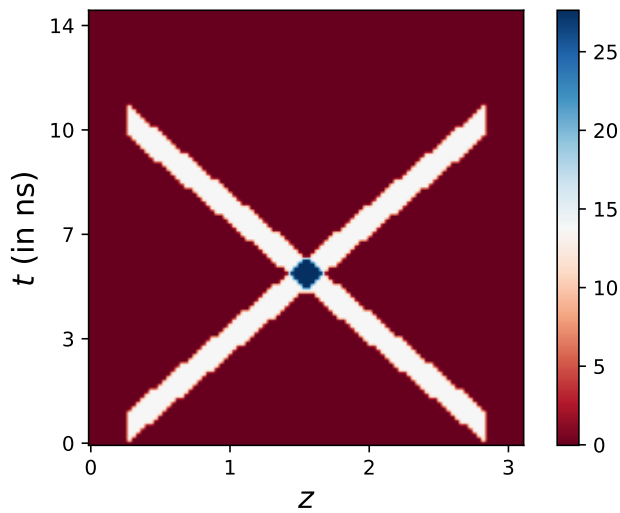


Figure 22: Plot of the integrand of the relative phase $\Delta\phi_{RL}$ with parameters $D = 3$m and $L = 1$ m in the tz-plane. We have set $\frac{4GA}{c^4}u_0 = c = 1$. Lengths are in units of ct.

In the massive DIGME protocol, the particles are kept at constant separation, hence the phase accumulation grows with the interferometer length (as its square root in the case of freely falling masses). In the photonic protocol, increasing D beyond many pulse lengths does not give more phase signal, as the pulses are counter-propagating and most of the relative phase accumulation occurs when the pulses are close to each other.

As the numeric evaluation of the total phase term requires incorporating large sections of the full spacetime integral $\int_{z=-\infty}^{\infty}\int_{t=0}^{\tau} dt dz$ for which no substantial phase is accumulated, we can restrict the integration domain to $0 \leqslant t \leqslant 2D/c$ and $-D-L \leqslant z \leqslant D+L$, a spacetime region encapsulating the pulse crossing and mutual interaction process, which will give a reasonable approximation to the actual accumulated phase.

Once this phase is evaluated, we certify entanglement in the same way as in the massive DIGME propocol. In Sec. 5.2.2 we have established an optimal witness $W_1 = \mathbb{1}\otimes\mathbb{1} - X\otimes X - Z\otimes Y - Y\otimes Z$, where $\{\mathbb{1}, X, Y, Z\}$ forms the set of single qubit Pauli operators. In the noiseless scenario, the witness expectation value is simply

$$\mathrm{Tr}[W_1 |\theta\rangle\langle\theta|] = 1 - (\sin(\Delta\phi_{LR}) + \sin(\Delta\phi_{RL})) - \frac{1}{2}(1 + \cos(\Delta\phi_{LR} - \Delta\phi_{RL})),$$

where $|\theta\rangle$ is the bipartite pure polarization state. This witness will pick up entanglement, in the noiseless case, as soon as the relative phase accumulation is appreciable.

Let us now give some parameters which would yield an appreciable relative phase. For the calculation to be valid, we remind that diffraction and interference effects must be neglected, thus we must operate in the limit $d - \Delta x \gg \lambda$ where λ is the central wavelength of the pulse. To conservatively satisfy this condition, let us choose λ such that $d - \Delta x = 10\lambda$. To arrive at a figure of merit on the feasibility of the protocol, let us enforce the condition $\Delta\phi_{RL} \sim 1$ rad and determine corresponding parameters satisfying this. In a later section, we shall discuss this figure of merit with regards to its current feasibility and the challenges to overcome.

Considering typical over-the-counter nanosecond pulsed lasers, we assume a central wavelength $\lambda = 1\,\mu\mathrm{m}$ and a pulse length $L = 0.3\,\mathrm{m}$. Choosing a splitting distance $\Delta x = 1\,\mathrm{cm}$ satisfying $\Delta x = d - 10\lambda$ in order to have negligible beam overlap, we also set a typical laboratory friendly interferometer length D on the order of a few meters so that $D/L \approx 10$. Since for a laser with power P we have $P = Au_0c$, we can write $\kappa = 4GA^2u_0^2/c^4 = 4GP^2/c^6$. Numerics show that achieving an appreciable relative phase of $\Delta\phi_{RL} \approx 0.29\,\mathrm{rad}$ requires a power on the order of $P \approx 30\,\mathrm{PW}$. Such a pulse contains an average photon number $N = PL\lambda/(\hbar c^2) \approx 10^{26}$, an admittedly demanding figure, as we shall discuss in the next section. This estimate may be refined by considering higher-order contributions in the quantum field theoretic formulation, and accounting for the bandwidth of the pulse.

5.3.5 *Future challenges*

We have seen that the photonic DIGME protocol may sidestep some difficult problems arising in the matter version, and shown that one could in principle generate appreciable phase with light pulses. This being said, the implementation of the photonic DIGME protocol is by no means straightforward. To formulate more precise claims on its feasibility, we lay out some further questions that may constitute interesting future investigations.

The most critical drawback of using light in the DIGME protocol is by far the weakness of the gravitational effects of light, and so the need for quite intense light pulses. It would be tempting to think that current laser technology boasting petawatt ultrashort pulses [277] may already allow the implementation of the protocol. However there are at least two issues that arise. First is the control of high-intensity light pulses, which are known to damage the optical components constituting the whole apparatus. Second, and more serious, is the fact that high-power laser pulses are simply not usable for DIGME proposals as they are classical light states (in the sense that their Glauber-Sudarshan P function is positive), and as such, are not entangled through beam splitting. To carry out a DIGME experiment, one thus has to resort to non-classical states light, for which high average photon number states are much harder to achieve. To have an ideal comparison with the massive case, in the photonic DIGME proposal, one would like to obtain the maximally entangled state after beam splitting in each interferometer $|\psi\rangle_{\text{out}} = \frac{1}{\sqrt{2}}\left(|N\rangle_x |0\rangle_z + |0\rangle_x |N\rangle_z\right)$, often called *NOON* state, the generation of which has been widely studied [278–283]. That being said, current high-NOON states contain $N < 10$ photons, and as such the generation of an appreciable metric perturbation from a NOON state will remain hardly conceivable in the near future.

Nevertheless, it can be argued that the photonic DIGME protocol deserves further attention. As we have said, having a very low single-shot phase signal does not necessarily constitute an insurmountable obstacle. Some features of the photonic version, such as absence of non-gravitational entangling forces between the light pulses, combined with the use of an optimal entanglement witness, and the rate at which measurements can be repeated, may tip the scale in its favor. While current NOON states are very weak, this limitation is not fundamental, barring any spontaneous collapse process a la Penrose [131] which would in any case also affect the matter DIGME protocol. For instance, the approach presented in Ref. [284] to generate NOON states with large N is, in principle, scalable up to arbitrarily high photon numbers. Worth considering, is also the generation of approximate NOON states from two-mode squeezed vacuum states [271].

To increase the gravitational phase signal, one may also consider using fiber loops in the split branches of the interferometers. Along a single loop, the light pulses cross one another in opposite directions twice. In a rough first approximation, we can generalize our estimate to l loops by multiplying the phase by a factor $2l$, where the length D for the single-shot experiment would correspond to the length of half a loop. In all due rigour, one should carry out the derivation of the metric perturbations in the loop geometry where the light beams are not always counter-propagating in a fixed direction, one also needs to take into account the stress-energy contribution of light propagating in a medium as laid out in Ref. [255]. This is by no means a straightforward analysis, as adding fibers and having the light follow a longer optical path also comes with drawbacks, such as pulse broadening, power loss, thermal noise, birefringence etc...

Another issue, that is not specific to the photonic version however, is the presence of background noise. Although the photonic variant is devoid of additional unwanted known interactions, there remains background noise from the surrounding mass distribution. One way to offset the noise is to consider a background with a quasi-static mass density distribution. The experiment may be run first with co-propagating light pulses. In vacuum, the pulses will not interact and thus any signal will be due to noise. This noise may then be offset from the signal obtained with counter-propagating pulses.

Another advantage of the photonic version is worth mentioning: to increase the interaction strength, the separation between the closest branches of the light beams may be tuned to be very small, even completely superimposed. This is conditioned to interference being accounted for, and the experimental ability to distinguish between the pulses at close distances with the inclusion of diffraction effects [285]. One would also need to rule out the contribution of direct photon-photon scattering.

In analogy to the generalisation to arbitrary geometries and qudits for the massive DIGME protocol [286, 287], one may also consider an array of light beams to boost the gravitational phase induction. In this manner, it may be interesting to examine whether there is any setup that entangles faster than the one studied in this work.

The photonic implementation may open up a new window into investigating gravity mediated entanglement, and using photons, as opposed to massive objects in a near-future experiment could also shed light on other theoretical aspects and features of gravity that cannot be witnessed using the latter.

