DISSERTATION

Titel der Dissertation

Local and Causal Structures in Quantum Theory

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Contents

Abstract

Several conceptual issues at the interface between quantum mechanics and special and general relativity revolve around the notions of locality and causality. In relativistic quantum field theory, the identification of local degrees of freedom with quantum observables yields counterintuitive predictions, such as vacuum entanglement. Combining general covariance and the dynamic causal structure of general relativity with quantum mechanics is one of the main open problems in theoretical physics and a consistent framework that unifies the two theories is still missing. In this thesis several foundational questions at the border between quantum mechanics, special and general relativity are addressed. Basic concepts such as localisation and causal structure are examined from an operational point of view, with a special focus on the experimental procedures that allow defining them. Methods are developed which allow exploring the relation between the mathematical and the operational notions, as well as understanding under which conditions counterintuitive features can be observed and in which limit they reduce to more intuitive, classical notions.

In the first chapter, the notions of particle and particle detector models in relativistic quantum field theory are investigated. Theoretical models of particle detectors are often used to give an operational meaning to the notion of particle in curved spacetime. However, the commonly adopted models feature temporary transitions from ground to excited state even when the detector is at rest in the Minkowski vacuum, making the interpretation of "clicks" of the detectors as absorption of particles unambiguous only if the detector is switched on for infinite times (in which limit, a detector initially in the vacuum is found in the ground state). A toy model is considered in which a local interaction between relativistic fields describes a simple process of absorption of a particle by a detector. Both the detector and the particles to be detected are represented in terms of dressed states of relativistic fields, i.e. eigenstates of the full interacting Hamiltonian, as opposed to the bare states (eigenstates of the non-interacting theory) considered in typical detector models. An effective model for a two-level detector is then derived, which reproduces the transition amplitudes of the fundamental model in the first order of the perturbation theory. Such a model does not predict particle detection in the Minkowski vacuum and provides a well-defined notion of particle also for finite detection times. However, the observables effectively "seen" by the (dressed) detector are not the local relativistic fields: although the underlying theory is local and relativistically invariant, the effective theory, as observed from the detector's point of view, appears as non-local.

The second chapter considers the problem of associating a thermodynamic entropy to a region of space containing a relativistic quantum field in a thermal state. If one considers a volume of space in thermal equilibrium, its entropy is

finite and extensive. However, if a subregion is considered, the calculation of
the entropy contains a divergent vacuum contribution which, once an ultraviolet
cut-off is introduced, is proportional to the area of the boundary of the subre-
gion. A new scheme for calculating the thermal entropy is considered, where the
degrees of freedom corresponding to a region of space are associated with the
Newton-Wigner position operators rather than with the local covariant fields. The
calculation shows that the entropy is always finite, without the need of any cut-off
or other additional regularisations. It is found that, in the high temperature/high
volume limit, the entropy is extensive and matches the result for the full space
calculated with standard techniques. For the vacuum state, the entropy vanishes
as a result of the fact that in the Newton-Wigner localisation scheme the vacuum
is a pure product state.

In the third chapter the discrepancies between the classical and quantum no-
tions of entropy in quantum field theory are investigated. It is shown how a clas-
sical notion of entropy can emerge under the assumption that measurements of the
quantum fields are subject to a minimal error. In particular, it is shown that the
entropy of a region of space becomes extensive, i.e. proportional to the volume, if
the field's amplitude cannot be measured with arbitrary precision. It is also shown
that a minimal error in distinguishing points in space produces a different defini-
tion of local degrees of freedom, according to which the vacuum is a pure product
state.

The fourth chapter addresses the implications of using quantum, rather than
classical, reference frames in experimental tests of quantum mechanics. In partic-
ular directional reference frames are considered, modelled as spin coherent states,
which allow measuring a spin's orientation without an additional, external ref-
erence frame (i.e. in a rotationally invariant manner). It is shown that quantum
reference frames of finite size limit the ability to demonstrate genuine quantum
features such as violation of local realism. It is found that if quantum features
of macroscopic objects have to be tested, quadratically larger reference frames
are needed, a requirement generally not met in everyday experience. This sug-
gests that there exist fundamental limits in performing arbitrarily accurate meas-
urements and provides a possible explanation for the non-observance of quantum
phenomena at macroscopic scales, that is to say, emergence of classicality.

The last chapter addresses the general question of whether a definite causal
order between events is a fundamental property of nature. The notion of causal
order is defined operationally in terms of signalling: if *A* can signal to *B* but *B*
cannot signal to *A*, then *A* precedes *B* in a causal structure. For operations local-
ised in spacetime, only one-way signalling is possible in an individual run of an
experiment; the main focus of the chapter is understanding whether, in quantum
mechanics, such an assumption can be relaxed and under which conditions it be-
comes necessary. For this purpose, a new framework for multipartite quantum

correlations is developed that does not presume any notion of global space, time, or causal structure but simply that experimenters in their local laboratories can perform arbitrary quantum operations. All known situations that respect definite causal order, including signalling and non-signalling correlations between time-like and space-like separated experiments respectively, as well as probabilistic mixtures of these, can be expressed in this framework. It is found that the formalism also includes situations where the two experiments are neither causally ordered nor in a probabilistic mixture of definite causal orders. These correlations are shown to allow performing a communication task that would be impossible if the operations were ordered according to a fixed background time. However, it is proven that classical correlations, i.e. correlations between classical operations, are always causally ordered, suggesting that a definite causal structure can emerge in a quantum-to-classical transition.

Zusammenfassung

Etliche konzeptuelle Fragestellungen, die an der Schnittstelle zwischen Quantenmechanik und der Speziellen sowie der Allgemeinen Relativitätstheorie entstehen, drehen sich um die Konzepte "Lokalität" und "Kausalität". In relativistischer Quantenfeldtheorie führt die Identifizierung lokaler Freiheitsgrade mit Quanten-Observablen zu kontraintuitiven Vorhersagen. Die Verbindung der allgemeinen Kovarianz und der dynamischen Kausalstruktur der Allgemeinen Relativitätstheorie mit der Quantenmechanik ist eines der großen offenen Probleme in Theoretischer Physik. Ein konsistenter Rahmen, welcher die beiden Theorien vereinheitlicht, fehlt bis heute. In dieser Doktorarbeit werden einige fundamentale Fragen an der Grenze zwischen Quantenmechanik, Spezieller und Allgemeiner Relativitätstheorie aufgegriffen. Grundlegende Konzepte, wie z.B. die Lokalisierung und die Kausalstruktur, werden von einem operationellen Standpunkt untersucht—mit einem speziellen Fokus auf die experimentellen Techniken, welche die Definition der Konzepte erlauben. Es werden Methoden entwickelt, die die Erforschung der Beziehung zwischen den mathematischen und operationellen Begriffen erlauben sowie zum Verständnis beitragen, unter welchen Bedingungen kontraintuitive Eigenschaften beobachtet werden können und in welchem Limit sich diese Eigenschaften auf intuitivere, klassische Begriffe reduzieren.

Im ersten Kapitel werden die Konzepte von Teilchen und Teilchendetektionsmodellen in der relativistischen Quantenfeldtheorie untersucht. Theoretische Modelle von Teilchendetektoren werden oftmals dazu herangezogen, um dem Konzept eines Teilchens in einer gekrümmten Raumzeit eine operationelle Bedeutung zu geben. Allerdings weisen die üblicherweise angewendeten Modelle zeitweilige Übergänge auf, selbst wenn sich der Detektor im Minkowski-Vakuum in Ruhe befindet. Ein Toy-Modell wird betrachtet, in welchem eine lokale Wechselwirkung zwischen relativistischen Feldern einen einfachen Prozess der Absorption eines Teilchens von einem Detektor beschreibt. Der Detektor sowie die zu detektierenden Teilchen werden durch bekleidete Zustände relativistischer Felder d.h. durch Eigenzustände des vollen Wechselwirkungs-Hamiltonischen Operators dargestellt. Ein erfolgreiches Modell für einen Zwei-Level-Detektor wird hergeleitet, welches die Übergangsamplitude des fundamentalen Models in der ersten Näherung der Störungstheorie reproduziert und welches keine Teilchen im Minkowski-Vakuum detektiert und daher ein wohldefiniertes Konzept eines Teilchens für eine beliebig endliche Zeit liefert. Als Ergebnis folgt, dass die Observablen, die tatsächlich vom (bekleideten) Detektor "gesehen" werden, nicht die lokalen relativistischen Felder sind. Obwohl die zugrunde liegende Theorie lokal und relativistisch invariant ist, erscheint die eigentliche Theorie vom Standpunkt des Detektors nicht-lokal.

Das zweite Kapitel betrachtet das Problem der Thermodynamik in der Quan-

tenfeldtheorie. Wenn man ein räumliches Volumen im thermischen Gleichgewicht betrachtet, ist dessen Entropie endlich und extensiv. Wenn man allerdings einen Teilbereich betrachtet, enthält die Berechnung der Entropie einen divergierenden Vakuumbeitrag, welcher proportional zur Grenzfläche des Teilbereichs wird, sobald ein ultravioletter Cut-Off eingeführt ist. Ein neues Schema für die Berechnung der thermischen Entropie wird betrachtet, in dem die mit einem Bereich des Raums korrespondierenden Freiheitsgrade mit den Newton-Wigner-Ortsoperatoren anstatt mit den lokalen kovarianten Feldern assoziiert sind. Die Berechnungen zeigen, dass die Entropie auch ohne einen Cut-Off oder andere zusätzliche Regularisierungen immer endlich ist. Es wird festgestellt, dass im Limes hoher Temperaturen/großen Volumens die Entropie extensiv ist und zu den Ergebnissen für den ganzen Raum passt, die mit den Standardtechniken berechnet wurden. Für den Vakuumzustand verschwindet die Entropie, da im Newton-Wigner-Lokalisierungsschema das Vakuum ein reiner Produktzustand ist.

Im dritten Kapitel werden Diskrepanzen zwischen den klassischen und den quantenphysikalischen Begriffen der Entropie in der Quantenfeldtheorie untersucht. Es wird gezeigt, wie ein klassischer Begriff der Entropie unter der Annahme zustande kommt, dass Messungen der Quantenfelder minimalen Fehlern unterworfen sind. Insbesondere wird gezeigt, dass die Entropie eines Bereichs im Raum extensiv werden kann, d.h. proportional zum Volumen, falls die Feldamplitude nicht mit beliebiger Genauigkeit gemessen werden kann. Desweiteren wird gezeigt, dass ein minimaler Fehler bei der Unterscheidung von Punkten im Raum eine unterschiedliche Definition lokaler Freiheitsgrade hervorrufen kann, gemäß derer das Vakuum ein reiner Produktzustand ist.

Das vierte Kapitel beschäftigt sich mit den Auswirkungen der Verwendung von quantenphysikalischen anstatt klassischer Bezugssysteme in experimentellen Tests der Quantenmechanik. Insbesondere werden gerichtete Bezugssystemen betrachtet, modelliert als Spin-kohärente Zustände, welche die Messung der Orientierung eines Spins ohne zusätzliches äußeres Bezugssystem (d.h. in einer rotationsinvarianten Weise) erlauben. Es wird gezeigt, dass Quantenbezugssysteme endlicher Größe die Möglichkeit beschränken, echte Quanteneigenschaften wie z.B. die Verletzung des lokalen Realismus aufzuzeigen. Es wird gezeigt, dass—falls Quanteneigenschaften makroskopischer Objekte getestet werden sollen—quadratisch größere Bezugssysteme nötig sind—eine Bedingung, die in der Alltagserfahrung allgemein nicht erfüllt ist. Dies legt nahe, dass fundamentale Grenzen für beliebig genaue Messungen existieren und schafft eine mögliche Erklärung für das Nicht-Beobachten von Quantenphänomenen auf makroskopischen Skalen, d.h. das Auftreten der Klassischen Physik.

Das fünfte Kapitel widmet sich der allgemeinen Frage, ob eine bestimmte kausale Abfolge von Ereignissen eine fundamentale Eigenschaft der Natur sei. Der Begriff der kausalen Abfolge ist operationell durch Signalübertragung defi-

niert: Wenn *A* ein Signal zu *B* schicken kann, aber *B* kein Signal zu *A* schicken kann, dann geht *A* in einer kausalen Struktur *B* voran. Üblicherweise wird angenommen, dass in einzelnen Durchläufen eines Experiments nur eine Einweg-Signalübertragung möglich ist. Der Hauptaugenmerk des Kapitels liegt darin zu verstehen, ob in der Quantenmechanik solch eine Annahme aufgelockert werden könnte und unter welchen Umständen dies notwendig werden könnte. Zu diesem Zweck wird ein neuer Rahmen für vielteilige Quantenkorrelationen entwickelt, welcher kein Konzept eines globalen Raums, einer globalen Zeit oder einer globalen Kausalstruktur voraussetzt, sondern nur voraussetzt, dass die Experimentatoren in ihren lokalen Laboratorien beliebige Quantenoperationen durchführen können. Alle bekannten Situationen, welche eine bestimmte kausale Abfolge einhalten (Signalübertragungs- und Nicht-Signalübertragungs-Korrelationen zwischen zeitartig und raumartig getrennten Experimenten miteingeschlossen), als auch deren wahrscheinlichkeitstheoretische Mischungen können in diesem Rahmen ausgedrückt werden. Es wird gezeigt, dass der Formalismus auch Situationen beinhaltet, in denen die zwei Experimente weder kausal gereiht sind noch sich in einer wahrscheinlichkeitstheoretischen Mischung bestimmter kausaler Abfolgen befinden. Es wird gezeigt, dass diese Korrelationen ermöglichen, eine Kommunikationsaufgabe zu erfüllen, welche unmöglich wäre, sofern die Operationen gemäß einer fixen Hintergrundzeit gereiht wären. Jedoch wird bewiesen, dass klassische Korrelationen d.h. Korrelationen zwischen klassischen Operationen, immer kausal gereiht sind, was nahe legt, dass eine bestimmte kausale Struktur in einem Übergang von der Quantenphysik zur klassischen Physik auftreten kann.

Acknowledgments

List of Publications

The titles of publications directly relevant for this dissertation are written in bold-face. In parentheses are indicated the chapters in which the content of such publications is presented.

1. M. Zych, F. Costa, I. Pikovski, T. C. Ralph, and Č. Brukner,
   "General relativistic effects in quantum interference of photons",
   Class. Quant. Grav. **29**, 224010 (2012).

2. O. Oreshkov, F. Costa, and Č. Brukner,
   "**Quantum correlations with no causal order**",
   Nat. Commun. **2**, 1092 (2012).
   (Chapter 5.)

3. M. Zych, F. Costa, I. Pikovski, and Č. Brukner,
   "Quantum interferometric visibility as a witness of general relativistic proper time",
   Nat. Commun. **2**, 505 (2011).

4. M. Zych, F. Costa, J. Kofler and Č. Brukner,
   "Entanglement between smeared field operators in the Klein-Gordon vacuum",
   Phys. Rev. D **81**, 125019 (2010).

5. F. Costa, N. Harrigan, T. Rudolph, and Č. Brukner,
   "**Entanglement detection with bounded reference frames**",
   New J. Phys. **11**, 123007 (2009).
   (Chapter 4.)

6. F. Costa and F. Piazza,
   "**Modeling a Particle Detector in Field Theory**",
   New J. Phys. **11**, 113006 (2009).
   (Chapter 1.)

7. S. Cacciatori, F. Costa, and F. Piazza,
   "**Renormalized thermal entropy in field theory**",
   Phys. Rev. D **79**, 025006 (2009).
   (Chapter 2.)

8. F. Piazza and F. Costa,
   "Volumes of Space as Subsystems",
   proceedings of *From Quantum to Emergent Gravity: Theory and Phenomenology*, PoS(QG-Ph)032 (2007).

Introduction

Much of the recent progress in the foundations of quantum physics has been tightly connected with the development of the field of quantum information. The perspective provided by information theory enables to extract deep conceptual features of the theory from complicated phenomena, which can be analysed through simple gedankenexperiments that can be often formulated as communication tasks or "games". The operational attitude developed in such a context helps clarifying apparent "paradoxes" which can be understood as prime examples of the theory's foundations, rather than as problematic aspects of it. In return, the research in quantum foundations, by highlighting features of quantum mechanics absent in classical physics, has strongly stimulated the field of quantum information, showing the possibility of numerous applications based on inherently quantum phenomena. The most celebrated example is Bell's theorem [1]: the observation that quantum systems feature correlations that cannot be explained in classical terms is at the same time a key insight into the structure of the theory and the basic premise for most of the developing quantum technologies, from quantum cryptography, through quantum communication, to quantum computing.

The interplay of quantum mechanics and special relativity gives rise to new conceptual challenges over and above those present in quantum mechanics. It has been recognised that information plays a crucial role in linking the two theories [2] and recently relativistic quantum information has started to emerge as an independent field [3]. Information theory, and in a similar way thermodynamics, provides a theory-independent perspective which becomes particularly useful in situations in which a coherent theoretical framework has not yet been develop, as is the case for a theory unifying quantum mechanics and general relativity.

In this thesis, we address several questions at the interface between quantum mechanics, special and general relativity adopting an operational point of view. This implies a re-examination of the physical and experimental condition under which the phenomena into consideration can emerge, as well as the use of tools and methods inspired by the point of view of quantum information and thermodynamics.

Issues at the Interface of Quantum Mechanics, Special and General relativity

We review some conceptual issues that constitute the main background of the work developed in the present dissertation.

Entanglement of the Quantum Vacuum   Several counterintuitive features of quantum field theory are tightly linked the Reeh-Schlieder theorem [4]. The theorem states that, given the vacuum state $|\Omega\rangle$ of a relativistic quantum field and the algebra of local operators $\mathcal{A}(O)$ associated with a region of spacetime O, the linear space $\mathcal{A}(O)|\Omega\rangle$ generated by acting on the state $|\Omega\rangle$ with the operators in $\mathcal{A}(O)$ is dense in the Hilbert space. This means that, in principle, by performing operations localised in an arbitrary spacetime region O, no matter how small, it is possible to reconstruct any state with arbitrary precision, which can in turn be detected with measurements in regions space-like separated from O. The theorem is not limited to the vacuum and extends to arbitrary states of finite energy. For free fields, the theorem also holds if O is a region of space.

The consequences are quite striking: not only measurements on the vacuum— the state one would naively think to be empty—can give non-trivial outcomes (in fact, *all* possible outcomes of a local measurement have a non-zero probability to occur), but local measurements in different regions are correlated. In fact, the vacuum turns out to be an entangled state, which in principle allows violating Bell's inequalities via measurements localised in arbitrary space-like separated regions [5, 6]. Since such a property does not appear in standard experiments, in which typical observations agree with a more intuitive notion of vacuum, it is natural to ask to which extent the vacuum entanglement has an operational meaning and what would be the physical conditions that could make it possible to observe vacuum correlations. As we are going to see in Chapter 1, a study of particle detection within quantum field theory produces an effective model that does not detect particles in the vacuum.

localisation in Quantum Field Theory   An interpretative difficulty encountered in quantum field theory, related to the Reeh-Schlieder theorem, is the notion of localised objects. One can think of a state $|\psi\rangle$ as localised in a region O if, after tracing the degrees of freedom in O, the reduced state outside that region is indistinguishable from the vacuum: $\mathrm{Tr}_O|\psi\rangle\langle\psi| = \mathrm{Tr}_O|\Omega\rangle\langle\Omega|$ [7, 8]. As it turns out, states with such a property cannot have a finite number of particles (although they can approximate finite-particle states arbitrarily closely). More importantly, states that, according to this definition, are localised in non-overlapping, space-like separated regions, are not necessarily orthogonal. Thus, after preparing a state local-

ised in a region O, it should in principle be possible to detect, via a von Neumann measurement, a state localised in a different region O'. These difficulties, absent in non-relativistic quantum mechanics, have led some authors to speculate that the mathematical objects associated with local measurements are not those prescribed by algebraic quantum field theory, on which the Reeh-Schlieder theorem relies [9, 10]. Such approaches however encounter difficulties related to relativistic invariance and their physical significance is still debated [11, 12, 13].

In this thesis we do not attempt to answer the question of what are the correct local degrees of freedom at a fundamental level, we however investigate how specific assumptions about physical measurements affect the concept of localisation (Chapters 1, 3). In Chapter 2 the consequences of an alternative localisation scheme on the notion of thermodynamic entropy are considered.

Correspondence Principles The counterintuitive features of Einstein's theory of special relativity come together with a well-defined condition for their non-observability: non-relativistic mechanics is an accurate description as long as relative velocities are small compared with the speed of light. In a similar way, general relativity can be approximated by Newton gravity for small gravitational fields and small velocities.

In quantum mechanics the situation is less simple. A first, tentative formulation of a "correspondence principle" was proposed by Bohr in 1920 [14] and posits that states with large quantum number should behave as classical (a condition often rephrased as the "$\hbar \to 0$" limit). Although this principle can be applied to some extent, for example to coherent states, the general idea is contradicted by the possibility of having entangled states with arbitrarily large quantum numbers that can violate some Bell-type inequalities [15]. It is widely recognised that a crucial role in the emergence of classicality is played by decoherence [16]—the process through which a macroscopic system loses the internal coherence through its interaction with the environment. There are however cases where this process alone is not sufficient to explain the emergence of classicality. A striking example is provided again by the vacuum entanglement in quantum field theory. Since the vacuum is a stable state, it does not evolve and thus does not "decohere". Additionally, since the Reeh-Schlieder theorem applies to any state with finite energy, one would conclude that all physical states of quantum fields, including those encountered in everyday life, are entangled across different regions of space. This contrasts with the common knowledge that quantum effects are only observable under very specific laboratory conditions. In particular, detecting the entanglement of the vacuum, if at all possible, would require measurements with a formidable accuracy.

Following an idea by Peres [17], it has been proposed that an important clue

in understanding the emergence of classicality is indeed the lack of precision in typical—*coarse-grained*—measurements [18, 19, 20]. The interesting aspect of this approach is that it provides an epistemological, rather than dynamical, emergence of classical states within the quantum formalism. It is particularly interesting to understand whether this approach extends to the several counterintuitive features of quantum field theory. This question is addressed in Chapter 3, where particular attention is devoted to the "area law" for the entanglement entropy in quantum field theory.

A related question is whether nature itself provides limitations for the observation of quantum phenomena, i.e. if there are regimes that can effectively be considered as classical. From the point of view of the coarse-graining approach, this translates into the question of what are the limits imposed by nature on the achievable measurement precision. This question is addressed in Chapter 4, where the limitations derived from the use of quantum systems as reference frame are considered.

General Relativity, Quantum Mechanics, and Causal Structures   One of the most pressing problems in modern theoretical physics is the lack of a framework that unifies quantum mechanics and general relativity. Unravelling the conceptual issues at the interface of the two theories is for this reason of special interest. The concept of time, in particular, has received a considerable attention across the years [21, 22, 23, 24, 25, 26, 27]. Since tentative full theories of quantum gravity are faced with great technical hindrances, the methods and points of view of quantum information could provide deep insights in this respect. Their application in the context of general relativity, however, faces some serious difficulties. Even though abstract formulations of quantum information do not make explicit reference to a spacetime geometry, the basic notions of the theory can still be clearly distinguished in "space-like", i.e. the properties of states, such as entropy or entanglement, and "time-like", i.e. the properties of quantum evolutions or more generally quantum channels, such as information rate or channel capacity. This contrasts with the unified picture of space and time provided by general relativity, in which space-like and time-like intervals are just examples of general spacetime intervals with specific properties defined with respect to the covariant metric. Even more critical is the fact that the spacetime metric, and more generally the causal structure, of general relativity are dynamical: given a spacetime interval, fixed with respect to some operationally-defined coordinate system, its space-like or time-like nature generally depends on the mass-energy content of the surrounding region via the Einstein equations. In quantum mechanics, on the other hand, the causal structure is fixed and can be abstractly formalised in the form of a quantum circuit, in which operations (or "gates") are applied to an initial state in

a pre-determined order [28, 29]. These issues have stimulated the research of an operational-probabilistic framework with a dynamic causal structure [30, 31] and constitute the main background behind Chapter 5, in which a particular attention is devoted to the notion of *causal order* as an operationally-defined concept.

Outlook of the Work

Chapter 1 is an analysis of the concept of particle and of particle detector models in quantum field theory. According to the traditional models, typically used to determine the particle content of quantum field theory on a curved background, particles can in principle be detected even by devices at rest in the Minkowski vacuum, if only finite times are considered. It is proposed that detectors that do not undergo such temporary transitions provide a more natural notion of particle. The basic assumption behind the proposed detector models is that the configuration corresponding to the detector at rest in the vacuum should correspond to an eigenstate of the full Hamiltonian describing the detector-field interaction. A concrete model is introduced, in which the detector and its interaction with the field is fully described within a locally interacting quantum field theory. An effective model is further considered, derived from the previous one by identifying the relevant subspaces of the fields describing the detector as "ground" and "excited" state of a two-level system. At the effective level, the two-level detector does not couple to the local field operator, although the original underlying theory was fully local. This suggests that an operational definition of "local degrees of freedom" may not coincide with the mathematical one.

Chapter 2 explores a new approach to the calculation of thermal entropy in quantum field theory, based on a re-examination of the identification of local degrees of freedom with field operators. In particular, the Newton-Wigner localisation scheme is considered, which, as opposed to the conventional scheme, allows a local definition of the particle content of a region of space in agreement with the global notion of particle. Crucially, the vacuum state is a product state over subsystems associated with the local Newton-Wigner degrees of freedom, each local state corresponding to a local vacuum.

A scalar quantum field in a thermal state is considered and the entropy associated with the reduced state in a sub-region, defined according to the Newton-Wigner localisation, is calculated. It is proved that the entropy so defined is free of the ultraviolet divergences typically found in analogous calculations for sub-regions associated with the local field operators. A diagrammatic formalism is developed that allows calculating analytical expression for the entropy in several

physical limits, including high and low temperature regimes of massive and massless fields in arbitrary space dimensions.

Chapter 3 addresses the general problem of the emergence of classicality in quantum field theory. More specifically, the main focus is the apparent discrepancy between the quantum and the classical behaviour of the entropy associated to a region of space containing a field in a thermal state or in the vacuum. Differently from Chapter 2, the standard localisation is assumed in order to identify subsystems with volumes of space. However, it is assumed that possible measurements are subject to a minimal precision, both in the localisation of a point in space and in the measurement of the field's amplitude. It is found that, for large enough imprecisions in the measurements of the field, all states appear effectively as separable and their entropy becomes proportional to the volume, rather than the area (even for arbitrarily fine space resolution). However, for poor space resolution, i.e. when only distances larger than the typical correlation length in the field can be discriminated, the entropy vanishes for the vacuum state, in agreement with the results of Chapter 2. In the large temperature limit, the von Neumann entropy of a region becomes equivalent to the Shannon entropy of a classical thermal field.