5.4 CONCLUSION

Recent proposals aiming to witness GME between two systems [219, 220] have given a second wind to the age-old investigation of unified

quantum gravity. Although the experimental requirements remain futuristic, some important theoretical questions, such as the plausibility of using position eigenstates, the possibility of a better witness, the necessity of a CP closest approach limit, and the significance of experimental data, were left open. In our investigation, we have addressed those questions and shown that the position eigenstate is a valid approximation, for the calculation of entanglement, to a good range of thermal states in the predicted experiment durations. By introducing an optimal entanglement witness, we were able to show that entanglement revelation is possible in less free-fall time, with higher decoherence rates. We have furthermore demonstrated that a statistical approach to the witness method decomposed into Pauli measurements allowed to discern gravitational from uncertain non-gravitational contributions. We have spelled out and closed a potential loophole in the witness based approach to establishing the entangling capacity of the gravitational interaction.

While our first analysis aimed to refine and improve certain aspects of the massive DIGME proposal, we have also studied a photonic variant motivated by some potential advantages, despite the well-known weak coupling of light to gravity. First and foremost the usage of light instead of matter relieves us of unwanted and otherwise unavoidable entangling effects such as dipole-dipole interactions or Casimir coupling, and difficulties in controlling the motion of massive objects such as microdiamonds with an nitrogen vacancy center. Second, the doubly interferometric setup may also serve to demonstrate gravitational coupling between light beams, through dephasing, rather than spatial deflection. Furthermore, a photonic experiment allows us to build up statistics more reliably than with matter, and the certification of entanglement unavoidably will require many repetitions of bipartite Pauli measurements. Last but not least, the photonic DIGME protocol is a fully relativistic test of GME, and as such may be seen as testing relevant aspects of the quantum nature of gravity. In our analysis, we considered the basics of the experimental implementation using two Mach-Zehnder interferometers and derived the metric perturbation sourced by two counter-propagating light pulses using linearized gravity. Through the path integral formalism, we have derived the action of the pulses leading to gravitational phase induction, and for some parameters we have given a figure of merit of the average photon number required for an appreciable signal.

6 EPILOGUE

Never let the future disturb you. You will meet it, if you have to, with the same weapons of reason which today arm you against the present.

— **Marcus Aurelius** [288]

In this thesis, which now draws to a close, we have presented various investigations of fundamental physics using the tools of quantum information theory and quantum control. In particular, we have examined how table-top experiments revolving around correlations – between quantum measurements, between the degrees of freedom of a quantum probe, or of quantum theory itself – may shed light on basic conceptions we hold about nature.

In our introductory chapter, we have given some historical background, both from the point of view of epistemology on the time scale of the millennium, and from the point of view of modern physics of the last century. This was followed by an extensive presentation of key results and concepts from mathematics, quantum physics, quantum optics and quantum information theory, in our second chapter, which served as a foundation to the work presented in this dissertation. In the following three chapters, which formed the core of this thesis, we have contextualized and reported the results of various explorations. These have ranged from fundamental considerations at the crossroads between foundations of physics and quantum optics, to the quest for empirical evidence of gravitational deviations to quantum dynamics in optomechanics, and the pursuit of non-classical signatures of the gravitational interaction.

In Chapter 3, we investigated the Leggett-Garg inequalities which constrain the two-point correlations of measurement results obtained on a given system at various points in time. It was already established, in the foundations of quantum mechanics, that these inequalities could only test the most constrained type of macroscopic realism.

From a practical stance, their violation is widely considered a witness of non-classical behavior. In order to scrutinize its value as a witness of non-classicality, we have taken as a benchmark the well formalized definitions of classicality from the realm of quantum optics. To do so we have examined the possibility of violating the Leggett-Garg inequalities using coherent states of light in a Mach-Zehnder interferometer. The main challenge on the way to establish a non-trivial violation with coherent states, was to find an observable assignment which would simultaneously be macroscopically definite when using coherent states, and that could allow ideal negative measurements. After having found such an assignment, we have demonstrated that

coherent states, despite being the golden standard of classicality in quantum optics, do violate the Leggett-Garg inequalities.

In an endeavour to more precisely determine the origin of the violations, we have considered surrendering phase reference by taking decohered input states. The possibility of a violation with a thermal state was an unexpected discovery. In the setting considered in our analysis, it turned out that the Leggett-Garg inequalities were essentially testing the minuteness of the vacuum component in a given state, be it coherent or not. There are two manners in which to interpret this result, the first (and rather trivial one), is that even the most classical state of light is in fact simply non-classical, and unsurprisingly violates the Leggett-Garg inequalities. The second speaks rather of the Leggett-Garg inequality as a witness of non-classicality: while it may be a useful signature, their violation certainly does not carry as strong a consequence as that of Bell's.

In point of fact, the Leggett-Garg inequalities, contrary to Bell's, are not necessary and sufficient conditions for macroscopic realism, for lack of an equivalent Fine theorem [289]. Tighter conditions, called "no-signalling-in-time" were put forward [157], and may prove both more easily violable and interpretable. An interesting follow up investigation at the confluence with the quest for empirical evidence of non-classical gravity, would be the conception of a no-signalling-in-time violating protocol involving gravitational motion, building on an approach which made use of the Leggett-Garg inequalities [290].

In Chapter 4, we revisited an optomechanical protocol which aims to uncover deviations to standard quantum mechanical predictions due to gravity, taking the form of a generalized uncertainty principle. The optomechanical protocol under study was designed to detect a nonlinear phase contribution that would arise from the deformation of the equal time commutation relations between the position and the momentum of a mesoscopic oscillator driven by an optical field. Not long after such proposals were put forward, approaches of this kind to test Planck scale physics were faced with a critical no-go theorem, stating that the amplitude of the non-standard deformations had no reason to be the same for elementary particles and for massive composite systems of such particles. Particularly, when the systems under study are described by their center of mass coordinates and total momenta, non-standard corrections were shown to decay with the square of the number of elementary constituents, under the quasi-rigid approximation.

In order to circumvent the no-go theorem, we began by re-deriving the non-standard signature captured by the optomechanical protocol from first principles, using the interaction picture and directly calculating the time propagator of the optomechanical system using a Magnus expansion. A significant hurdle on the way to our objective was the quartic momentum term arising in the non-standard interaction

Hamiltonian, which set the motion-independent phase to be the fifth order Magnus term. An admittedly heavy expression. Relinquishing the mechanical oscillator's rigidity, by describing it as a correlated many-body system the internal energy of which is given by a general hessian, only added to the arduousness of the algebra. These efforts did not go unrewarded, as we have presented a main result featuring a closed form expression of the non-standard signature, which is valid for all many-body systems perturbed by an optical field, with an arbitrary optomechanical coupling function, to first order in the non-standard correction.

We have applied our result to the case of coupled mechanical oscillators, evolving under a pulsed optical interaction, and derived a more specific closed form expression. Interestingly, numerics have revealed a superquadratic scaling of the non-standard signature, with the number of constituents of the system, demonstrating that resonance effects involved in internal motional correlations may amplify non-standard signals in spite of decaying non-standard corrections. The generality of the results we have shown may serve future investigations of fundamental physics using optomechanics.

From the theoretical perspective, our analysis revolved around a protocol aiming to test the generalized uncertainty principle. While it has been widely investigated by the physics community, only modifications to the uncertainty relating the position and momentum conjugate observables have been considered. There is no mention in the literature, to this day, of the generalization of the time-energy uncertainty relation. This is problematic as the heuristic arguments giving rise to generalized uncertainty principles should not only affect the uncertainty in lengths, but by relying on general-relativistic considerations (namely black hole mechanisms) should also result in additional uncertainties in durations. The difficulty in establishing modified time-energy uncertainty relations arises from the fact that time is not a quantum observable[1] hence the standard operator approach to derive Heisenberg inequalities, from commutation relations that are to be deformed, do not apply. A possible path of investigation would be to incorporate effects expected from quantum gravity into a recent derivation of the time-energy uncertainty relations [291] based on the Page-Wootters relational time [292].

In Chapter 5, we introduced improvements and variants to an experimental proposal designed to expose non-classical features of gravitation, specifically through its possible entangling capacity. We have first considered the original proposal which uses massive systems as a platform for gravity mediated entanglement, and shown that it was viable even for realistic thermal motional states. To demonstrate its robustness, we have proposed an optimal entanglement witness,

1 A time observable would result in an unbounded Hamiltonian, as per Pauli's objection.

and shown that the careful statistical analysis of Pauli measurement outcomes involved in the witness expectation value estimation, may allow to certify gravitational entanglement despite the presence of other, potentially stronger entangling interactions (such as Casimir coupling). We have also shown that the actual differential nature of the protocol makes the statistical analysis tolerant to uncertainties in non-gravitational couplings, and that using state tomography would further allow to close a non-monotonicity loophole.

Apart from conceptual improvements that may alleviate the challenging requirements of the massive version of the experiment, we have also considered using light pulses as an alternate platform for the doubly interferometric gravitational entanglement. Motivated by the establishment of a witness that may detect entanglement for arbitrarily weak phase signal and the importance of repeatability, it was a natural continuation to consider a photonic variant, given the statistical reliability of optical experiments, and the absence of Casimir coupling. We have derived a formula for the entangling phase using the path integral formalism, based on previous results on the metric perturbations sourced by a light pulse, and given a figure of merit of the required optical power required to achieve an appreciable phase.

Some future directions worth exploring include testing the entangling capacity of the Casimir-Polder interaction itself, as a first step towards the more ambitious gravitational test. The doubly interferometric protocol in combination with statistical analysis may also be able to rule out some models of non-local gravity [234]. Further analysis of this setup may also contribute to investigations into the discreteness of time [293].

All in all, the investigations presented in this thesis serve to illustrate how fundamental questions about nature, be it about the elusive quantum-classical boundary, or about the possibly related quest for a theory of quantum gravity, could benefit from the theoretical framework and the experimental platforms of the flourishing field of quantum information science.

The general outlook for quantum information science is a very exciting one. Many challenges for fundamental physics lie ahead, and the combined efforts from the high energy physics and the quantum information communities may enkindle the new paradigm shift from which, one would hope, a better understanding of gravity and the measurement problem would emerge.

From the perspective of funding volume all around the world, it seems like the early 2020s marked the beginning of a new era, driven by the vast amount of resources pouring into the development of quantum technologies for their strategic applications. These range from quantum sensing [294, 295], to quantum secure communications [296], all the way up to hybrid computational methods like quantum approximate optimization algorithms [297] which already

draw interest from financial businesses [298]. Recent years have also seen the humble beginnings of the quantum internet [299] and the first audacious claims of quantum supremacy [300].

The immense practical outcomes of quantum theory had once siphoned talents and attention away from its most fundamental aspects. It now seems like the new generation of quantum technologies, with their ever more miraculous potential applications, may incidentally grant precious resources to research efforts in the foundations of quantum theory: perhaps the most exciting theory of nature mankind has ever designed. One that finds itself at the crossroads between physics, computer science and philosophy. Predicting the future has always been a risky endeavor, but the new formulations of quantum theory [301, 302], based on measurement outcomes, their correlations and fundamental information theoretic principles, could turn out to be the ones to stand the test of time.

Part III

APPENDIX

A

COMPLEMENTS TO CHAPTER 1

DIGRESSIO PERSONALIS

This section contains a few opinionated words to explain why I find Relational Quantum Mechanics (RQM) convincing. Let us begin with a modest but fascinating question, the investigation of which may shed some light on common ontological beliefs: is π a physical constant or a mathematical number?

My take on this question, is that the tempting and seldom questioned dichotomy between what is physical, and what is mathematical, may be yet another Aristotelian delusion. π, one may say, is a geometric constant, and hence belongs to mathematics. However, what is geometry, but the physics of the vacuum[1]? As it appears, π may serve as a prime example to show why the mathematical-physical dichotomy must be left behind. Had the universe not been locally flat, or more drastically dynamical, triangles would not have had constant sums of angles, and the perimeters of circles would have had variable relationships to their radii. Looking back at history, with what we now know of the much more sophisticxated theory of differential geometry that underpins general relativity, it is not surprising that π was discovered so early on: it is after all one of the first numbers one arrives at through a direct experience of the world.

At this stage, it merely seems that I am stating the obvious: some mathematical objects have marked physical manifestations. Furthermore, this does little to prove that the mathematical-physical distinction is invalid. Indeed, one may ask the same question about another number: is the imaginary unit i a physical constant, or a mathematical number? While it seems harder to make a case for the physicality of i by geometrical arguments, it was recently proven that physical theories, based on real numbers only, cannot be consistent with quantum mechanical experiments [85]. As such, the presence of complex numbers in our current description of nature is not a simple matter of algebraic convenience, it says something much deeper about physics.

If mathematical objects and relations are necessary components of our description of phenomena, on what grounds may one claim that they should not be physical? This rhetorical question may look like I am making a case for ψ-ontology, however I follow this with another query: to the reader who is convinced that the concepts of π and i among others, are mathematical *rather than* physical, what then qualifies a concept to be physical?

1 With no matter, and no fields, but spacetime.

It is my sentiment that many, perhaps even some physicists, would come up with an example of a physical concept, such as the electron. *Surely*, the electron is more physical than π, is it not? It is an all too common fallacy to attribute some substance to a concept by having merely named it. While in the everyday vernacular, we refer to the electron as if it were an ontological object, as some sort of tangible substance in the vicinity of another palpable substance called the atomic nucleus, the electron is above all a mathematical concept, best defined in the theory of quantum electrodynamics. The simple statement "*the electron exists*", in all due rigor is but a practical formulation of "*to the best of our knowledge, based on empirical data from which correlations were analysed, there exists a consistent correspondence between the relationships inferentially linking together a set of mathematical concepts to the concept of electron, and the relationships causally linking together a set of observed events*". That is to say, (successful) physical concepts are mathematical concepts which, in their inferential relationships to their neighbouring concepts, weave the same patterns as the network of observed influences in which the corresponding phenomenon is observed[2]. In short, physicality is the consistency of a correspondence between metaphysical relations and observed phenomenological relations. So where does this leave us with regards to RQM?

In my view RQM epitomizes an understanding of physics as a discipline that is not tasked with the establishment of an ontology, but rather as a human enterprise seeking to speak of nature. RQM, I gather, constitutes the final steps of the "epistemologization" of physics. To clarify this statement, let us take a step back and wonder what it means to have knowledge of a concept A.

Knowledge of a concept A does not simply come from having given it a label. Rather, the very definition of a concept emerges from its relationship to surrounding concepts: this is the very purpose of dictionaries, which do not give any absolute, immediate, fundamental meaning to any word, but rather weave a web of relationships between different words, called definitions. The same observation holds for the truth or falsehood of any logical statements, which are essentially relational values: True and False are values which simply divide statements within a scientific theory into two equivalence classes. A statement is only true, or false, with respect to a consistent set of axioms[3].

If there is no absolute meaning to a word, or absolute truth to a statement, should there be any reason why the lack of absolute facts in RQM be of particular concern? While RQM may seem radical at first reading, I have grown to believe that on the contrary, postulating

2 For a much more rigorous presentation of causal-inferential theories, I strongly recommend Ref. [303].

3 Barring issues of undecidability, which do not arise without multiplication, such as in Presburger arithmetics [304].

a fundamental absolute ontology, be it deities, celestial spheres, physical properties or measurement results, is a much more radical stance, perhaps the vestige of an Aristotelian fantasy that is drawing its last breaths.

B

COMPLEMENTS TO CHAPTER 2

B.1 ALGEBRAIC STRUCTURES

Definition 42 (Groups). *A set* E *equipped with an internal binary operation* $+ : E^2 \to E$ *is said to be a group when the following three conditions are satisfied:*

1. $\forall (x, y, z) \in E^3,\ (x + y) + z = x + (y + z)$ *(associativity).*
2. $\exists e \in E,\ \forall x \in E,\ x + e = e + x = x$ *(identity element).*
3. $\forall x \in E,\ \exists y \in E,\ x + y = y + x = e$ *(inverse element)*[1].

Moreover, if $\forall (x, y) \in E^2,\ x + y = y + x$ *then the group is said to be abelian or commutative.*

We can now use the concept of group to build up more sophisticated structures, such as the field.

Definition 43 (Fields). *A set* $\mathcal{F}$ *equipped with two internal binary operations* $+, \cdot : \mathcal{F}^2 \to \mathcal{F}$ *is said to be a field when the following three conditions are satisfied:*

1. $(\mathcal{F}, +)$ *is an abelian group (we shall denote its identity element* 0*).*
2. $(\mathcal{F} \backslash \{0\}, \cdot)$ *is an abelian group.*
3. $\forall (a, b, c) \in \mathcal{F}^3,\ a \cdot (b + c) = a \cdot b + a \cdot c$ *(distributivity).*

From this, one arrives at the concept of vector space.

Definition 44 (Vector spaces). *A set* V *equipped with an internal binary operation* $+ : V^2 \to V$ *and an external binary operation* $\cdot : \mathcal{F} \times V \to V$ *is said to be a vector space over the field* $\mathcal{F}$ *when the following six conditions are satisfied:*

1. $(V, +)$ *is an abelian group.*
2. $\mathcal{F}$ *is a field (multiplicative identity denoted as* 1*).*
3. $\forall (a, b, v) \in \mathcal{F} \times F \times V,\ a \cdot (b \cdot v) = (ab) \cdot v$ *(compatibility).*
4. $\forall v \in \mathcal{F},\ 1 \cdot v = v$ *(identity element of scalar multiplication).*
5. $\forall (a, u, v) \in \mathcal{F} \times V \times V,\ a \cdot (u + v) = a \cdot u + a \cdot v$ *(distributivity).*

1 It can technically be shown that the left inverse is equal to the right inverse, and so forms a unique bilateral inverse. For simplicity we have embedded this into the definition of a group.

6. $\forall (a, b, v) \in \mathcal{F} \times \mathcal{F} \times V,\ (a + b) \cdot v = a \cdot v + b \cdot v$ *(distributivity).*

When $\mathcal{F} = \mathbb{R}$ or $\mathcal{F} = \mathbb{C}$ then V is called respectively a real vector space or a complex vector space.