Chapter 4 addresses the consequences of considering finite-size quantum reference frames in the measurement of quantum properties: the quantum nature of physical measurement devices is expected to provide a limitation on the measurement precision, equivalent to a fundamental *coarse-graining* of the possible measurements. In particular, the case of directional reference frames is studied. A classical directional reference frame defines a direction in space along which the spin of a particle can be measured with arbitrary precision. As a quantum analogue of a directional reference frame a spin coherent state is considered. In the absence of additional, external reference frame it is still possible to measure the relative orientation between the spin of a particle and the reference frame's spin. The finite size of the reference frame, however, imposes a limitation on the accuracy with which such a measurement can be performed. It is studied how this limitation affects the observation of non-classical effects in various situations.

It is found what the minimal sizes are of the reference frames that allow violating several local-realistic bounds, such as those given by the Bell-CHSH inequalities for a pair dichotomic observables (e.g. two spin-1/2 particles), the Mermin inequalities for N dichotomic observables (such as N spin-1/2 particles), and the Bell inequalities for a pair of observables with arbitrarily many outcomes (e.g. two particles with arbitrarily large spin). In the latter case, it is found numerically that the size of the spin reference frames necessary to violate the inequalities must be at least quadratically larger than the particles' spin length, suggesting a fun-

damental limitation for the observation of quantum properties at the macroscopic scale.

Chapter 5 proposes an approach to the study of causal structures, in which causal relations are defined in terms of the possibility of signalling. According to this definition, it is possible to find an operational task—a "causal game"—whose probability of success is limited for operations performed in a definite causal sequence (or even in a probabilistic mixture of causal sequences). A formalism is then developed that allows describing all the possible multipartite correlations that can be produced by different agents whose operations are locally described by quantum mechanics, without making any prior assumption on the existence of a global spacetime, or even of a causal structure, in which the operations are embedded. A full characterisation of such correlations is found, as well as a convenient representation in which the possibility of signalling between different parties can be directly recognised. An example of such correlations is found that allows winning the causal game with a probability of success larger than the causally-ordered bound. This shows that assuming the local validity of quantum mechanics does not imply the existence of a global causal structure. In contrast, if locally classical mechanics is assumed, all the possible multipartite correlations can always be embedded in a global causal structure. This shows that if a fundamental theory, possibly unifying general relativity and quantum mechanics, were not to feature a definite causal structure, such a structure would nonetheless naturally emerge in a quantum-to-classical transition.

Chapter 1

Particle Detector Models in Field Theory

Summary

We analyse the concept of particle in quantum field theory from an operational point of view, that is, as the result of a detection event of a particle detector. The commonly adopted Unruh-DeWitt type of detector, based on the coupling of a discrete quantum system with the local field operators, is known to undergo temporary transitions to excited states even when at rest and in the Minkowski vacuum, making an interpretation of the vacuum as a state "devoid of particle" difficult. We argue that in fact a well-defined notion of particle is possible if one adopts the natural assumption that the configuration "detector in its ground state + vacuum of the field" is, in the non-accelerated case, a stable bound state of the underlying fundamental theory describing the interaction of the field with the detector. As a concrete example, we study a local relativistic field theory where a stable particle can capture a quantum from a lighter field and form a quasi-stable state. As expected, to such a stable particle correspond energy eigenstates of the full theory, as it is shown explicitly by using a dressed particle formalism at the first order in perturbation theory. We derive an effective model of a particle detector (at rest), where the stable particle and the quasi-stable configurations correspond to the two internal levels, "ground" and "excited", of the detector. This detector model provides a well-defined notion of particle, according to which the vacuum of the field can be interpreted as a state with zero particle content, even for finite times. The price to pay is an apparent non-locality of the interaction between the effective detector model and the field.

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1.1   Particles and Detectors in Relativistic Quantum Field Theory

In Minkowski spacetime, particles can be identified with the excited modes of the field Hamiltonian. However, when field quantisation is applied to general backgrounds, a univocal definition of particle is no longer possible [32]. Still, with sound operational attitude, one can model a particle detector, calculate its response along some trajectory and define accordingly the particle content of the observed state. A requirement usually imposed on a detector model is that it should reveal no particles in the vacuum when the detector is at rest and *long enough* times are considered. However, typical predictions include the possibility that, for short times, particles can be detected by a detector in inertial motion, even in Minkowski spacetime. This implies that, according to such models, *the vacuum state contains a finite number of particles for finite-times* [33].

Here we attempt to clarify some aspects of particle detector modelling and, in particular, emphasise the role of the eigenstates of the full Hamiltonian when the configurations of "field+detector" are taken into consideration. To be specific, we will introduce two levels of description for the detector model (see Fig. 1.1): the first level is a *bona fide* "fundamental" theory, which we take as a weakly coupled quantum field theory (QFT) with three neutral scalar fields. This theory features two stable particles ("*A*" and "*C*") and one meta-stable state ("*B*"). The massive particle *A* can capture the lighter quantum *C* and form the unstable particle *B*, Fig. 1.1a. Stable particles correspond to eigenstates of the full Hamiltonian, as is shown explicitly by using a dressed particle formalism. Within this first level of description, we interpret the capture process as "detection" of the particle *C*. The second level of description is effective: it features only a two-level system—the effective particle detector—and the (otherwise) free field to be detected, Fig. 1.1b. The detector-field interaction is such that the transition rates $A \rightarrow B$ of the fundamental theory are faithfully reproduced, at the effective level, as transitions between the two levels ("ground" and "excited" states) of the detector. The discussion will only concern inertial detectors in Minkowski spacetime.

The main observation at the basis of the present analysis is that the configuration "the detector is in its ground state and the field is in the vacuum" is stable and therefore should correspond to an *eigenstate* of the Hamiltonian, both at the level of the effective detector model and at the level of the more fundamental in-
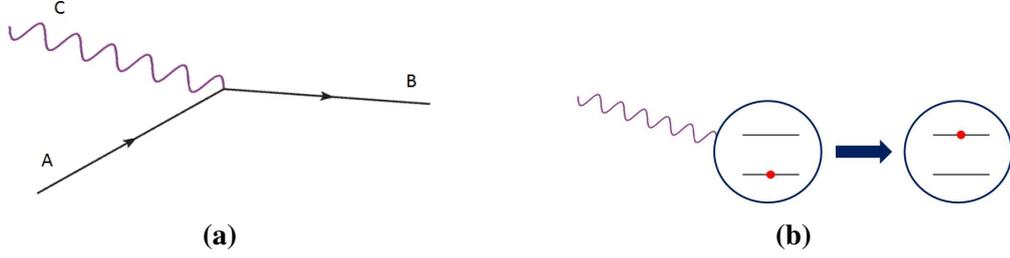
Figure 1.1: The two levels of description of the particle detector. (a) At a fundamental level, the detector is described by a toy model of locally interacting quantum fields. The model, besides the particles *C* to be detected, includes two more species of particles: *A*, representing the unexcited detector, and *B*, representing the detector after having absorbed a particle. The *A* and *C* particles can interact and produce a *B* particle. (b) At an effective level, the detector is described as a two-level system that can undergo a transition from ground to excited state after absorbing a particle with the same probability amplitudes as the corresponding process in the fundamental theory.

teracting field theory. The commonly adopted Unruh-DeWitt detector [34, 35] only satisfies a weaker version of this basic request: it sees no particles in the (Minkowski) vacuum after an infinite time. For finite times, however, it always undergoes temporary transitions to excited states with finite (albeit small) probability. It is interesting that the property we are asking for is instead shared by one of the first photodetector models, proposed by Glauber in 1963 [36], in which photon detection is associated with the positive-energy components of the electromagnetic field.

Here we show that the Glauber type of detector corresponds, at the deeper QFT-level description, to dealing with the properly "dressed" states of the full theory. Therefore, we argue that the Glauber type of detector is more appropriate for describing finite-time processes. The proposed detector model, although derived from a perfectly local relativistic field theory, does not couple to the local degrees of freedom of the field to be detected and, therefore, it is not *localised* [37, 38] in the usual sense. This is due to the fact that we are capturing and modelling the finite time behaviour of the dressed—as opposed to the bare—states of the field theory itself.

1.2 Detector Models: a Critique

A model detector [34, 35, 36] is a quantum system whose states live in a product Hilbert space $\mathcal{H}_D \otimes \mathcal{H}_\phi$ (i.e. detector and field) and provided with a Hamiltonian operator $H_m = H_m^D + H_m^\phi + H_m^I$ (suffix m stands for "model"). In the simplest

scenario, ϕ is an—otherwise free—scalar field,

$$H_m^\phi = \int d^3k E(k) c^\dagger_{\vec{k}} c_{\vec{k}}, \quad \text{where} \quad E(k) = \sqrt{k^2 + m^2} \tag{1.1}$$

and $c^\dagger_{\vec{k}}$ and $c_{\vec{k}}$ are the usual creation and annihilation operators,

$$\phi(\vec{x}) = \frac{1}{(2\pi)^3} \int \frac{d^3k}{\sqrt{2E(k)}} \left(c^\dagger_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} + c_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}} \right) .$$

The detector Hamiltonian H_m^D accounts for at least two energy levels: unexcited, $|0\rangle_D$, and excited, $|E\rangle_D$; say that $H_m^D|E\rangle_D = \Delta E|E\rangle_D$, $H_m^D|0\rangle_D = 0$. Regardless of the choice of H_m^I, the model state $|0\rangle_D \otimes |0\rangle$ is thus interpreted, by construction, as "the detector is in its ground state and the field is in its vacuum state".

The traditionally used Unruh-DeWitt detector features an interaction Hamiltonian of the type

$$H_m^I = \sigma \, \phi(\vec{x}(t), t), \tag{1.2}$$

where σ is a self adjoint operator acting on $\mathcal{H}_D$ and containing off diagonal elements and $\vec{x}(t)$ is the detector's trajectory. Without loss of generality, we can take $\sigma = \sigma_\uparrow + \sigma_\downarrow$, where $\sigma_\uparrow = |E\rangle_D\langle 0|$ and $\sigma_\downarrow = (\sigma_\uparrow)^\dagger$. The Hamiltonian (1.2) is based on the following requests:

1. The detector is a quantum system with discrete energy levels.

2. Transitions between different levels must be possible in order to account for particle absorption and emission (the simplified version containing two levels only allows single-particle detection).

3. The detector interacts locally with the field.

4. *Asymptotically*, no transition has to take place when the detector is at rest.

A striking feature of this traditionally adopted detector is that the state $|0\rangle_D \otimes |0\rangle$ is not an eigenstate of (1.2), due to the presence of the creation operators $c^\dagger_{\vec{k}}$ inside ϕ. Accordingly, if the system is initially prepared in the configuration $|0\rangle_D \otimes |0\rangle$, there is always a non-vanishing transition rate to a state of type $|E\rangle_D \otimes |\text{one particle}\rangle$ at finite times, regardless of the state of motion of the detector. In the interaction picture, and at first order in perturbation theory, the amplitude for this process reads

$$\mathcal{A}_{\vec{k}}(2t) = -i \int_{-t}^{t} dt' \langle \vec{k}| \otimes_D \langle E| H_m^I(t') |0\rangle_D \otimes |0\rangle, \tag{1.3}$$

where $|\vec{k}\rangle = c^\dagger_{\vec{k}}|0\rangle$, $H_m^I(t') = e^{i(H_m^D \tau(t) + H_m^\phi t)} H_m^I e^{-i(H_m^D \tau(t) + H_m^\phi t)}$ and τ is the proper time along the trajectory considered. If the detector is at rest, $\mathcal{A}_{\vec{k}}(2t) \propto \sin[(\Delta E +$

$E(k))t]/(\Delta E + E(k))$; only for $t \to \infty$, i.e. $t \gg 1/\Delta E$, does $\mathcal{A}$ become proportional to a delta function of the positive quantity $\Delta E + E(k)$, and therefore vanishes. On the opposite, $|\mathcal{A}|$ keeps staying above zero along accelerated trajectories, which is one of the several derivations of the Unruh effect [34].

Here we consider in detail only the case of a detector at rest. The possibility that a detector may "click" at finite times in the vacuum but then "erase" the record later, appears rather mysterious. One may object that the measurement process cannot be considered finished as long as the detector undergoes quantum fluctuations, so that only if $|\mathcal{A}_{\vec{k}}(t)|$ stays definitely above zero in the future can we fairly say that a particle has been detected. However, in real apparatuses quantum coherence is usually destroyed over very short times by some amplification process; for decoherence times $t_d \ll 1/\Delta E$, the vacuum fluctuations (1.3) would become detectable and give rise to observable effects. (The numerical analysis performed in Ref. [39] showed that such effects could indeed become relevant in forthcoming experiments in circuit QED.)

An elementary and reasonable detector one may think of is a hydrogen atom that, by absorbing a photon, can make a transition to an excited state. We can think of a consistent QED theory with two Dirac fields of opposite charges (electrons and protons) and appropriate masses; the hydrogen atom in its ground state is arguably contemplated in the spectrum of that theory as a stable bound state. When written in terms of fundamental fields, we therefore expect the model state $|0\rangle_D \otimes |0\rangle$ to concretely correspond to a stable state, i.e., strictly, an eigenstate, of the full Hamiltonian: this is what the unexcited hydrogen atom is in QED and the detector is not in the Unruh-DeWitt model. It is plausible that even more realistic detectors, such as a block of germanium crystal, correspond to stable bound states in appropriate QED-like theories.

The amplitude (1.2) is clearly analogous to the usual perturbative calculation of S matrix elements. In that formalism, the asymptotic in- and out- states are borrowed from the free theory under the consistent assumption of adiabatic switching of the interactions. Consider, as an example, a $\lambda\phi^4$ theory. Similarly to the Unruh-DeWitt detector, the Hamiltonian features off-diagonal elements, among others, of the type $\langle$four particles$|H|0\rangle$, which could suggest that the vacuum could spontaneously generate four particle states. Such matrix elements, however, are those taken the unphysical states of the free theory, while it is well-known that $\lambda\phi^4$ has a stable vacuum and stable single-particle states. When written in terms of those states, the full Hamiltonian has, by definition, only diagonal elements and no particle is generated from the "true" vacuum, even at finite times. One would come to wrong conclusions if the states of the free theory were used to study finite-time processes.

The above reasoning brings us to postulate, as a condition for a good model of a particle detector, that the configuration "unclicked detector + vacuum", $|0\rangle_D \otimes |0\rangle$,

be an eigenstate of the full Hamiltonian H_m of the model at rest. We will refer to this as *the Frog Principle*[1]. This principle can be regarded as a stronger version of the above Condition 4: the condition of not clicking in the vacuum is extended from infinite to finite times. It seems that if we make Condition 4 stronger, all four requirements cannot be satisfied simultaneously. What seems problematic, in particular, is to reconcile locality (Condition 3) with the frog principle. This is in fact an instance of the "localisation problem" in quantum field theory and arises from a well-known consequence of the Reeh-Schlieder theorem, which implies that no nontrivial, positive, local observable can exist having zero expectation value on the vacuum [4, 41]. This means that, if a detector performs a von Neumann-type measurement corresponding to a projector Π, then, either $\langle 0|\Pi|0\rangle \neq 0$ (the detector reveals particles in the vacuum) or Π is not local (see also Ref. [2], Sec. IV E). We suggest that, for particle detector models, Condition 3 can indeed be relaxed, and that this is perfectly compatible with local relativistic quantum field theory. In order to make our point stronger, in the following we consider a toy—local relativistic—"fundamental" field theory where a stable particle plays the role of the detector in its ground state and the detection process corresponds to the capture of a light particle and the formation of a meta-stable state. We will then provide a two-level effective detector model faithfully reproducing the detection rates of the fundamental theory and satisfying the *Frog Principle*. A similar toy field theory was sketched already in Unruh's celebrated paper [34]. The crucial difference here is that we use the "dressed" rather than the "bare" states of the model.

Studies of Unruh-DeWitt models have gone beyond the perturbative amplitude (1.3), exact and numerical solutions are available for a variety of trajectories (see e.g. [42]). Considering exact asymptotic states is particularly appropriate since, in most cases, preparing the system into the state $|0\rangle_D \otimes |0\rangle$ and then switching on the interaction is not realistically possible. Crucially, the "dressed" stable configurations of the Unruh-DeWitt detector depend on the trajectory considered and exhibit radiation at infinity in the accelerated case. Here we show that if dressing is consistently done—in the first place—on all sectors of the underlying field theory, this produces a different detector model altogether, i.e. a different model Hamiltonian H_m^I (Eq. 1.14 below).

1.3   The Toy Field Theory

Beside the already introduced light field to be detected, $\phi(x)$ of mass m (sector "C" of the theory), we introduce two other neutral scalars, $\chi(x)$, of mass M (sector

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[1]Some frogs are known to have eyes sensitive enough to detect a single photon [40]. The postulated triviality of a good detector's response on the vacuum—and the absence of dark counts—may be pictorially rephrased as "a frog does not see photons when it is dark".

"A"), and $\eta(x)$ of mass $\overline{M}$ (sector "B"). We choose a local interaction of the type $\mathcal{L}^I(x) \sim -\mu \chi(x)\eta(x)\phi(x)$, the coupling μ being small with respect to the other masses[2]. The full Hamiltonian reads $H = H^0 + H^I$, where $H^0 = H^A + H^B + H^C$, and

$$H^A = \int d^3k \, w(k) a^\dagger_{\vec{k}} a_{\vec{k}}, \quad w(k)^2 = k^2 + M^2, \tag{1.4}$$

$$H^B = \int d^3k \, W(k) b^\dagger_{\vec{k}} b_{\vec{k}}, \quad W(k)^2 = k^2 + \overline{M}^2, \tag{1.5}$$

$$H^C = \int d^3k \, E(k) c^\dagger_{\vec{k}} c_{\vec{k}}, \quad E(k)^2 = k^2 + m^2, \tag{1.6}$$

$$H^I = (2\pi)^{3/2}\mu \int d^3x \, \phi(\vec{x})\eta(\vec{x})\chi(\vec{x})$$

$$= \mu \int \frac{d[k_1 k_2 k_3]}{\sqrt{2w(k_1) \, 2W(k_2) \, 2E(k_3)}} \, (a_{\vec{k}_1} + a^\dagger_{-\vec{k}_1})(b_{\vec{k}_2} + b^\dagger_{-\vec{k}_2})(c_{\vec{k}_3} + c^\dagger_{-\vec{k}_3}). \tag{1.7}$$

In the above expression $d[k_1 k_2 k_3] = d^3k_1 \, d^3k_2 \, d^3k_3 \, \delta^3(\vec{k}_1 + \vec{k}_2 + \vec{k}_3)$ is the volume element on the momentum shell. Creation and annihilations operators have been introduced in the usual way and satisfy usual commutation relations. In the picture we have in mind ϕ is a light field ($m \ll M, \overline{M}$) that can be captured by an A-particle and form a B meta-stable state. The mass difference $\Delta M = \overline{M} - M$ is therefore supposed to be of the same order as—but slightly bigger than—m, $\overline{M} > M + m$. In order to allow a perturbative treatment, the coupling μ is taken much smaller than the other masses, $\mu \ll m$. Particles A and C are stable. C cannot decay to anything else for kinematical reasons. Moreover, processes such as $A \rightarrow 2C$ are not allowed by the form of the interaction: formally, the discrete symmetry $\phi \rightarrow -\phi, \chi \rightarrow -\chi, \eta \rightarrow \eta + permutations$ is protected.

We aim to give an effective description of the *ABC* dynamics in which sectors *A* and *B* are described as "internal" to the model detector and in such a way that the transition amplitudes are faithfully reproduced (at first order in μ). The one-particle sector *A* is the detector in its ground state. The excited detector is described instead by the meta-stable configurations of the *B* sector. With the above assumed relations among the mass parameters, the decay rate of a *B*-particle is $\Gamma_B \sim \mu^2 \Delta M/M^2$. At the expense of detector's efficiency, we can assume *B*'s

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[2]Strictly speaking, this potential is not bounded from below *e.g.* along the direction $\chi = \phi$, $\eta = -\phi$. However, the tunnelling decay rate of the perturbative vacuum is suppressed by an exponential factor of at least e^{-m^2/μ^2} which we fix to be small enough to be irrelevant. Moreover, we can always stabilise the potential with higher order terms that will not be relevant for present purposes.

lifetime $\tau_B \sim 1/\Gamma_B$ to be long enough for the detector to be considered as "permanently clicked" for all practical purposes.

As announced, we want the one-particle space of the A sector of this theory to correspond to the state $|0\rangle_D \otimes |0\rangle$ of the model detector. However, $a_{\vec{k}}^\dagger |\Omega\rangle$ (here $|\Omega\rangle$ is the field theory vacuum, as opposed to the vacuum $|0\rangle$ of the field ϕ in the detector model (1.2)) is an eigenstate of the free theory but not of H^I, due to the presence in (1.7), e.g., of terms such as $ab^\dagger c^\dagger$. On the other hand, we know that the A-particle is stable and therefore corresponds to a set of eigenstates also in the full theory. Such states can be expressed, order by order in perturbation theory, through a "clothing" or "dressing" transformation[3]. For this purpose, we act with a unitary transformation U on the whole Hilbert space, $|\Omega\rangle \rightarrow |\Omega_d\rangle = U|\Omega\rangle$, $a^\dagger \rightarrow \alpha^\dagger = Ua^\dagger U^\dagger$, $b^\dagger \rightarrow \beta^\dagger = Ub^\dagger U^\dagger$, $c^\dagger \rightarrow \gamma^\dagger = Uc^\dagger U^\dagger$ etc . . . and impose that the "dressed" states $|\Omega_d\rangle, \alpha^\dagger|\Omega_d\rangle, \gamma^\dagger|\Omega_d\rangle$ be eigenstates of the full Hamiltonian. On the other hand, $\beta_d^\dagger|\Omega_d\rangle$ will not be an eigenstate because B-particles are unstable. Following [45], we write $U = e^R$, where R is an anti-hermitian operator, $R = \mathcal{R} - \mathcal{R}^\dagger$ that can be written at first order in μ in terms of the bare operators. We make the ansatz

$$\mathcal{R} = \mu \int d[k_1 k_2 k_3] \left(F_1 a_{\vec{k}_1} b_{\vec{k}_2} c_{\vec{k}_3} + F_2 a_{\vec{k}_1} b_{\vec{k}_2} c^\dagger_{-\vec{k}_3} + F_3 a_{\vec{k}_1} b^\dagger_{-\vec{k}_2} c_{\vec{k}_3} + F_4 a^\dagger_{-\vec{k}_1} b_{\vec{k}_2} c_{\vec{k}_3} \right), \tag{1.8}$$

where the Fs are functions of the moduli k_1, k_2 and k_3, regular on the momentum shell $\vec{k}_1 + \vec{k}_2 + \vec{k}_3 = 0$. Instead of transforming the states we can equivalently transform the Hamiltonian although, in spirit, what we are doing is really rewriting the same Hamiltonian in terms of the dressed operators α, β, etc. . . To first order in μ the transformation reads $H \rightarrow H_d = H + [R, H]$. The zeroth order free part H^0 is left unchanged by this transformation. The interaction part gets a contribution of the type $H^I \rightarrow H_d^I = H^I + [R, H^0]$. To give an example, let us see this commutator in detail for terms of type $a^\dagger bc$ and $ab^\dagger c^\dagger$ inside R. Terms of this type would make the A-particle decay into $B + C$ and therefore are not physical.

$$[R_4, H^0] = \mu \int d[k_1 k_2 k_3] \left(-w(k_1) + W(k_2) + E(k_3)\right) \left(a^\dagger_{-\vec{k}_1} b_{\vec{k}_2} c_{\vec{k}_3} + a_{\vec{k}_1} b^\dagger_{-\vec{k}_2} c^\dagger_{-\vec{k}_3} \right) F_4. \tag{1.9}$$

Note that, by setting $1/F_4 = \left(-w(k_1) + W(k_2) + E(k_3)\right) \sqrt{2w(k_1)\, 2W(k_2)\, 2E(k_3)}$ in (1.8), we can get rid of the corresponding terms inside H^I.

Other terms in H^I get contributions similar to (1.9), except that the energies w, W and E appear in different combinations i.e. with appropriate relative signs.

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[3]A QFT formulation in terms of clothed particles dates back to the late 50s [43], although similar approaches date even earlier. The beautiful paper [44] explores a similar transformation at the pure level of matrix elements. Our two main references are [45, 46], where a complete bibliography on the subject can be found.

Crucially, we cannot get rid of the term $ab^\dagger c$, $a^\dagger bc^\dagger$, since the corresponding combination of energies, $w(k_1) - W(k_2) + E(k_3)$, vanishes on a subset of the momentum shell and the function F_3 would be singular there. Note that bare and dressed particles are bound to give the same S-matrix elements and decay rates, since the "good terms" such as $ab^\dagger c$, $a^\dagger bc^\dagger$ can only get harmless corrections that vanish on the energy shell! By setting $F_3 = 0$ in (1.8) we get the following dressed interaction Hamiltonian:

$$H_d^I = \mu \int \frac{d[k_1 k_2 k_3]}{\sqrt{2w(k_1)\, 2W(k_2)\, 2E(k_3)}} \left(\alpha_{\vec{k}_1} \beta^\dagger_{-\vec{k}_2} \gamma_{\vec{k}_3} + \alpha^\dagger_{-\vec{k}_1} \beta_{\vec{k}_2} \gamma^\dagger_{-\vec{k}_3} \right). \tag{1.10}$$

The above operator is equal to the original Hamiltonian H^I (1.7) up to first order in μ. A drawback of this formalism is that it gets rather involved at higher orders: new dressed operators and Hamiltonians have to be derived at each step. Lorentz invariance is guaranteed, since the dressing transformation U preserves the commutation relations among the generators of the Poincaré group. However, as opposed to (1.7), (1.10) is not written in the local form $\int d^3x V(\vec{x})$, $V(x)$ being a scalar commuting at space-like separated events. What is important here is that H_d^I makes the stability of the A and C sectors manifest and reproduces the dynamics with the required accuracy.

1.4 The Effective Detector Model

We are now ready to build our detector. We first specify the state of the theory that matches the state $|0\rangle_D \otimes |0\rangle$ of the detector model. In momentum space this will be expressed by

$$|0\rangle_D \otimes |0\rangle \simeq |g\rangle_A \otimes |0\rangle_B \otimes |0\rangle_C = \int d^3k\, g(\vec{k}) \alpha^\dagger_{\vec{k}} |\Omega\rangle. \tag{1.11}$$

It is not too restrictive to choose the detector at rest in a spherically symmetric configuration centered around some point in space $\vec{x}$, i.e. $g(\vec{k}) = g(k)e^{-i\vec{k}\vec{x}}$, $g(k)$ being a real function. As this state may well describe a macroscopic object, we can also assume the momentum fluctuations to be small compared to its mass (or, equivalently, the spatial extension to be much larger than the Compton wavelength). This is accomplished by a distribution $g(k)$ non-vanishing only for $k^2 \ll M^2$, which makes the above state also an approximate eigenstate of the free evolution.