B.2 TOPOLOGY

Definition 45 (Metric spaces). *A set E equipped with a real valued function $d : E \to \mathbb{R}$ is said to be a metric space, and d is called a distance, when the four following conditions are satisfied:*

1. $\forall (x, y) \in E^2,\ d(x, y) \geqslant 0$ *(positivity).*
2. $\forall (x, y) \in E^2,\ d(x, y) = d(y, x)$ *(symmetry).*
3. $\forall (x, y) \in E^2,\ d(x, y) = 0 \implies x = y$ *(identity of indiscernibles).*
4. $\forall (x, y, z) \in E^3,\ d(x, z) \leqslant d(x, y) + d(y, z)$ *(triangle inequality).*

Definition 46 (Normed spaces). *A vector space V over field $\mathcal{F}$ equipped with a real valued function $\mathcal{N} : V \to \mathbb{R}$ is said to be a normed vector space, and $\mathcal{N}$ is called a norm, when the four following conditions are satisfied:*

1. $\forall x \in V,\ \mathcal{N}(x) \geqslant 0$ *(positivity).*
2. $\forall x \in V,\ \mathcal{N}(x) = 0 \implies x = 0_V$ *(identity of indiscernibles).*
3. $\forall (\lambda, x) \in F \times V,\ \mathcal{N}(\lambda x) = |\lambda| \mathcal{N}(x)$ *(homogeneity).*
4. $\forall (x, y) \in V^2,\ \mathcal{N}(x + y) \leqslant \mathcal{N}(x) + \mathcal{N}(y)$ *(triangle inequality).*

Claim 18. *A normed vector space $(V, \mathcal{N})$ is also a metric space where the distance is defined as $d : (x, y) \mapsto \mathcal{N}(y - x)$ and is called the norm induced metric.*

Proof. Properties 1, 3 and 4 of the distance are directly inherited from properties 1, 2 and 4 of the norm. Property 2 follows from the homogeneity of the norm, as $\mathcal{N}(x - y) = \mathcal{N}(-(y - x)) = |-1| \mathcal{N}(y - x)$. □

Claim 19. *A vector space V equipped with an inner product is a normed vector space, where the norm is defined by $\forall x \in V, \|x\| = \sqrt{\langle x | x \rangle}$.*

Proof. Positivity is trivial. Identity of indiscernibles follows immediately from the definiteness of the inner product. Homogeneity follows from sesquilinearity and the fact that $\forall \lambda \in \mathbb{C}, \sqrt{\lambda \lambda^*} = |\lambda|$. The triangle inequality follows from the Cauchy-Schwarz inequality. □

Definition 47 (Cauchy sequences). *A sequence $(u_n) \in E^{\mathbb{N}}$ of elements of the metric space (E, d) is said to be a Cauchy sequence when*

$$\forall \varepsilon > 0,\ \exists n_0 \in \mathbb{N},\ \forall p, q \geqslant n_0,\ d(u_p, u_q) \leqslant \varepsilon,$$

where d is the distance with which the metric space E is equipped.

Intuitively one can say that a Cauchy sequence is any sequence for which the terms uniformly get closer to each other.

Definition 48 (Converging sequences). *A sequence* $(u_n) \in E^{\mathbb{N}}$ *of elements of the metric space* (E, d) *is said to converge when*

$$\exists \ell \in E,\ \forall \varepsilon > 0,\ \exists n_0 \in \mathbb{N}, \forall n \geqslant n_0,\ d(u_n, \ell) < \varepsilon.$$

B.3 LINEAR ALGEBRA

Definition 49 (Linear independence). *A family* $(v_i)_{i \in I}$ *of vectors of a vector space* V *over the field* $\mathcal{F}$ *is said to be linearly independent when*

$$\sum_{i \in I} \lambda_i v_i = 0_V \implies \forall i \in I, \lambda_i = 0_F.$$

Definition 50 (Spanning vectors). *A family* $(v_i)_{i \in I}$ *of vectors of a vector space* V *over the field* $\mathcal{F}$ *is said to span* V *when*

$$\forall v \in V,\ \exists (\lambda_i)_{i \in I} \in F^{|I|},\ v = \lambda_i v_i.$$

Definition 51 (Bases). *A basis*[2] *of a vector space* V *is any family of vectors* $(v_i)_{i \in I}$ *which is linearly independent and spans* V.

In a nutshell, a basis B of a vector space V is simply a family of vectors with respect to which any other vector admits a decomposition, and this decomposition is unique. Another way to say it, is that bases are the spanning families of minimal cardinality, or equivalently, the linearly independent families of maximal cardinality. This fact leads to the following definition.

Definition 52 (Dimension). *The dimension* $\dim(V)$ *of a vector space* V *is the cardinality of its bases.*

Combining this with the definition of the scalar product one has the following important definition.

Definition 53 (Orthonormal bases). *A basis* $B = (v_i)_{i \in I}$ *of a vector space* V *is said to be orthogonal if* $\forall (i, j) \in B^2,\ i \neq j \implies \langle v_i | v_j \rangle = 0$. *Additionally, if* $\forall i \in I, \|v_i\| = 1$ *then the vectors are said to be normalized, the basis* B *is said to be orthonormal and the following relationship holds* $\forall (i, j) \in I^2,\ \langle v_i | v_j \rangle = \delta_{ij}$.

Definition 54 (Kernels). *Let* $U \in \mathcal{L}(E, F)$ *where* E *and* F *are two vector spaces. The kernel* $\ker(U)$ *is defined by*

$$\ker(U) = \{x \in E \mid Ux = 0_F\},$$

it is the vector subspace of E *which is mapped onto* 0_F *by* U.*r*

2 One can prove that all vector spaces admit bases, using Zorn's lemma.

Definition 55 (Eigenelements). *Let* $U \in \mathcal{L}(E)$ *be an endomorphism of the vector space* E *over the field* $\mathcal{F}$*. An element* $\lambda \in \mathcal{F}$ *is an eigenvalue of* U *if and only if*

$$\dim(\ker(U - \lambda \mathbb{1}_E)) \geqslant 1,$$

the vector space $\ker(U - \lambda \mathbb{1}_E)$ *is then called the eigenspace associated to the eigenvalue* λ*, and its non-zero elements are called eigenvectors. The set* $\sigma(U)$ *of eigenvalues of* U *is called its spectrum*[3]*. If* $\dim(\ker(U - \lambda \mathbb{1}_E)) = 1$ *then the eigenvalue* λ *is said to be non-degenerate. Otherwise, it is degenerate and its order of degeneracy* $deg(\lambda)$ *is the dimension of the associated eigenspace.*

3 Formally the spectrum is a set, not a list, and so does not take into account repetitions due to degeneracy.

C

COMPLEMENTS TO CHAPTER 3

C.1 PROJECTED OUTPUT STATE

We prove the expression $\tilde{\rho}_3(n) = |0,n\rangle\langle 0,n|$ as follows.

The intermediate state is

$$\rho_2(n) = \frac{1}{2^n n!} \sum_{k,\ell=0}^{n} \binom{n}{k}\binom{n}{l} (-1)^{k+\ell} a_L^{\dagger\, k} a_R^{\dagger\, n-k} |0,0\rangle\langle 0,0|\, a_L^{\ell} a_R^{n-\ell}.$$

Applying the beam splitter transformation (26) yields

$$\rho_3(n) = \frac{1}{2^{2n} n!} \sum_{k,\ell=0}^{n} \binom{n}{k}\binom{n}{\ell} (-1)^{k+\ell} (a_L^\dagger - a_R^\dagger)^k (a_L^\dagger + a_R^\dagger)^{n-k} \\ |0,0\rangle\langle 0,0|\, (a_L - a_R)^{\ell} (a_L + a_R)^{n-\ell},$$

which can be expanded into

$$\begin{aligned}\rho_3(n) = \frac{1}{2^{2n} n!} &\sum_{k,\ell=0}^{n} \binom{n}{k}\binom{n}{\ell} (-1)^{k+\ell} \\ &\times \sum_{i=0}^{k}\sum_{j=0}^{\ell}\sum_{p=0}^{n-k}\sum_{q=0}^{n-\ell} \binom{k}{i}\binom{\ell}{j}\binom{n-k}{p}\binom{n-\ell}{q} \\ &\times (-1)^{k+\ell-i-j} \sqrt{(i+p)!(n-i-p)!(j+q)!(n-j-q)!} \\ &\times |i+p, n-i-p\rangle\langle j+q, n-j-q|\,.\end{aligned}$$

Then in the evaluation of $\mathrm{Tr}(Q_3\, |i+p, n-i-p\rangle\langle j+q, n-j-q|)$ the only non-vanishing terms satisfy either $(p = n-i) \wedge (q = n-j)$ or $(q = -j) \wedge (p = -i)$. Note that both cases account for $n = 0$. Hence, the relevant submatrix for the calculation of $\langle Q_3 \rangle$ is deduced to take the simple form

$$\begin{aligned}\tilde{\rho}_3(n) = \frac{1}{2^{2n}} \Bigg[|n,0\rangle\langle n,0| \left(\sum_{k,\ell=0}^{n} \binom{n}{k}\binom{n}{\ell} (-1)^{k+\ell} \right) \\ + |0,n\rangle\langle 0,n| \left(\sum_{k,\ell=0}^{n} \binom{n}{k}\binom{n}{\ell} \right) \Bigg] - |0,0\rangle\langle 0,0|\, \delta_n,\end{aligned}$$

where a vacuum contribution was subtracted to correct for the $n = 0$ case. Since the first double-sum equals δ_n and the second equals 2^{2n}, the announced result is obtained.