In order to study detector's response we now populate also the C sector and consider the state $|\psi\rangle = |g\rangle_A \otimes |0\rangle_B \otimes |f\rangle_C$, where $|f\rangle_C = \int d^3k\, f(\vec{k}) \gamma^\dagger_{\vec{k}} |0\rangle_C$ and now f can be centered around some $\vec{k} \neq 0$. Still, we take the energy of the particle to be detected much smaller than the mass of the detector, so that typically $f(\vec{k})$

is nonzero only for $E(k) \ll M$. In interaction picture the evolution of $|\psi\rangle$ reads $|\psi(2t)\rangle = (1 - i \int_{-t}^{t} dt' H_d^I(t'))|\psi\rangle$. The interaction picture Hamiltonian $H_d^I(t)$ is, in form, very similar to (1.10), with the difference that the operators inside the brackets get a phase factor, i.e. $e^{i\Omega t} \alpha_{\vec{k}_1} \beta_{-\vec{k}_2}^\dagger \gamma_{\vec{k}_3} + c.c.$, where $\Omega(k_1, k_2, k_3) = -w(k_1) + W(k_2) - E(k_3)$. The amplitude $\mathcal{A}_{\vec{k}}(2t) \equiv \langle \Omega_d | \beta_{\vec{k}} | \psi(2t) \rangle$ for the creation of a B particle of momentum $\vec{k}$ thus reads

$$\mathcal{A}_{\vec{k}}(2t) = -2i\mu \int \frac{d^3 k_c}{\sqrt{2w(k_a)2W(k)2E(k_c)}} g(\vec{k}_a) f(\vec{k}_c) \frac{\sin \Omega(k_a, k, k_c)t}{\Omega(k_a, k, k_c)}. \quad (1.12)$$

In the above formula $\vec{k}_a = \vec{k} - \vec{k}_c$. Under the above assumptions, the functions g, f cut the high momenta in the integral, so that we can make the following approximations: $w(k_a) \simeq M$, $W(k) \simeq \overline{M}$, $\Omega \simeq \overline{M} - M - E(k_c) = \Delta M - E(k_c) \equiv \Omega(k_c)$.

We now want to consider as "detection" all possible final states of the B field, regardless of the small recoils $\vec{k}$ that the A-B particle gets from the C particle. When we integrate the squared amplitude (1.12) to get the detection probability $P(2t) = \int d^3 k |\mathcal{A}_{\vec{k}}(2t)|^2$, there appears an interference term of the form $\int d^3 k g^*(\vec{k} - \vec{k}_c) g(\vec{k} - \vec{k}_c')$; this term cannot be reproduced by detector models where such recoil is just ignored. However, it looks reasonable to assume that f be much less spread than g, since the spread in the momenta is naturally weighted by the respective masses. Under this assumption, and recalling that $g(\vec{k}) = g(k)e^{-i\vec{k}\vec{x}}$, inside the expression for $P(2t)$ we always have $g(|\vec{k} + \vec{k}_c - \vec{k}_c'|) \simeq g(k)$, and so we can put $\int d^3 k g^*(\vec{k} - \vec{k}_c) g(\vec{k} - \vec{k}_c') \simeq e^{i(\vec{k}_c - \vec{k}_c')\vec{x}}$. In other words, the configuration $g(k)$ of the A particle becomes irrelevant in the process whenever the light quantum has a much more definite momentum. Therefore, in the detector model that follows, the $\vec{x}$ variable is effectively coarse-grained by the typical spread $1/\Delta k_c$ of the particles that are detected. In the limit where $f(\vec{k}_c) = \delta^3(\vec{k}_c - \vec{k}_{\text{particle}})$ the $\vec{x}$ dependence drops from the rate and detector's position becomes irrelevant. The two integrals inside $P(2t)$ factorise and we finally obtain

$$P(2t) = \frac{\mu^2}{M^2} \left| \int \frac{d^3 k}{\sqrt{2E(\vec{k})}} f(\vec{k}) e^{i\vec{k}\cdot\vec{x}} \frac{\sin \Omega(\vec{k})t}{\Omega(\vec{k})} \right|^2 \quad (1.13)$$

Our model detector has to reproduce the same detection rate for a generic initial state $|0\rangle_D \otimes |f\rangle$, where $|f\rangle = \int d^3 k f(\vec{k}) \gamma_{\vec{k}}^\dagger |0\rangle$ is the field state in the model. This is achieved through the effective interaction Hamiltonian

$$H_m^I = \frac{\mu}{M} \left(\sigma_\uparrow \Phi^+(\vec{x}) + \sigma_\downarrow \Phi^-(\vec{x}) \right), \quad (1.14)$$

where we recall that $\sigma_\uparrow$, $\sigma_\downarrow$ are the raising and lowering operators of the two level detector and the energy gap inside the detector is $\Delta E = \Delta M$. The complex

fields $\Phi^+(\vec{x})$ and $\Phi^-(\vec{x})$ are defined in terms of the dressed annihilators as $\Phi^+(\vec{x}) = \int d^3k e^{i\vec{k}\cdot\vec{x}} \gamma_{\vec{k}} / \sqrt{2E(k)}$, $\Phi^- = (\Phi^+)^\dagger$. Eq. (1.14) has the same matrix structure as (1.10), where the $A \to B$ transition between Fock spaces is modelled inside a two level system through the raising operator $\sigma_\uparrow$.

Passing from bare to dressed states changed the way in which the original local field theory (1.7) is partitioned in subsystems corresponding to the fields A, B, and C. As a consequence, $\Phi^+(\vec{x})$ and $\Phi^-(\vec{x})$ are not the positive and negative energy parts of the local field ϕ, because they are built from the dressed operators γ and $\gamma^\dagger$. However, at the pure level of the detector model, the underlying theory is not relevant: in order to describe what the detector measures one can define the—otherwise free—field $\Phi(\vec{x}) = \Phi^+(\vec{x}) + \Phi^-(\vec{x})$, coupled to the detector through (1.14). The initial local field theory (1.7) has effectively produced a non-local detector for the field Φ.

In summary, the derived detector model (1.14) has the same response as a physical "dressed"—rather than "bare"—particle in an interacting field theory, since it is built stressing the privileged role of the full theory's Hamiltonian eigenstates in describing typical objects and measuring devices. The detector clearly obeys the *Frog Principle*, as the state $|0\rangle_D \otimes |0\rangle$ is stable and no transitions can possibly occur at any finite time. The derivation is fully consistent only in the case of an inertial detector, since this is the natural state of motion of the A particle under the only influence of the field theory Hamiltonian. A consistent way to study the accelerated case would be to model how this acceleration is produced at the level of the fundamental field-theory model. For example, one can make the A and B fields charged and make the detector accelerate under the effect of an external classical electric field. An analogous set-up has been considered in Refs. [47, 48], where a direct relation between the Unruh and the Schwinger effects has been highlighted. It would be interesting, however, to study such an accelerating model not only in terms of asymptotic "free" states, and consider also its short time behaviour in terms of "dressed" objects.

More generally, our analysis seems to suggest that real measuring devices used for particle detection have no direct access to the local degrees of freedom $\phi(\vec{x})$ and effectively "see" only the positive energy fields Φ^+ of the dressed quanta. Such a circumstance was already pointed out by Glauber [4] in his pioneering paper [36], where, in fact, a photodetector model analogous to (1.14) was introduced.

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[4]"It has become customary, in discussions of classical theory, to regard the electric field $\vec{E}(\vec{x}, t)$ as the quantity one measures experimentally, and to think of the complex fields $\vec{E}^\pm(\vec{x}, t)$ as convenient, but fictitious, mathematical constructions. Such an attitude can only be held in the classical domain [...]. Where quantum phenomena are important the situation is usually quite different. [...] The use of any absorption process, such as photoionisation, means in effect that the field we are measuring is the one associated with photon annihilation, the complex field $\vec{E}^+(\vec{x}, t)$" [36].

Chapter 2

Renormalised Entropy in Quantum Fields

Summary

In this chapter we consider a finite region of space as a subsystem of a larger region, in which a quantum field has reached thermal equilibrium at some finite temperature. Standard calculations for the entropy of such a system exhibit ultraviolet divergences which, once a cut-off is introduced, are proportional to the area of the region. We show that a renormalised entropy can be defined if, instead of the local field operators, the Newton-Wigner position operators are used to identify the region of space. This prescription implies that, in order to identify the subsystem corresponding to a certain region, we have to trace away degrees of freedom that are localised outside the region according to the Newton-Wigner localisation, but not in the usual sense. However, the difference in the two localisations only involves distances smaller than the Compton wavelength of the field.

We consider a free scalar field in $d + 1$ spacetime dimensions prepared in a thermal state and we show that the entropy associated with the Newton-Wigner degrees of freedom is free of divergences and has a sound thermodynamic behaviour. In the limit of high temperatures/big volumes an extensive entropy is found, in agreement with the standard quantum field theory calculations once the divergent contributions are subtracted from the latter. In the limit of low temperatures/small volumes the entropy vanishes, but with a dependence on temperature and volume different from the high temperature regime. Explicit results are found for both massive and massless fields.
This chapter is based on and contains material from the publication

- S. Cacciatori, F. Costa, and F. Piazza,
  "Renormalized thermal entropy in field theory",

2.1   Thermal States and Local Degrees of Freedom

Thermodynamics is a powerful tool for describing complex physical systems. Beside its experimental success in the laboratory, thermodynamics is often applied to cosmology, for instance when the conservation of entropy is applied to a comoving volume of the expanding Universe (see e.g. [49]). On a more speculative level, the search for a consistent theory of quantum gravity often makes use of entropic and thermodynamic arguments, since they are supposed to be somewhat independent of the details of the underlying dynamics. Especially in view of such applications, it is certainly worth understanding better and better the connection between thermodynamics and microphysics within those physical regimes which are best known and under control. The tendency to thermal equilibrium, which in classical statistical physics relies on ergodic or mixing hypotheses, in quantum mechanics seems to be naturally driven by the correlations that a subsystem inevitably develops with its environment. This view, which has occasionally appeared in the literature at the level of common wisdom, is now being put on a firmer ground, e.g. in the book [50] and in related ongoing works. During time evolution, the reduced quantum state of a subsystem tends in fact to approach that of a thermal Gibbs state $\rho_{\text{thermal}} \propto e^{-\beta H}$, H being the Hamiltonian operator of the subsystem. This happens, under some generic circumstances and on time scales which are thoroughly discussed in [50], even if the initial state of the subsystem is very different from ρ_{thermal}, e.g. in the case when the entire system is initially prepared in a product state |subsystem⟩ ⊗ |environment⟩.

Our most successful microscopic description of physical interactions, quantum field theory (QFT), faces some difficulties when asked to reproduce coarse-grained meaningful thermodynamic quantities. In particular, as first noted in [51], the ultraviolet divergences encountered in the calculation of entropy are of a relatively uncommon type. If a finite system is in a thermal state, its entropy can be calculated with standard methods giving a thermodynamically sound result (see e.g. [52]). For the reasons described above, however, it is also interesting to consider, instead of the entire system, a subsystem occupying a finite portion of the entire volume. In this case, the entropy exhibits a UV-divergent "vacuum" contribution proportional to the boundary of the subsystem.

2.1.1   Thermal Entropy and UV Divergences

To be more definite, consider a system S whose dynamics is described by a QFT Hamiltonian H and put it in a thermal state $\rho_{\text{total}} \propto e^{-\beta H}$. Then consider a region

of space P (P stands for "place") of definite volume inside S and call R the rest of the system. The reduced state in P is obtained by tracing out the degrees of freedom belonging to R, $\rho = Tr_R\rho_{\text{total}}$. Calculate then the Von Neumann entropy $S = -Tr\rho \ln \rho$, which is the appropriate generalisation of the thermodynamical entropy for generic quantum states (see e.g. [53, 54]). Schematically, in four spacetime dimensions, one finds

$$S = S_{\text{vac}}(A, \Lambda) + S_{\text{therm}}(V, T). \tag{2.1}$$

Here A and V are the boundary area and the volume of P respectively, Λ is a UV cut-off (with the dimension of a mass) and $T = 1/\beta$ is the temperature. The term S_{vac} is the UV-divergent entanglement entropy of the vacuum (see, among others [55, 56, 57, 58]), obtained with the same procedure in the limit of zero temperature, i.e. when $\rho_{\text{total}} = |0\rangle\langle 0|$. The general form of S_{vac} is [59]

$$S_{\text{vac}} = c\Lambda^2 A + O(\Lambda^2 A)^{1/2}, \tag{2.2}$$

c being a regularisation-dependent number of order one, for more general boundaries see, e.g. [60]. The expansion (2.2) follows quite generally, e.g. from the heat kernel methods used in [57]. The finite component $S_{\text{therm}}(V, T)$, on the other hand, is the meaningful thermodynamic quantity; for a massless field it typically scales as $\sim VT^3$ in the big volume/high temperature limit. A few comments are now in order.

While the leading area-dependent vacuum divergence (2.2) can be checked in a variety of ways, bringing out the subleading finite term S_{therm} is not trivial and, to our knowledge, has been done explicitly only for conformal field theories. In 1+1 dimensions Calabrese and Cardy [61], by exploiting the analytic properties of the theory, found a structure of the type (2.1). More precisely, for a free massless bosonic field, it was found

$$S = \frac{1}{3}\left[\ln\left(\frac{\Lambda}{\pi T}\right) + \ln(\sinh \pi L T)\right] + c_1,$$

where $L \equiv V$ is the length of the subsystem and c_1 is a non-universal constant[1]. By using insights from the AdS/CFT correspondence, Ryu and Takayanagi have been able to extend the result to higher dimensions [62]. In any case, it would be surprising if the entropy did not have the structure (2.1) in general. The entanglement of the vacuum is in fact a UV effect and should be there also for generic finite energy states. The two separate terms in (2.1) are thus expected in any

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[1]Here $S_{\text{vac}} = \frac{1}{3}\ln\left(\frac{\Lambda}{\pi T}\right)$ diverges logarithmically with the cut-off because the theory, being massless, is critical, while an "area term", in one dimension, would just be a constant. (In generic d space dimensions, an area term has the form $\Lambda^{d-1}L^{d-1}$.)

plausible QFT theory where the highest energy modes decouple from the low energy physics. Of course, if thermal entropy did not have the form (2.1) and, say, some divergent term were also temperature dependent, then the intent of deriving meaningful coarse-grained quantities would be even more troublesome.