C.2 COHERENT INPUT WITH DEPHASING

We consider the input state $\rho_1 = |\alpha\rangle\langle\alpha|$. Then the intermediate state with dephasing can be written using Eq. (39) as

$$\rho_2(\alpha,\gamma) = \left|\tfrac{\alpha}{\sqrt{2}}\right\rangle\left\langle\tfrac{\alpha}{\sqrt{2}}\right| \otimes \left[\gamma \left|\tfrac{-\alpha}{\sqrt{2}}\right\rangle\left\langle\tfrac{-\alpha}{\sqrt{2}}\right| + (1-\gamma)\sum_{n=0}^{+\infty} p_n\left(\tfrac{\alpha}{\sqrt{2}}\right)|n\rangle\langle n|\right].$$

It should be noted that the summed over element $|n\rangle\langle n|$ designates a Fock state, while $\left|\frac{\alpha}{\sqrt{2}}\right\rangle\left\langle\frac{\alpha}{\sqrt{2}}\right|$ are coherent states. The first correlator $C_{12} = \langle Q_1 Q_2\rangle = \langle Q_2\rangle$ is

$$\begin{aligned}
&\mathrm{Tr}[Q_2\rho_2(\alpha,\gamma)] \\
&= \sum_{n=1}^{+\infty} \gamma\left(\left\langle 0\middle|\tfrac{\alpha}{\sqrt{2}}\right\rangle\left\langle n\middle|\tfrac{-\alpha}{\sqrt{2}}\right\rangle\left\langle\tfrac{\alpha}{\sqrt{2}}\middle|0\right\rangle\left\langle\tfrac{-\alpha}{\sqrt{2}}\middle|n\right\rangle + \{n \longleftrightarrow 0\}\right) \\
&+ (1-\gamma)\times \\
&\left\{\langle 0,n|\left(\left|\tfrac{\alpha}{\sqrt{2}}\right\rangle\left\langle\tfrac{\alpha}{\sqrt{2}}\right| \otimes \sum_{m=0}^{+\infty} p_m\left(\tfrac{\alpha}{\sqrt{2}}\right)|m\rangle\langle m|\right)|0,n\rangle + \{n \longleftrightarrow 0\}\right\},
\end{aligned}$$

which can be simplified to

$$\mathrm{Tr}[Q_2\rho_2(\alpha,\gamma)] = \sum_{n=1}^{+\infty} 2\gamma e^{-\frac{|\alpha|^2}{2}} p_n\left(\tfrac{\alpha}{\sqrt{2}}\right) + (1-\gamma)2e^{-\frac{|\alpha|^2}{2}} p_n\left(\tfrac{\alpha}{\sqrt{2}}\right).$$

Hence we find $C_{12} = 2e^{-|\alpha|^2/2}(1-e^{-|\alpha|^2/2})$ which, as announced, is the same as with the depolarized case. This is not surprising as phase noise does not change the photon number statistics and there has not been any interference at this stage.

Let us now proceed with the $C_{13} = \langle Q_3\rangle$ correlator. The output state can be written as

$$\rho_3(\alpha,\gamma) = \gamma(|0\rangle\langle 0| \otimes |-\alpha\rangle\langle -\alpha|) + (1-\gamma)\sum_{n=0}^{+\infty} p_n\left(\tfrac{\alpha}{\sqrt{2}}\right) B\left|\tfrac{\alpha}{\sqrt{2}}\right\rangle\left\langle\tfrac{\alpha}{\sqrt{2}}\right| \otimes |n\rangle\langle n|\, B^\dagger.$$

In the calculation of $\mathrm{Tr}[Q_3\rho_3(\alpha,\gamma)]$ the first term is unproblematic (it gives $-\gamma$ as all the flux is in the right output mode). Let us focus on the second term where there is interference between a coherent state and a Fock state. We write $B\left|\frac{\alpha}{\sqrt{2}}\right\rangle|n\rangle = e^{-|\alpha|^2/4}\sum_{k=0}^{+\infty}\frac{\alpha^k}{\sqrt{2^k k!}} B\,|k,n\rangle$, so that

$$\left\langle\tfrac{\alpha}{\sqrt{2}}\right|\langle n|\, B^\dagger Q_3 B\left|\tfrac{\alpha}{\sqrt{2}}\right\rangle|n\rangle = e^{-\frac{|\alpha|^2}{2}}\sum_{k,\ell=0}^{+\infty}\frac{\alpha^{*\ell}\alpha^k}{\sqrt{2^{k+\ell}k!\ell!}}\langle \ell,n|B^\dagger Q_3 B|k,n\rangle.$$

Standard calculations using Eqs. (26) and (42) give $\forall(\ell, m, k, n) \in \mathbb{N}^4$

$$\langle \ell, m|B^\dagger Q_3 B|k, n\rangle = -\delta_\ell \delta_m \delta_k \delta_n + \frac{\sqrt{(k+n)!(\ell+m)!}}{\sqrt{2^{k+n} k! n! \ell! m!}} \times (\delta_{\ell+m,k+n} - (-1)^{k+\ell} \delta_{\ell+m,k+n}),$$

from which one finds

$$\left\langle \frac{\alpha}{\sqrt{2}} \right| \langle n| B^\dagger Q_3 B \left| \frac{\alpha}{\sqrt{2}} \right\rangle |n\rangle = -e^{-|\alpha|^2/2} \delta_n.$$

Hence $C_{13} = -e^{-|\alpha|^2} - \gamma(1 - e^{-|\alpha|^2})$.

Finally, as previously argued, $C_{23} = 0$ by the fact that Q_3 is on average null for trials where $Q_2 = +1$.

D

COMPLEMENTS TO CHAPTER 4

D.1 NESTED COMMUTATORS

Recall that the interaction Hamiltonian in the Dirac picture reads

$$\tilde{H}_1(t) = \frac{1}{\sqrt{m\Omega}} g(t) a^\dagger a \tilde{q}(t) + \frac{1}{3} m\Omega^2 \beta \tilde{p}^4(t).$$

Then to first order in β one has

$$\begin{aligned}[\tilde{H}_1(t_1), \tilde{H}_1(t_2)] &= \frac{1}{m\Omega}(a^\dagger a)^2 g(t_1) g(t_2) [\tilde{q}(t_1), \tilde{q}(t_2)] \\ &\quad + \frac{\sqrt{m\Omega^3}}{3} \beta (a^\dagger a) \Big(g(t_1) [\tilde{q}(t_1), \tilde{p}^4(t_2)] + (t_1 \leftrightarrow t_2) \Big).\end{aligned}$$

Using the commutator expressions (50), the previous equation takes the explicit form

$$\begin{aligned}&[\tilde{H}_1(t_1), \tilde{H}_1(t_2)] = i\hbar \frac{1}{m\Omega}(a^\dagger a)^2 g(t_1) g(t_2) \sin(\Omega(t_2 - t_1)) \\ &+ \frac{4}{3} i\hbar \sqrt{m\Omega^3} \beta (a^\dagger a) \left(g(t_1) \tilde{p}^3(t_2) \cos(\Omega(t_2 - t_1)) - (t_1 \leftrightarrow t_2) \right). \quad (74)\end{aligned}$$

Since the first term commutes with $\tilde{H}_1$, the next nested commutator to first order in β takes the simple form

$$\begin{aligned}&[\tilde{H}_1(t_1), [\tilde{H}_1(t_2), \tilde{H}_1(t_3)]] = 4(a^\dagger a)^2 (i\hbar)^2 \Omega \beta g(t_1) g(t_2) \\ &\quad \times \Big(\tilde{p}^2(t_3) \cos(\Omega(t_3 - t_1)) \cos(\Omega(t_3 - t_2)) - (t_2 \leftrightarrow t_3) \Big). \quad (75)\end{aligned}$$

The following term is then found to be

$$\begin{aligned}&[\tilde{H}_1(t_1), [\tilde{H}_1(t_2), [\tilde{H}_1(t_3), \tilde{H}_1(t_4)]]] = 8(a^\dagger a)^3 (i\hbar)^3 \beta \sqrt{\frac{\Omega}{m}} \\ &\quad \times \Big(g(t_1) g(t_2) g(t_3) \tilde{p}(t_4) \prod_{i=1}^{3} \cos(\Omega(t_4 - t_i)) - (t_3 \leftrightarrow t_4) \Big),\end{aligned}$$

yielding the following form of the fifth order commutator:

$$\begin{aligned}&[\tilde{H}_1(t_1), [\tilde{H}_1(t_2), [\tilde{H}_1(t_3), [\tilde{H}_1(t_4), \tilde{H}_1(t_5)]]]] = \\ &\quad \frac{4!}{3} (a^\dagger a)^4 (i\hbar)^4 \beta \frac{1}{m} \prod_{j=1}^{4} g(t_j) \cos\big(\Omega(t_5 - t_j)\big) - (t_4 \leftrightarrow t_5),\end{aligned}$$

as announced.