One could object that the volume-dependent term in (2.1) dominates over the area term in the thermodynamic limit for, say, sufficiently large volumes. In thermodynamics, however, volumes usually have to be big in comparison to, say, the typical distances (powered by the dimension of space) between particles. If one takes, for instance, a typical cosmological setup ($T^2 \sim M_{Pl} \times$ Hubble) and $\Lambda \sim M_{Pl}$, it is easy to see that, taking $S_{\text{vac}} \sim \Lambda^2 A$ and $S_{\text{therm}} \sim VT^3$, the thermodynamic term overcomes in (2.1) only for volumes much larger than the Hubble scale! One would expect thermodynamics to be applicable in much less extreme conditions. One could also argue that, since $S_{\text{vac}}(A, \Lambda)$ originates from the entanglement of the region considered with the outside, it should be suppressed in the limit where the full system is in a thermal state with a high enough temperature. However, such an argument is once again undermined by the divergent nature of the UV cut-off Λ and could only be applied for unreasonably high temperatures. Finally, one may also object that only entropy differences are meaningful and get rid in this way of the divergent area-dependent term. Still, this would not allow for a clear thermodynamic description of systems whose size is (adiabatically) changing in time, since the divergent term would not drop from entropy differences in this case. In this regard, once again, a finite, comoving volume in an expanding universe is perhaps the cleanest example.

Due to the non trivial dependence of the divergence on area, the quantity (2.1) cannot be renormalised by standard methods, i.e. by adding local counter terms to the Lagrangian. Moreover, since the result (2.2) has been carried out for free and conformal theories, we are bound to have divergences regardless of the asymptotic behaviour of the couplings or the UV completion of the theory, as long as such a completion is still a field theory. Of course, as proposed in [51], one can always *subtract* the divergent terms. The latter, however, are not more "spurious" than the widely accepted entanglement of the vacuum[2]. Furthermore, the subtraction of S_{vac} from (2.1) is not a completely consistent procedure, since one

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[2]At times, arguments are put forth that the Von Neumann entropy of a subsystem has a different meaning depending on whether or not the entire system is in a pure state. In this view, one may be tempted to conclude that the divergent term S_{vac}, since it originates from entanglement, should not be included in the evaluation of the thermodynamical entropy. Consider, however, the entire Universe in a pure state. One can expect thermalisation to occur over some region S after local equilibrium is reached, i.e. $\rho_S \simeq e^{-\beta H}$. Deep inside S, one can eventually consider a smaller subsystem P. The Von Neumann entropy of P is clearly both a thermodynamic entropy—because S is in a thermal state—and an entanglement entropy—because the whole Universe is in a pure state.

could start with the entangled vacuum of QFT and construct from it less and less entangled states. Such states, although probably not very relevant from a thermodynamical point of view, are nonetheless physical but would end up having a negative entropy after the subtraction of S_{vac}. In plain contradiction with the general view/common wisdom illustrated at the beginning of this section, equation (2.1) is just saying that the state of a generic subsystem in QFT is actually very far from being thermal!

Since the Hamiltonian operator H is an integral of a local density, i.e. $H = \int d^3 x H(\vec{x})$, one may naively expect that a state of the form $e^{-\beta H}$ would factorise over contiguous regions of space, giving $e^{-\beta H_P} \otimes e^{-\beta H_R}$, where H_P and H_R are the integrals of the Hamiltonian density extended only to regions P and R respectively, i.e. $H_P = \int_P d^3 x H(\vec{x})$ and $H_R = \int_R d^3 x H(\vec{x})$. If this were the case, tracing over R would trivially give a thermal state in P. However, the energy H hides a relevant amount of non-extensiveness that does not allow for this factorisation. The "inside" and "outside" contribution, H_P and H_R, do not add up to the total Hamiltonian because of the UV-divergent contact term H_I coming from the gradients across the boundary between P and R. In QFT, because of the singular nature of the interaction H_I between P and its environment R, the general arguments of [50] are not applicable (or at least not in a straightforward way).

2.1.2 Renormalising the Entropy

The above difficulties can be ascribed to an inconvenient choice of degrees of freedom. To see what that means, note that the system/region of space in question has two complementary descriptions [63, 64, 37]. In compliance to common intuition, P is described in classical general relativity by a subset $\overline{P}$—more specifically, a submanifold—of the points/events at a given time-like coordinate t. On the other hand, as a quantum subsystem, P is described by a Hilbert space $\mathcal{H}_P$, which is a factor in the tensor product decomposition ($\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_R$) of the total Hilbert space of the field theory under examination[3]. In this chapter we show that if we associate the region of space $\overline{P}$ with a more suitable—although unconventional—set of quantum degrees of freedom $\mathcal{H}_P$, the entropy is already "renormalised" and has a perfectly sound thermodynamic behaviour. For a massless, free scalar in the large volume/high temperature limit we find $S = c(d)VT^d$, where $d + 1$ is the dimension of spacetime and $c(d)$ is a numerical factor that can be explicitly calcu-

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[3]Note that partitioning a quantum system [65, 66] is more subtle than making the partition of a set. While a finite set admits a finite number of possible partitions, a finite number of quantum degrees of freedom can be divided in an infinite number of inequivalent ways. The simplest example is a four-dimensional quantum system, $\mathcal{H} = \mathbb{C}^4$, whose partitions into "two spins", $\simeq \mathbb{C}^2 \otimes \mathbb{C}^2$, are in one to one correspondence with the elements of the infinite group $SU(4)/SU(2)^2$ (see Ref. [37]).

lated (see Eqs. (2.36)). In this limit, our results are consistent with those obtained in Refs. [61, 62] once their divergent contribution is subtracted. However, there is no trace of any area-dependent term in our calculations and no infinities are encountered except, of the IR type, in the $1 + 1$-dimensional massless case in the limit $T \to 0$. In the same limit, our results differ from the "finite piece" S_{therm} that is found in (2.1) by using the conventional approach, although entropies tend to zero in both cases. For $T \to 0$ we find in fact $S \sim -VT^d \ln(VT^d)$, while [61, 62] find $S_{\text{therm}} \sim (VT^d)^{(d+1)/d}$. We comment on this in the last section of the chapter.

Before describing our calculation in section 2.2 it is perhaps worth spending few more words and see in which sense our anomalous renormalisation procedure underlies a different "localisation scheme" (see Ref. [37] for more details). The main point here is how to pick a bunch of (local) quantum degrees of freedom $\mathcal{H}_P$ out of a larger system. A tensor product structure (TPS)—or quantum partition— can be assigned by specifying the observables of the individual subsystems [66, 67]. In a composite system $\mathcal{H}_P \otimes \mathcal{H}_R$ two sets of observables $\mathcal{A}^j(P)$ and $\mathcal{A}^k(R)$, separately defined in P and R respectively, commute by construction:

$$[\mathcal{A}^j(P), \mathcal{A}^k(R)] = 0 \qquad \text{for any } j, k. \tag{2.3}$$

The point here is that such a trivial result can be applied the other way around [66]: if, within the algebra of observables acting on $\mathcal{H}$, we manage to isolate two commuting subalgebras $\mathcal{A}^j(P)$ and $\mathcal{A}^k(R)$, they induce a unique bipartition $\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_R$ on the whole system[4]. In the conventional calculation of entropy (2.1), it is implicitly assumed that the quantum degrees of freedom $\mathcal{H}_P$ of a region of space $\overline{P}$ at time t are those defined by the set of local relativistic fields $\phi(t, \vec{x} \in \overline{P})$ and their conjugate momenta $\pi(t, \vec{x} \in \overline{P})$. In fact, thanks to the canonical commutation relations, the two subalgebras generated by ϕ and π with labels $\vec{x}$ inside and outside P satisfy (2.3), and therefore induce a TPS. Such a TPS is the conventional localisation scheme in QFT.

In order to renormalise the entropy, we use an alternative set of commuting operators—and their corresponding TPS—as a new rationale to isolate the quantum degrees of freedom of P. We consider a free scalar field in $d + 1$-dimensional Minkowski spacetime. The normal-ordered Hamiltonian reads

$$H = \int d^d k \, w_k \, a_{\vec{k}}^\dagger a_{\vec{k}}, \tag{2.4}$$

where $w_k = \sqrt{\vec{k}^2 + m^2}$ and the operators $a_{\vec{k}}$ satisfy the usual canonical commutation relations: $[a_{\vec{k}}, a_{\vec{k}'}] = 0$, $[a_{\vec{k}}, a_{\vec{k}'}^\dagger] = \delta^3(\vec{k} - \vec{k}')$. Instead of the relativistic fields

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[4]More precisely, this is true only if the two subalgebras generate the entire algebra of operators on $\mathcal{H}$ [66].

and their conjugate momenta we introduce the "Newton-Wigner" fields $a(\vec{x})$ just as the Fourier transforms of $a_{\vec{k}}$:

$$a(\vec{x}) = \frac{1}{(2\pi)^{d/2}} \int d^d k \, a_{\vec{k}} \, e^{i\vec{k}\cdot\vec{x}}, \qquad a^\dagger(\vec{x}) = \frac{1}{(2\pi)^{d/2}} \int d^d k \, a_{\vec{k}}^\dagger \, e^{-i\vec{k}\cdot\vec{x}}; \qquad (2.5)$$

The above defined operator $a^\dagger(\vec{x})$ is directly related to the Newton-Wigner (NW) position operator [68] in that, acting on the vacuum, it produces an eigenvector of eigenvalue $\vec{x}$. Note that the relativistic invariant measure $1/\sqrt{2w_k}$ is absent from the integrand and therefore those operators are not relativistically invariant. This amounts to the fact that a particle perfectly NW-localised according to some observer is instead "spread" when described by a boosted one [69]. Nonetheless, the dynamics is still relativistically invariant because we are not changing the Hamiltonian of the free scalar (2.4) nor the other generators of the Poincaré group. It is also worth stressing that the non-covariant nature of the NW operators, usually considered one of the main drawbacks of the whole approach, is not extremely relevant in the present context, since any thermal state with $T > 0$ already breaks Lorentz invariance. Indeed, a system in thermal equilibrium is described as in a thermal state only in the reference frame with four-velocity parallel to the expectation value of the momentum operator, $\langle P^\mu \rangle$, which fixes the natural reference in which the operators (2.5) are defined. We refer to the extensive literature for more technical details (e.g. [46, 68, 70]) and philosophical implications [10] of NW operators. A very introductory comparison between the two localisation schemes is found in [37].

2.2 Sketches of the Calculation and Main Results

Since the entire problem is stationary, the time coordinate can be dropped throughout the analysis. At some given time, we divide a d-dimensional, space-like surface of a $d + 1$-dimensional Minkowski spacetime into two connected regions: $\overline{P}$, of finite volume, and $\overline{R}$, such that $\overline{P} \cup \overline{R} = \mathbb{R}^3$. (The results are independent of the particular shape of $\overline{P}$.) We distinguish spatial coordinates belonging to different regions using labels $\vec{p}, \vec{p}', \vec{p}_j \ldots$ for points inside $\overline{P}$, using $\vec{r}, \vec{r}', \vec{r}_j \ldots$ for those in $\overline{R}$ and, finally, $\vec{x}, \vec{y} \ldots$ for generic points in $\mathbb{R}^d$. One of the basic properties of NW localisation is that the vacuum of the theory is a product state, i.e. $|0\rangle = |0_P\rangle \otimes |0_R\rangle$ [37]. Moreover, starting from the vacuum, we can repeatedly apply $a^\dagger(\vec{x} \in \overline{P})$ and $a^\dagger(\vec{x} \in \overline{R})$ and generate two independent Fock spaces:

$$\mathcal{H}_P = \mathbb{C} \oplus P_1 \oplus P_2 \oplus \ldots \oplus P_n \oplus \ldots$$
$$\mathcal{H}_R = \mathbb{C} \oplus R_1 \oplus R_2 \oplus \ldots \oplus R_n \oplus \ldots$$

This Fock-space decomposition of the regions is the distinctive feature of NW localisation and allows an intuitive representation of particles localised in space. Such a construction cannot be carried out in the standard localisation, since the Reeh-Schlieder theorem forbids the existence of localised states with a finite number of particles. The most striking consequence is that the vacuum is here a product state, while it is entangled in the standard scheme. In each Fock subspace of given particle number we choose the obvious basis

$$
\begin{aligned}
P_n &\to |\vec{p}_1 \ldots \vec{p}_n\rangle = \frac{1}{\sqrt{n!}} a^\dagger(\vec{p}_1) \ldots a^\dagger(\vec{p}_n)|0\rangle, \\
R_n &\to |\vec{r}_1 \ldots \vec{r}_n\rangle = \frac{1}{\sqrt{n!}} a^\dagger(\vec{r}_1) \ldots a^\dagger(\vec{r}_n)|0\rangle.
\end{aligned}
\tag{2.6}
$$

In order to calculate traces, one has therefore to integrate on a basis in a Fock subspace of given particle number and then sum over all Fock subspaces. For example, if we restrict to block diagonal states (as are all those appearing here), we have

$$
\mathrm{Tr}_R \cdot = \langle 0_R| \cdot |0_R\rangle + \int_R d^d r \langle \vec{r}| \cdot |\vec{r}\rangle + \int_R d^d r d^d r' \langle \vec{r}\vec{r}'| \cdot |\vec{r}\vec{r}'\rangle + \ldots
\tag{2.7}
$$

(Here and in the following we write P, R, for $\overline{P}, \overline{R}$, understanding the identification of regions with subsystems via the NW scheme).