D.2 FIFTH MAGNUS TERM IN THE PULSED REGIME

To work out an analytical expression for the fifth Magnus term, we begin with Eq. (54) that we rewrite as

$$\Theta_5(t) = -\frac{i}{\hbar} 8(a^\dagger a)^4 \frac{\beta}{m}(\lambda_1 T_1 + \lambda_2 T_2 + \lambda_3 T_3 + \lambda_4 T_4).$$

The λ_k are known. We seek to express the T_k terms when the interaction g takes the form $g(t) = \lambda \sum_{i=0}^{3} \delta(t - \tau_i)$ with no further specification for τ_i. Let us define $f(t_1, ..., t_5) := \prod_{j=1}^{4} \cos\big(\Omega(t_5 - t_j)\big)$. Then

$$\begin{aligned} T_k = \lambda^4 \sum_{i_1 i_2 i_3 i_4 = 0}^{3} \int_{(5,t)} dt^5 \\ \Big\{ \delta(t_{\sigma_k(1)} - \tau_{i_1}) \delta(t_{\sigma_k(2)} - \tau_{i_2}) \delta(t_{\sigma_k(3)} - \tau_{i_3}) \delta(t_{\sigma_k(4)} - \tau_{i_4}) \\ \times f(t_{\sigma_k(1)}, t_{\sigma_k(2)}, t_{\sigma_k(3)}, t_{\sigma_k(4)}, t_{\sigma_k(5)}) \Big\} \\ - \Big\{ \delta(t_{\sigma_k(1)} - \tau_{i_1}) \delta(t_{\sigma_k(2)} - \tau_{i_2}) \delta(t_{\sigma_k(3)} - \tau_{i_3}) \delta(t_{\sigma_k(5)} - \tau_{i_4}) \\ \times f(t_{\sigma_k(1)}, t_{\sigma_k(2)}, t_{\sigma_k(3)}, t_{\sigma_k(5)}, t_{\sigma_k(4)}) \Big\}. \end{aligned}$$

Showing explicit calculations for the first term $\sigma_1 = (54321)$ we have

$$\begin{aligned} T_1 = \lambda^4 \sum_{i_1 i_2 i_3 i_4 = 0}^{3} \int_{(5,t)} dt^5 \delta(t_5 - \tau_{i_1}) \delta(t_4 - \tau_{i_2}) \delta(t_3 - \tau_{i_3}) \\ \times \Big\{ \delta(t_2 - \tau_{i_4}) f(t_5, t_4, t_3, t_2, t_1) - \delta(t_1 - \tau_{i_4}) f(t_5, t_4, t_3, t_1, t_2) \Big\}. \end{aligned}$$

Integrating the δ distributions yields

$$\begin{aligned} T_1 = \lambda^4 \sum_{i_1 i_2 i_3 i_4 = 0}^{3} H(t, \tau_{i_4}, \tau_{i_3}, \tau_{i_2}, \tau_{i_1}) \\ \times \left(\int_{\tau_{i_4}}^{t} ds - \int_{\tau_{i_3}}^{\tau_{i_4}} ds \right) f(\tau_{i_1}, \tau_{i_2}, \tau_{i_3}, \tau_{i_4}, s), \end{aligned}$$

where $H(a, b, c, d, e)$ designates the succession of Heaviside functions $H(a, b, c, d, e) = H(a - b)H(b - c)H(c - d)H(d - e)$. In a similar fashion, from $\sigma_2 = (15423)$ we obtain

$$\begin{aligned} T_2 = \lambda^4 \sum_{i_1 i_2 i_3 i_4 = 0}^{3} H(t, \tau_{i_1}, \tau_{i_4}, \tau_{i_3}, \tau_{i_2}) \\ \times \left(\int_{\tau_{i_3}}^{\tau_{i_4}} ds - \int_{\tau_{i_4}}^{\tau_{i_1}} ds \right) f(\tau_{i_1}, \tau_{i_2}, \tau_{i_3}, \tau_{i_4}, s). \end{aligned}$$

For the third permutation $\sigma_3 = (14325)$, one finds

$$T_3 = \lambda^4 \sum_{i_1 i_2 i_3 i_4 = 0}^{3} \left(H(t, \tau_{i_1}, \tau_{i_4}, \tau_{i_3}, \tau_{i_2}) \int_0^{\tau_{i_2}} ds - H(t, \tau_{i_1}, \tau_{i_3}, \tau_{i_2}, \tau_{i_4}) \int_{\tau_{i_3}}^{\tau_{i_1}} ds \right) f(\tau_{i_1}, \tau_{i_2}, \tau_{i_3}, \tau_{i_4}, s).$$

Finally, from $\sigma_4 = (15324)$ it follows that

$$T_4 = \lambda^4 \sum_{i_1 i_2 i_3 i_4 = 0}^{3} \left(H(t, \tau_{i_1}, \tau_{i_4}, \tau_{i_3}, \tau_{i_2}) \int_{\tau_{i_2}}^{\tau_{i_3}} ds - H(t, \tau_{i_1}, \tau_{i_3}, \tau_{i_4}, \tau_{i_2}) \int_{\tau_{i_3}}^{\tau_{i_1}} ds \right) f(\tau_{i_1}, \tau_{i_2}, \tau_{i_3}, \tau_{i_4}, s).$$

Summing up these expressions, noting that $\lambda_1 = \lambda_3 = \lambda_4 = -\frac{1}{30}$ and $\lambda_2 = \frac{4}{30}$ one arrives at

$$\begin{aligned} \sum_{k=1}^{4} \lambda_k T_k = \frac{\lambda^4}{30} \sum_{i_1 i_2 i_3 i_4 = 0}^{3} \Bigg\{ & H(t, \tau_{i_4}, \tau_{i_3}, \tau_{i_2}, \tau_{i_1}) \left(\int_{\tau_{i_3}}^{\tau_{i_4}} ds - \int_{\tau_{i_4}}^{t} ds \right) \\ & + H(t, \tau_{i_1}, \tau_{i_4}, \tau_{i_3}, \tau_{i_2}) \left(4 \int_{\tau_{i_3}}^{\tau_{i_1}} ds - \int_0^{\tau_{i_3}} ds \right) \\ & + H(t, \tau_{i_1}, \tau_{i_3}, \tau_{i_2}, \tau_{i_4}) \left(\int_{\tau_{i_3}}^{\tau_{i_1}} ds \right) \\ & + H(t, \tau_{i_1}, \tau_{i_3}, \tau_{i_4}, \tau_{i_2}) \left(\int_{\tau_{i_3}}^{\tau_{i_1}} ds \right) \Bigg\} f(\tau_{i_1}, \tau_{i_2}, \tau_{i_3}, \tau_{i_4}, s). \end{aligned} \tag{76}$$

Thus the fifth order Magnus term can be expressed as follows:

$$\begin{aligned} \Theta_5(t) = -\frac{i}{\hbar} \frac{4!}{3} (a^\dagger a)^4 \frac{\beta}{m} \frac{\lambda^4}{30} \sum_{i_1 i_2 i_3 i_4 = 0}^{3} \Bigg\{ & \\ & H(t, \tau_{i_4}, \tau_{i_3}, \tau_{i_2}, \tau_{i_1}) \left(\int_{\tau_{i_3}}^{\tau_{i_4}} ds - \int_{\tau_{i_4}}^{t} ds \right) \\ & + H(t, \tau_{i_1}, \tau_{i_4}, \tau_{i_3}, \tau_{i_2}) \left(4 \int_{\tau_{i_3}}^{\tau_{i_4}} ds - 4 \int_{\tau_{i_4}}^{\tau_{i_1}} ds - \int_0^{\tau_{i_3}} ds \right) \\ & + H(t, \tau_{i_1}, \tau_{i_3}, \tau_{i_2}, \tau_{i_4}) \left(\int_{\tau_{i_3}}^{\tau_{i_1}} ds \right) \\ & + H(t, \tau_{i_1}, \tau_{i_3}, \tau_{i_4}, \tau_{i_2}) \left(\int_{\tau_{i_3}}^{\tau_{i_1}} ds \right) \Bigg\} f(\tau_{i_1}, \tau_{i_2}, \tau_{i_3}, \tau_{i_4}, s). \end{aligned} \tag{77}$$

For completeness, the closed form result is obtained by taking Eq. (77) and specifying $\forall k \in \{0,1,2,3\},\ \tau_k = t_0 + k\theta$ where $\theta = \frac{\pi}{2\Omega} > 0$ and assuming $t > t_0 + 3\theta$.

It is then established that

$$\begin{aligned}\sum_{k=1}^{4} \lambda_k T_k = \frac{\lambda^4}{30} \sum_{i_1 i_2 i_3 i_4 = 0}^{3} \Bigg\{ & \\ & H(i_4, i_3, i_2, i_1) \left(\int_{t_0+i_3\theta}^{t_0+i_4\theta} ds - \int_{t_0+i_4\theta}^{t} ds \right) \\ & + H(i_1, i_4, i_3, i_2) \left(4 \int_{t_0+i_3\theta}^{t_0+i_1\theta} ds - \int_{0}^{t_0+i_3\theta} ds \right) \\ & + H(i_1, i_3, i_2, i_4) \left(\int_{t_0+i_3\theta}^{t_0+i_1\theta} ds \right) \\ & + H(i_1, i_3, i_4, i_2) \left(\int_{t_0+i_3\theta}^{t_0+i_1\theta} ds \right) \Bigg\} \\ & f(t_0 + i_1\theta, t_0 + i_2\theta, t_0 + i_3\theta, t_0 + i_4\theta, s).\end{aligned}$$

One can simplify the expression of the integrand by noticing that $f(t_0 + i_1\theta, t_0 + i_2\theta, t_0 + i_3\theta, t_0 + i_4\theta, s) = \prod_{k=1}^{4} \cos\left(\Omega(s - t_0) + \frac{i_k \pi}{2}\right)$, and with the affine change of variable $u = \Omega(s - t_0)$, one has

$$\int_{t_0+\alpha\theta}^{t_0+\beta\theta} f(t_0 + i_1\theta, t_0 + i_2\theta, t_0 + i_3\theta, t_0 + i_4\theta, s) ds = \frac{1}{\Omega} \int_{\alpha\frac{\pi}{2}}^{\beta\frac{\pi}{2}} \prod_{k=1}^{4} \cos\left(u - \frac{i_k \pi}{2}\right) du,$$

and the result follows.

D.3 FIFTH MAGNUS TERM IN THE EXTENDED CASE

To compute the fifth order Magnus term in this case, we can start by making Eq. (59) more explicit by writing out

$$\prod_{s=1}^{4} D_j(t_{\sigma_s}, t_{\sigma_5}) = \sum_{i_1 i_2 i_3 i_4 = 1}^{N} g_{i_1}(t_{\sigma_1}) \ldots g_{i_4}(t_{\sigma_4}) f_{i_1 i_2 i_3 i_4}(t_{\sigma_1}, \ldots, t_{\sigma_5}),$$

where $f_{i_1 i_2 i_3 i_4 j}(t_{\sigma_1}, \ldots, t_{\sigma_5}) := \prod_{s=1}^{4} C_{i_s j}(t_{\sigma_s} - t_{\sigma_5})$ and

$$C_{i_s j}(t_{\sigma_s} - t_{\sigma_5}) = i\hbar \sum_{\nu=1}^{N} O_{i_s \nu} O'_{j\nu} \cos(\omega_\nu (t_{\sigma_s} - t_{\sigma_5})).$$

Thus one can write

$$\begin{aligned} & f_{i_1 i_2 i_3 i_4 j}(t_{\sigma_1}, \ldots, t_{\sigma_5}) \\ & \quad = \hbar^4 \sum_{\nu_1 \nu_2 \nu_3 \nu_4 = 1}^{N} \left(\prod_{s=1}^{4} O_{i_s \nu_s} O'_{j\nu_s} \right) \varphi_{\nu_1 \nu_2 \nu_3 \nu_4}(t_{\sigma_1}, \ldots, t_{\sigma_5}),\end{aligned}$$

where we have defined

$$\varphi_{\nu_1\nu_2\nu_3\nu_4}(t_{\sigma_1},...,t_{\sigma_5}) := \prod_{s=1}^{4} \cos(\omega_{\nu_s}(t_{\sigma_s} - t_{\sigma_5})).$$

From this, one can express the fifth Magnus term as

$$\Theta_5(t) = \left(\frac{-i}{\hbar}\right)^5 \hbar^4 \frac{4!}{3}\frac{\beta}{m}(a^\dagger a)^4 \times$$
$$\sum_{\sigma\in S}\lambda_\sigma \sum_{i_1i_2i_3i_4j=1}^{N} \sum_{\nu_1\nu_2\nu_3\nu_4=1}^{N} \left(\prod_{s=1}^{4} O_{i_s\nu_s}O'_{j\nu_s}\right) \times$$
$$\int_{(5,t)} dt^5 g_{i_1}(t_{\sigma_1})...g_{i_4}(t_{\sigma_4})\varphi_{\nu_1\nu_2\nu_3\nu_4}(t_{\sigma_1},...,t_{\sigma_5}) - (t_{\sigma_5} \leftrightarrow t_{\sigma_4}).$$

We may write

$$g_{i_1}(t_{\sigma_1})...g_{i_4}(t_{\sigma_4}) = \lambda^4 \sum_{\alpha_1\alpha_2\alpha_3\alpha_4=0}^{3} \prod_{r=1}^{4} \delta(t_{\sigma_r} - \theta(\alpha_r, i_r)),$$

where $\theta(\alpha_r, i_r) := t_0 + \alpha_r T + (i_r - 1)\tau$ for convenience. We shall lighten the notation to θ_r bearing in mind that it is a function of α_r and i_r. The task is now reduced to expressing the integral

$$\int_{(5,t)} dt^5 \left(\prod_{r=1}^{4} \delta(t_{\sigma_r} - \theta_r)\right) \varphi_{\nu_1\nu_2\nu_3\nu_4}(t_{\sigma_1},...,t_{\sigma_5}) - (t_{\sigma_4} \leftrightarrow t_{\sigma_5}).$$

After similar calculations as for the single oscillator driven by pulsed light, one arrives at

$$\sum_{\sigma\in S}\lambda_\sigma \int_{(5,t)} dt^5 \left(\prod_{r=1}^{4} \delta(t_{\sigma(r)} - \theta_r)\right)$$
$$\times\ \varphi_{\nu_1\nu_2\nu_3\nu_4}(t_{\sigma(1)},...,t_{\sigma(5)}) - (t_{\sigma(4)} \leftrightarrow t_{\sigma(5)}) =$$
$$\Bigg\{\lambda_1 H(t,\theta_4,\theta_3,\theta_2,\theta_1)\int_{D_1} ds + \lambda_2 H(t,\theta_1,\theta_4,\theta_3,\theta_2)\int_{D_2} ds$$
$$+\lambda_3\left(H(t,\theta_1,\theta_4,\theta_3,\theta_2)\int_{D_3} ds + H(t,\theta_1,\theta_3,\theta_2,\theta_4)\int_{D'_3} ds\right)$$
$$+\lambda_4\left(H(t,\theta_1,\theta_4,\theta_3,\theta_2)\int_{D_4} ds + H(t,\theta_1,\theta_3,\theta_4,\theta_2)\int_{D'_4} ds\right)\Bigg\}$$
$$\varphi_{\nu_1\nu_2\nu_3\nu_4}(\theta_1,\theta_2,\theta_3,\theta_4,s)$$

where $(\lambda_1,\lambda_2,\lambda_3,\lambda_4) = (\frac{-1}{30}, \frac{4}{30}, \frac{-1}{30}, \frac{-1}{30})$ are the coefficients associated with the permutations and the integration domains are given by oriented intervals (and unions of)

$$D_1 = [\theta_4, t] \cup [\theta_4, \theta_3];\ D_2 = [\theta_3, \theta_4] \cup [\theta_1, \theta_4],$$
$$D_3 = [0, \theta_2];\ D'_3 = [\theta_1, \theta_3];\ D_4 = [\theta_2, \theta_3];\ D'_4 = [\theta_1, \theta_3].$$

Hence the fifth Magnus term takes the following expression:

$$\Theta_5(t) = -\frac{i}{\hbar}\frac{4!}{3}\frac{\beta}{m}(a^\dagger a)^4 \sum_{i_1 i_2 i_3 i_4 j=1}^{N} \sum_{\nu_1\nu_2\nu_3\nu_4=1}^{N} \left(\prod_{s=1}^{4} O_{i_s\nu_s} O'_{j\nu_s}\right) \frac{\lambda^4}{30} \times$$
$$\sum_{\alpha_1\alpha_2\alpha_3\alpha_4=0}^{3} \left\{ H(t,\theta_4,\theta_3,\theta_2,\theta_1)\left(\int_{\theta_3}^{\theta_4} ds - \int_{\theta_4}^{t} ds\right)\right.$$
$$+ H(t,\theta_1,\theta_4,\theta_3,\theta_2)\left(4\int_{\theta_3}^{\theta_4} ds - 4\int_{\theta_4}^{\theta_1} ds - \int_{0}^{\theta_3} ds\right)$$
$$\left. + H(t,\theta_1,\theta_3,\theta_2,\theta_4)\left(\int_{\theta_3}^{\theta_1} ds\right) + H(t,\theta_1,\theta_3,\theta_4,\theta_2)\left(\int_{\theta_3}^{\theta_1} ds\right)\right\}$$
$$\varphi_{\nu_1\nu_2\nu_3\nu_4}(\theta_1,\theta_2,\theta_3,\theta_4,s).$$