We consider the entire system in a (non-normalised) thermal state, $\rho_{\text{total}} = e^{-\beta H}$, where H is defined in (2.4). We call ρ the reduced state in P: $\rho = \mathrm{Tr}_R \rho_{\text{total}}$ and we calculate Von Neumann entropy by means of the formula [57]

$$
S \equiv -\mathrm{Tr}_P(\rho \ln \rho) = \left(-\frac{d}{dn} + 1 \right) \ln \mathrm{Tr}_P \rho^n \Big|_{n=1}.
\tag{2.8}
$$

This formula is particularly useful because it does not require the use of normalised states. Indeed, if one multiplies a state by a numerical factor, $\rho \to \Omega\rho$, one gets, from Eq. (2.8),

$$
S \to S + \left(-\frac{d}{dn} + 1 \right) \ln \Omega^n \Big|_{n=1} = S.
$$

It is easy to check that ρ (as well as ρ_{total}) is block diagonal on the particle number subspaces of its Fock space. Its matrix elements on each subspace are expressible in terms of the crucial two-point function defined in the one-particle sector

$$
K(\vec{p}, \vec{p}') \equiv \frac{\langle \vec{p}|\rho|\vec{p}'\rangle}{\Omega},
\tag{2.9}
$$

where $\Omega \equiv \langle 0_P | \rho | 0_P \rangle$ is the vacuum-vacuum matrix element. The function K is itself an infinite series obtained by tracing ρ_{total} over R (where each term of the series is obtained by integrating over the subspace R_n, see Eq. (2.20) below) and can be conveniently written (see Eq. (2.21)) in the diagrammatic formalism to be introduced in the next section. Since we are dealing with a free theory, the generic matrix element $\langle \vec{p}_1 \vec{p}_2 \ldots \vec{p}_n | \rho | \vec{p}_1' \vec{p}_2' \ldots \vec{p}_n' \rangle$ is expressed as a combination of products of K's in equation (2.22).

Since ρ is an operator acting on P, when calculating matrix elements of ρ^n, integrations over the variables $\vec{p}$ have to be carried out in each Fock subspace. A final integration over the same variables has to be done in order to obtain $\text{Tr}_P \rho^n$. The terms in the corresponding series rearrange (see Eq. (2.23)) and this number can be written in closed form, again, in terms of the two-point function K as

$$\text{Tr}_P \rho^n = \Omega^n \exp\left(\sum_{j=1}^{\infty} \frac{1}{j} \text{Tr}\, K^{j \cdot n} \right), \tag{2.10}$$

where, by definition,

$$\text{Tr}\, K^m \equiv \int_P d^d p_1 d^d p_2 \ldots d^d p_m \, K(\vec{p}_1, \vec{p}_2) K(\vec{p}_2, \vec{p}_3) \ldots K(\vec{p}_m, \vec{p}_1).$$

Note that the normalisation factor Ω^n in (2.10) drops when used in formula (2.8). Note also that each factor K in the above integral is itself a series of integrals over the $\vec{r}$ variables, obtained by plugging $\rho = \text{Tr}_R \rho_{\text{total}}$ in (2.9) and applying (2.7). A consistent part of the chapter is finally devoted to evaluate the above quantity in the high temperature, $V/\beta^d \to \infty$, and small temperature, $V/\beta^d \to 0$, limits. Two distinct behaviours of $\text{Tr}\, K^n$ as a function of n follow.

In the high-temperature limit, the leading term of the series giving $\text{Tr}\, K^n$ is the one containing only integrations over the $\vec{p}$ variables: the other terms converge and give a subleading contribution. The only integrations left are those inside P. Those are all of the same order in VT^d, although they scale as $1/n^d$, where n is the number of integration variables. The corresponding behaviour of $\text{Tr}\, K^n$, when used in (2.10) and (2.8), gives an extensive entropy. In this limit, apart from numerical factors to be found in Eqs. (2.35) and (2.36), one finds in fact

$$\text{Tr} K^n \simeq \frac{VT^d}{n^d} + O(1), \quad S \simeq VT^d + O(1), \quad 1/VT^d \to 0. \tag{2.11}$$

In the low-temperature limit, the external integrals are no longer negligible and they have to be summed up. The corresponding series can be explicitly calculated at leading order in VT^d. On the other hand, terms with a higher number of internal integrations are subleading and this gives

$$\text{Tr}\, K^n \simeq (VT^d)^n + O(VT^d)^{n+1}, \quad S \simeq -VT^d \ln VT^d + O(VT^d),$$
$$VT^d \to 0. \tag{2.12}$$

The numerical factors are found in Eqs. (2.39) and (2.40) below. In section 2.4.3, we will also consider massive fields In the low-temperature limit, their entropy behaves as in Eq. (2.12), except that the quantity VT^d is each time suppressed by the factor $e^{-m/T}$ (see Eq. (2.43) below).

2.3   Formalism and Diagrammatic

After the general setting described above (basically, Eqs. (2.4)–(2.6)) we give here more details of the calculation. First of all, we need to calculate the matrix elements of $\rho_{\text{total}} = e^{-\beta H}$ in position space; using the basis vectors (2.6) and going to Fourier space, we have

$$\langle \vec{x}_1 \ldots \vec{x}_n | e^{-\beta H} | \vec{x}_1'' \ldots \vec{x}_n'' \rangle \ = \ \frac{1}{m!(n-m)!} \sum_{\sigma \in S_n} I_\beta(\vec{x}_1 - \vec{x}_{\sigma(1)}'') \cdots I_\beta(\vec{x}_n - \vec{x}_{\sigma(n)}''). \quad (2.13)$$

Here, of the total n points, m is the number of points inside P, S_n denotes the group of permutations over n elements and

$$I_\beta(\vec{x} - \vec{x}') \equiv \langle \vec{x} | e^{-\beta H} | \vec{x}' \rangle \ = \ \frac{1}{(2\pi)^d} \int d^d k \, e^{i \vec{k} \cdot (\vec{x} - \vec{x}') - \beta w_k} \ . \quad (2.14)$$

Explicit expressions of the two-point function I and its massless limit follow for $d = 1$,

$$I_\beta(x) \ = \ \frac{m\beta}{\pi \sqrt{\beta^2 + x^2}} K_1(m \sqrt{\beta^2 + x^2}) \simeq \frac{\beta}{\pi(\beta^2 + x^2)} + O(m^2), \quad (2.15)$$

and $d = 3$,

$$I_\beta(\vec{x}) \ = \ \frac{m^2 \beta}{2\pi^2(\beta^2 + x^2)} K_2(m \sqrt{\beta^2 + x^2}) \simeq \frac{\beta}{\pi^2(\beta^2 + x^2)^2} + O(m^2). \quad (2.16)$$

Here K_j are the modified Bessel functions of the second kind. Note that (2.14) is not the usual QFT thermal correlator and, as such, it is not periodic in β. This reflects the fact that we are not working in the usual thermic representation, where traces are taken by functional integration over a compactified Euclidean manifold.

A crucial property of the two-point function I_β that follows straightforwardly from its expression (2.14) in Fourier space is

$$\int d^d z \, I_\beta(\vec{x} - \vec{z}) I_\gamma(\vec{z} - \vec{y}) \ = \ I_{\beta+\gamma}(\vec{x} - \vec{y}). \quad (2.17)$$

By iteration we also have

$$I_\beta^n(\vec{x} - \vec{y}) = I_{n\beta}(\vec{x} - \vec{y}), \quad (2.18)$$

where the nth power of I_β has been implicitly defined in an obvious way.

Matrix elements with a different number of particles on the two sides vanish, because in transformation (2.5) the number of creation and annihilation operators is preserved; our matrix ρ_{total} is thus block diagonal in the subspaces of given particle number. The same property is retained by the reduced density matrix ρ with respect to the local Fock space $\mathcal{H}_P$, so that we only need to calculate the matrix elements $\langle \vec{p}_1 \ldots \vec{p}_n | \rho | \vec{p}'_1 \ldots \vec{p}'_n \rangle$.

First, we define Ω as the matrix element of ρ on the local vacuum in P:

$$
\begin{aligned}
\Omega :=& \langle 0_P | \rho | 0_P \rangle = \langle 0_P | \text{Tr}_R e^{-\beta H} | 0_P \rangle \\
=& \left(\langle 0_R | \otimes \langle 0_P | \right) e^{-\beta H} \left(|0_P\rangle \otimes |0_R\rangle \right) + \int_R d^d r \left(\langle \vec{r} | \otimes \langle 0_P | \right) e^{-\beta H} \left(|0_P\rangle \otimes |\vec{r}\rangle \right) \\
& + \int_{R \times R} d^d r_1 d^d r_2 \left(\langle \vec{r}_1 \vec{r}_2 | \otimes \langle 0_P | \right) e^{-\beta H} \left(|0\rangle_P \otimes |\vec{r}_1 \vec{r}_2\rangle_P \right) + \ldots
\end{aligned}
$$

In terms of the two-point function $I_\beta(\vec{x} - \vec{x}'')$, we have

$$
\begin{aligned}
\Omega =& \sum_{n=0}^{\infty} \frac{1}{n!} \int_{R^n} d^d r_1 \ldots d^d r_n \sum_{\sigma \in S_n} \prod_{j=1}^{n} I_\beta(\vec{r}_j - \vec{r}_{\sigma(j)}) = 1 + \int_R d^d r I_\beta(\vec{r} - \vec{r}) \\
& + \frac{1}{2} \int_{R \times R} d^d r_1 d^d r_2 \left[I_\beta(\vec{r}_1 - \vec{r}_1) I_\beta(\vec{r}_2 - \vec{r}_2) + I_\beta(\vec{r}_1 - \vec{r}_2) I_\beta(\vec{r}_1 - \vec{r}_2) \right] + \ldots
\end{aligned}
\tag{2.19}
$$

We can write this kind of expressions in a diagrammatic form; in this way, the vacuum expectation value is given by the sum of all the "bubble diagrams":

$$
\Omega \;=\; 1 \;+\; \bigcirc \;+\; \frac{1}{2} \left(\bigcirc \bigcirc \;+\; \bigcirc \right) \;+\; \ldots
$$

Here and in the following, empty circles ∘ are points in R and full circles ● points in P, lines are the two-point function I and two lines getting at the same circle imply integration. The nth term of the series (2.19) is obtained diagrammatically by taking n empty circles and connecting them with each other in all possible ways such that each circle is reached by two lines.

The matrix element of ρ living in the one particle sector is a two-point function:

$$
\langle \vec{p} | \rho | \vec{p}' \rangle \;=\; I_\beta(\vec{p} - \vec{p}') \;+\; \int_R d^d r \left[I_\beta(\vec{p} - \vec{p}') I_\beta(\vec{r} - \vec{r}) + I_\beta(\vec{p} - \vec{r}) I_\beta(\vec{r} - \vec{p}') \right] \;+\; \ldots
\tag{2.20}
$$

diagrammatically,

$$\langle \vec{p}|\rho|\vec{p}'\rangle \;=\; (\text{diagram}) + \Big((\text{diagram}) + (\text{diagram}) \Big)$$

$$+\frac{1}{2}\Big((\text{diagram}) + 2\,(\text{diagram}) + 2\,(\text{diagram}) + (\text{diagram}) \Big)$$

$$+ \ldots$$

Each term, weighted by a factor $1/n!$, consists of all possible ways that the two external lines with the full circles can connect each other through n empty circles. Note that the "vacuum contribution" factorises out, leaving

$$\langle \vec{p}|\rho|\vec{p}'\rangle \;=\; \Omega\Big((\text{diagram}) + (\text{diagram}) + (\text{diagram}) + \ldots \Big). \qquad (2.21)$$

We call the two-point function inside the parenthesis K:

$$\langle \vec{p}|\rho|\vec{p}'\rangle \;\equiv\; \Omega\,K(\vec{p},\vec{p}').$$

When we consider the matrix elements in the n-particle sector, bubble diagrams again factorise out, leaving us with an expression of the form

$$\langle \vec{p}_1\vec{p}_2\ldots\vec{p}_n|\rho|\vec{p}_1'\vec{p}_2'\ldots\vec{p}_n'\rangle \;=\; \frac{\Omega}{n!}\sum\,(2n\text{-points connected diagrams}),$$

where now we are summing over all the possible diagrams that connect n points on the left to n points on the right. As we can have only two lines starting from each internal point, a diagram is composed by "paths", each of which connects one point on the left to one on the right (two points on the same side cannot be connected). This means that, if we select a pair of points $(\vec{p}_i,\,\vec{p}_j')$, we can factorise an expression equal to the sum of connected diagrams in (2.21), which gives the two-point function $K(\vec{p}_i,\vec{p}_j')$. To obtain all the diagrams, we have to consider all the possible pairs; the result is that we can write all the matrix elements in terms of functions $K(\vec{p}_i,\vec{p}_j')$:

$$\langle \vec{p}_1\vec{p}_2\ldots\vec{p}_n|\rho|\vec{p}_1'\vec{p}_2'\ldots\vec{p}_n'\rangle \;=\; \frac{\Omega}{n!}\sum_{\sigma\in S_n}\prod_{j=1}^{n} K(\vec{p}_j,\vec{p}_{\sigma(j)}'). \qquad (2.22)$$

Note that this expression has the same structure as (2.13), with $I_\beta(\vec{x} - \vec{x}')$ replaced by $K(\vec{p}, \vec{p}')$. The reason is that, using the NW localisation, local regions have the same Fock structure as the global space.