E

COMPLEMENTS TO CHAPTER 5

E.1 SPIN DENSITY MATRIX EXPRESSION

We present explicit derivations of Eq. (63) and Eq. (64). We express the two copies of an arbitrary initial state with their P-representations so that

$$(\pi \otimes \pi) = \iint d^2\varepsilon d^2\zeta P(\varepsilon)P(\zeta)\,|\varepsilon\zeta\rangle\langle\varepsilon\zeta|\,.$$

From Eq. (61) the spin density matrix elements are found to be

$$s_{\alpha\beta\mu\nu} = \frac{1}{4}e^{-iGm^2\tau Q^{(1)}_{\alpha\beta\mu\nu}/\hbar}\iint d^2\varepsilon d^2\zeta P(\varepsilon)P(\zeta)\,\mathrm{Tr}\Big[\mathcal{U}_{\alpha\beta}{}^{\dagger}\mathcal{U}_{\mu\nu}\,|\varepsilon\zeta\rangle\langle\varepsilon\zeta|\Big].$$

Combining this with (62), it follows that

$$\begin{aligned} s_{\alpha\beta\mu\nu} = \frac{1}{4}e^{-iGm^2\tau Q^{(1)}_{\alpha\beta\mu\nu}/\hbar}e^{-iG^2m^3\tau^3 Q^{(4)}_{\alpha\beta\mu\nu}/6\hbar} \\ \times \iint d^2\varepsilon d^2\zeta P(\varepsilon)P(\zeta)\,\big\langle\varepsilon\big|\varepsilon+\theta_{\alpha\beta\mu\nu}\big\rangle\,\big\langle\zeta\big|\zeta-\theta_{\alpha\beta\mu\nu}\big\rangle\,. \end{aligned}$$

The remaining double integral turns out to be quite simply expressed as

$$\begin{aligned} &\iint d^2\varepsilon d^2\zeta P(\varepsilon)P(\zeta)\,\langle\varepsilon|\varepsilon+\theta\rangle\,\langle\zeta|\zeta-\theta\rangle \\ &\qquad = e^{-|\theta|^2}\left(\int d^2\varepsilon P(\varepsilon)e^{\frac{1}{2}(\varepsilon^*\theta-\theta^*\varepsilon)}\right)\left(\int d^2\zeta P(\zeta)e^{\frac{1}{2}(\theta^*\zeta-\zeta^*\theta)}\right) \\ &\qquad = e^{-|\theta|^2}\mathcal{F}(P)\left(\frac{\theta}{2}\right)\mathcal{F}(P)\left(-\frac{\theta}{2}\right) \\ &\qquad = e^{-|\theta|^2}\left(C_N\left(\frac{\theta}{2}\right)\right)^2, \end{aligned}$$

where we have dropped the indices for θ and used the fact that the P-function is real, so has an even Fourier transform $\mathcal{F}(P)$, which coincides with the normally ordered characteristic function. This yields Eq. (63). Furthermore, if the initial local motional state is thermal with average photon number $\langle N\rangle = \overline{n}$, then the characteristic function is $C_N(\lambda) = e^{-\overline{n}|\lambda|^2}$, as was shown at length in Sec. 2.3.2, which yields Eq. (64).

E.2 DECOHERENCE RATE LIMIT

We demonstrate the decoherence rate limit for our witness. For any Hermitian 4 by 4 matrix $\rho = (\rho_{ij})_{1\leqslant i,j\leqslant 4}$ one can compute

$$\begin{aligned}\mathrm{Tr}(W_1\rho) = \mathrm{Tr}(\rho) + 2\,\mathrm{Im}\{\rho_{12}\} + 2\,\mathrm{Im}\{\rho_{13}\} \\ - 2\,\mathrm{Re}\{\rho_{14}\} - 2\,\mathrm{Re}\{\rho_{23}\} - 2\,\mathrm{Im}\{\rho_{24}\} - 2\,\mathrm{Im}\{\rho_{34}\}.\end{aligned}$$

Without decoherence, the spin state after free fall of duration t reads

$$\rho_s(\gamma = 0) = \frac{1}{4}\begin{pmatrix} 1 & e^{-i\Delta\phi_{LR}} & e^{-i\Delta\phi_{RL}} & 1 \\ e^{i\Delta\phi_{LR}} & 1 & e^{i(\Delta\phi_{LR}-\Delta\phi_{RL})} & e^{i\Delta\phi_{LR}} \\ e^{i\Delta\phi_{RL}} & e^{i(\Delta\phi_{RL}-\Delta\phi_{LR})} & 1 & e^{i\Delta\phi_{RL}} \\ 1 & ee^{-i\Delta\phi_{LR}} & e^{-i\Delta\phi_{RL}} & 1 \end{pmatrix}.$$

With the inclusion of a decoherence rate γ, the spin state takes the form $\rho_s = \rho_s(\gamma = 0) \odot \Gamma$, where $\odot$ designates a Hadamard product in the bipartite spin computational basis, and the matrix Γ is defined by

$$\Gamma = \begin{pmatrix} 1 & e^{-\gamma t} & e^{-\gamma t} & e^{-2\gamma t} \\ e^{-\gamma t} & 1 & e^{-2\gamma t} & e^{-\gamma t} \\ e^{-\gamma t} & e^{-2\gamma t} & 1 & e^{-\gamma t} \\ e^{-2\gamma t} & e^{-\gamma t} & e^{-\gamma t} & 1 \end{pmatrix}.$$

Then the witness expectation value is given by

$$\begin{aligned}\mathrm{Tr}(W_1\rho) = 1 - e^{-\gamma t}\left(\sin(\Delta\phi_{LR}) + \sin(\Delta\phi_{RL})\right) \\ - \frac{1}{2}e^{-2\gamma t}(1 + \cos(\Delta\phi_{LR} - \Delta\phi_{RL})).\end{aligned}$$

Writing $\omega_{\mu\nu}t = \Delta\phi_{\mu\nu}$ a first order expansion around $t = 0$ gives

$$\mathrm{Tr}(W_1\rho) = (2\gamma - (\omega_{LR} + \omega_{RL}))t + o(t),$$

so there is no more immediately witnessed entanglement for decoherence rates greater than the average of the two path coupling frequencies $\gamma \geqslant (\omega_{RL} + \omega_{LR})/2$.

E.3 NON-MONOTONICITY LOOPHOLE STATE

We simulate a 3×10^3 element string of Pauli measurement outcomes, obtained from 10^3 measurements of W_1 on ρ_a. Given this data, we construct a state ρ'_a that is at least as likely as ρ_a given the data but has a negativity that is lower than that of the null hypothesis state ρ_0. Explicitly, for separation distance $d = 350$ μm, decoherence rate $\gamma = 0.3$ s^{-1} with corresponding free-fall duration $\tau = 0.34$ s, one

has $\mathcal{N}(\rho_0) \approx 0.108 > \mathcal{N}(\rho'_a) \approx 0.104$ where with a rounding to 3 significant figures the loophole state ρ'_a takes the form

$$\begin{pmatrix} 0.256 & 0.009+0.012i & 0.042-0.174i & 0.212+0.010i \\ 0.009-0.012i & 0.244 & 0.109-0.022i & -0.008+0.004i \\ 0.042+0.174i & 0.109+0.023i & 0.246 & 0.017+0.161i \\ 0.212-0.011i & -0.008-0.004i & 0.017-0.161i & 0.254 \end{pmatrix}.$$

To obtain such a state, we have made used of a constrained optimization method (sequential least squares programming) over all valid 2-qubit quantum states. The cost function to minimize was the negative logarithmic likelihood ratio given the data, under the constraint that the state should be less negative than the null hypothesis state.

For completeness we remind a parametrization of the 2-qubit state space. By Cholesky decomposition of positive-semidefinite density matrices (see Sec. 2.1.2 for details) one can write any density matrix as $\rho = LL^\dagger$, where L is a lower diagonal matrix with real diagonal coefficients

$$L = \begin{pmatrix} l_1 & 0 & 0 & 0 \\ l_5 & l_2 & 0 & 0 \\ l_8 & l_6 & l_3 & 0 \\ l_{10} & l_9 & l_7 & l_4 \end{pmatrix}.$$

The set of such matrices is a 16-dimensional real vector space. There are 4 degrees of freedom for the diagonal terms and 12 for the off-diagonal ones. The unit trace condition imposes $\mathrm{Tr}(\rho) = \mathrm{Tr}(LL^\dagger) = 1$ so that $\sum_{i=1}^{10} |l_i|^2 = 1$. Thus, the state space can be viewed as constituting a 9-sphere. One can parametrize this with 15 real angles, as expected from Sec. 2.4.1 by defining $l_1 = \cos\theta_1$, $l_2 = \sin\theta_1 \cos\theta_2$ up to $l_9 = (e^{i\phi_9} \prod_{i=1}^{8} \sin\theta_i) \cos\theta_9$, $l_{10} = e^{i\phi_{10}} \prod_{i=1}^{9} \sin\theta_i$. Note that $l_1, ...l_4$ do not require $e^{i\phi}$ phase terms since they are real. Hence we have the 15 real parameters $\theta_1, ...\theta_9$, and $\phi_5, ..., \phi_{10}$ on which to run the constrained optimization.

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