We define the powers of the two-point function K by multiplying K as a one-particle operator acting inside P. Accordingly, we define the trace of the m-th power of K as

$$\mathrm{Tr}\, K^m \equiv \int_{P^m} dp\, dp' \ldots dp^{(m-1)}\, K(\vec{p}, \vec{p}')K(\vec{p}', \vec{p}'') \ldots K(\vec{p}^{(m-1)}, \vec{p}).$$

These traces are what is needed to calculate $\mathrm{Tr}_P\, \rho^n$, which in turn allows finding the Von Neumann entropy by means of Eq. 2.8. (Which can be applied to ρ regardless of its normalisation.)

Consider first the case $n = 2$. Since ρ is block diagonal in the fixed number of particles subspaces, so is ρ^2, and we can write, for the generic matrix element in the m-particle subspace

$$\langle \vec{p}_1 \vec{p}_2 \ldots \vec{p}_m | \rho^2 | \vec{p}_1' \vec{p}_2' \ldots \vec{p}_m' \rangle$$
$$= \int_{P^m} d^d q_1 \ldots d^d q_m \langle \vec{p}_1 \vec{p}_2 \ldots \vec{p}_m | \rho | \vec{q}_1 \ldots \vec{q}_m \rangle \langle \vec{q}_1 \ldots \vec{q}_m | \rho | \vec{p}_1' \vec{p}_2' \ldots \vec{p}_m' \rangle$$
$$= \left(\frac{\Omega}{m!} \right)^2 \int_{P^m} d^d q_1 \ldots d^d q_m \sum_{\sigma, \sigma' \in S_m} \prod_{i\, j=1}^m K(\vec{p}_i, \vec{q}_{\sigma(i)}) K(\vec{q}_j, \vec{p}_{\sigma'(j)}')$$
$$= \left(\frac{\Omega}{m!} \right)^2 \int_{P^m} d^d q_1 \ldots d^d q_m \sum_{\sigma, \sigma' \in S_m} \prod_{j=1}^m K(\vec{p}_j, \vec{q}_{\sigma(j)}) K(\vec{q}_{\sigma'(j)}, \vec{p}_j')$$
$$= \frac{\Omega^2}{m!} \sum_{\sigma \in S_m} \prod_{j=1}^m \int_P d^d q\, K(\vec{p}_j, \vec{q}) K(\vec{q}, \vec{p}_{\sigma(j)}')$$
$$\equiv \frac{\Omega^2}{m!} \sum_{\sigma \in S_m} \prod_{j=1}^m K^2(\vec{p}_j, \vec{p}_{\sigma(j)}').$$

Iterating this procedure we obtain the expression for ρ^n:

$$\langle \vec{p}_1 \vec{p}_2 \ldots \vec{p}_m | \rho^n | \vec{p}_1' \vec{p}_2' \ldots \vec{p}_m' \rangle = \frac{\Omega^n}{m!} \sum_{\sigma \in S_m} \prod_{j=1}^m K^n(\vec{p}_j, \vec{p}_{\sigma(j)}').$$

Finally, the trace is given by the sum of all the contributions of the m-particle matrix elements:

$$\mathrm{Tr}_P\, \rho^n = \Omega^n \sum_{m=0}^{+\infty} \frac{1}{m!} \sum_{\sigma \in S_m} \int_{P^m} d^d p_1 \ldots d^d p_m \prod_{j=1}^m K^n(\vec{p}_j, \vec{p}_{\sigma(j)})$$
$$= \Omega^n \det(1 - K^n)^{-1}$$

(2.23)

(see, for example, Ref. [71], page 187, formula (4-86)), and then

$$\mathrm{Tr}_P \rho^n \ = \ \Omega^n \ \exp\left(\sum_{j=1}^{\infty} \frac{1}{j} \mathrm{Tr}\, K^{jn}\right). \tag{2.24}$$

Inserting this expression in (2.8), we find

$$S \ = \ \left(-\frac{d}{dn}+1\right) \sum_{j=1}^{\infty} \frac{1}{j} \,\mathrm{Tr}\, K^{jn}\bigg|_{n=1}. \tag{2.25}$$

The quantities we need to calculate are $\mathrm{Tr}\, K^n$; we can give for these a diagrammatic expansion, like in (2.21). For $n=1$, we only have to "close" each diagram, so to match together the full circles at the ends of each factor. We get

$$\mathrm{Tr} K \ = \ \bigcirc \ + \ \bigcirc \ + \ \bigcirc \ + \ldots \tag{2.26}$$

Operator K^2 is obtained multiplying term by term two copies of the expression for K:

$$K^2(\vec{p}, \vec{p}') = \left(\bullet\!\!-\!\!-\!\!\bullet \ + \ \bullet\!\!-\!\!-\!\!\circ\!\!-\!\!-\!\!\bullet \ +\ldots \right)\left(\bullet\!\!-\!\!-\!\!\bullet \ + \ \bullet\!\!-\!\!-\!\!\circ\!\!-\!\!-\!\!\bullet \ +\ldots \right)$$

$$= \bullet\!\!-\!\!-\!\!\bullet\!\!-\!\!-\!\!\bullet \quad + 2\, \bullet\!\!-\!\!-\!\!\bullet\!\!-\!\!-\!\!\circ\!\!-\!\!-\!\!\bullet + \bullet\!\!-\!\!-\!\!\circ\!\!-\!\!-\!\!\bullet\!\!-\!\!-\!\!\circ\!\!-\!\!-\!\!\bullet + \ldots$$

When we take the trace, again we have to match the extremes of each diagram, so that we end up with closed loops with two full circles each and an arbitrary number of empty circles. The analogue expression for $\mathrm{Tr} K^n$ is a straightforward generalisation: it contains loops with n full circles and an arbitrary number of empty circles. The explicit formula is

$$\mathrm{Tr} K^n = \int d^d p_1 \ldots d^d p_n \sum_{j_1 \ldots j_n = 0}^{+\infty} \int d^d r'_1 \ldots d^d r'_{j_1} d^d r''_1 \ldots \ldots d^d r_1^{(n)} \ldots d^d r_{j_n}^{(n)}$$

$$I_\beta(\vec{p}_1 - \vec{r}_1^{\,1}) I_\beta(\vec{r}_1'' - \vec{r}_2^{\,1}) \ldots I_\beta(\vec{r}_{j_1}^{\,1} - \vec{p}_2) I_\beta(\vec{p}_2 - \vec{r}_1^{\,2}) \ldots I_\beta(\vec{r}_{j_n}^{\,n} - \vec{p}_1).$$

2.4   Explicit Evaluations of Entropy

We consider separately the two situations $\beta^d \ll V$ (high temperature) and $\beta^d \gg V$ (low temperature), where V is the volume of the region P under consideration. We

will mainly consider a massless field, but we will also consider a finite mass m in the low-temperature limit.

The high-temperature limit, $V/\beta^d \to \infty$, is also the limit of very large volume, so we may expect to find, at leading order, the entropy that we would find by considering as our subsystem the whole space. Although this turns out to be the case, the actual proof is pretty involved and is carried out in the subsection 2.4.2.

2.4.1 The Whole Space

As a first check of our formalism we calculate the entropy of a system (not a subsystem) in a thermal state. This can be done by standard methods, i.e., by calculating the partition function $Z = \text{Tr}\, e^{-\beta H}$ that, in our formalism, using Eq. (2.13), reads

$$Z = \sum_{n=0}^{+\infty} \int d^d x_1 \ldots d^d x_n \frac{1}{n!} \sum_{\sigma \in S_n} \prod_{j=1}^{n} I_\beta(\vec{x}_j - \vec{x}_{\sigma(j)}) = \exp\left(\sum_{j=1}^{+\infty} \frac{1}{j} \text{Tr} I_\beta^j\right). \quad (2.27)$$

We basically used the same derivation as for (2.24). In fact, in this case, $K = I_\beta$ since there is nothing to integrate over outside the system. The operator powers I_β^j are obtained by integration over all space. For this purpose, we use Eq. (2.18) and find

$$\text{Tr} I_\beta^n = \int d^d x I_{n\beta}(\vec{x} - \vec{x}) = V I_{n\beta}(0).$$

On the other hand, for $m = 0$, we have

$$I_\beta(0) = \int \frac{d^d k}{(2\pi)^d} e^{-\beta|\vec{k}|} = \frac{\Omega_d}{(2\pi)^d} \int_0^{+\infty} dk\, k^{d-1} e^{-\beta k} = \frac{\Omega_d}{(2\pi)^d} \frac{(d-1)!}{\beta^d},$$

where $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$ is the d-dimensional solid angle. From (2.27) we then find

$$\ln Z = \frac{V}{\beta^d} \frac{(d-1)!\Omega_d}{(2\pi)^d} \zeta(d+1),$$

where ζ is the Riemann zeta function. If we calculate the entropy by using

$$S = \left(-\beta \frac{d}{d\beta} + 1\right) \ln Z,$$

we find the leading order (2.36) of the more general result in the high-temperature limit.

2.4.2 High-Temperature Limit

We consider the limit $\beta^d/V \to 0$ in the massless case. Let us first consider the one-dimensional case where P is the the interval $(-L, L)$.

The One-Dimensional Case

We need to compute $\mathrm{Tr}K^n$. For $n = 1$ it is given by (2.26). By Eq. (2.15) the first term is simply

$$\bigcirc(\beta) = \int_{-L}^{L} \frac{\beta}{\pi(\beta^2 + (x - x)^2)} = \frac{2L}{\pi\beta},$$

where the term in parenthesis after the diagram, here and in what follows, specifies the suffix β of the corresponding I_β functions running in the loop. For the second term, we have

$$\bigcirc(\beta,\beta) = \bigcirc(2\beta) - \bigcirc(\beta,\beta)$$

$$= \frac{2L}{\pi 2\beta} - \int_{-L}^{L} dx \int_{-L}^{L} dy \frac{\beta}{\pi(\beta^2 + (x - y)^2)} \frac{\beta}{\pi(\beta^2 + (y - x)^2)},$$

where the property (2.18) has been used. Now,

$$\int_{-L}^{L} dx \int_{-L}^{L} dy \frac{\beta}{\pi(\beta^2 + (x - y)^2)} \frac{\beta}{\pi(\beta^2 + (y - x)^2)}$$

$$= -\frac{\beta}{2\pi^2} \frac{d}{d\beta} \int_{0}^{2L} dx \int_{0}^{2L} dy \frac{1}{\beta^2 + (x - y)^2}$$

$$= -\frac{\beta}{\pi^2} \frac{d}{d\beta} \int_{0}^{2L} dx \frac{1}{\beta} \arctan \frac{x}{\beta} = \frac{1}{\beta\pi^2} \int_{0}^{2L} dx \frac{d}{dx} \left(x \arctan \frac{x}{\beta} \right)$$

$$= \frac{2L}{\beta\pi^2} \arctan \frac{2L}{\beta} = \frac{L}{\pi\beta} + O(1),$$

thus,

$$\bigcirc = O(1).$$

Thus it seems that terms containing external integrations give finite contributions. Before checking this to the next order, let us note that

$$\frac{1}{\pi^{n+2}} \int_{-L}^{L} dx_0 \cdots \int_{-L}^{L} dx_{n+1} \frac{m_0 m_1 \cdots m_{n+1}\beta^{n+2}}{[\beta^2 m_0^2 + (x_0 - x_1)^2] \cdots [\beta^2 m_{n+1}^2 + (x_{n+1} - x_0)^2]}$$

$$= \frac{2L}{\beta\pi^{n+2}} \int_{0}^{\infty} dx_1 \cdots \int_{0}^{\infty} dx_{n+1} \Bigg[\tag{2.28}$$

$$\frac{m_0 m_1 \cdots m_{n+1}}{[m_0^2 + x_1^2][m_1^2 + (x_1 - x_2)^2] \cdots [m_0^2 + (x_n - x_{n+1})^2][m_{n+1}^2 + x_{n+1}^2]} \Bigg]$$

$$+ \text{ cyclic terms} + \ldots$$

Here cyclic means with respect to the dependence on m_i and the ellipses mean terms of the next order in β/L (when β/L goes to zero). This can be easily verified as follows: let us call $U(m_0, \ldots, m_{n+1})$ the left hand side of Eq. (2.28). One must show that the limit

$$\lim_{\beta \to 0} \frac{\beta}{L} U(m_0, \ldots, m_{n+1})$$

exists and is given by (2.28). To this end, it is convenient first to rescale all coordinates by β, so that

$$\frac{\beta}{L} U(m_0, \ldots, m_{n+1})$$

$$= \frac{1}{\pi^{n+2}} \frac{\beta}{L} \int_{-\frac{L}{\beta}}^{\frac{L}{\beta}} dx_0 \cdots \int_{-\frac{L}{\beta}}^{\frac{L}{\beta}} dx_{n+1} \frac{m_0 m_1 \cdots m_{n+1}}{[m_0^2 + (x_0 - x_1)^2] \cdots [m_{n+1}^2 + (x_{n+1} - x_0)^2]}. \tag{2.29}$$

Setting $z = L/\beta$, it suffices to compute the limit $z \to \infty$ by means of the de l'Hospital rule, to get the desired result. Indeed the de l'Hospital rule says that we must look at the limit

$$\lim_{z \to \infty} = \frac{1}{\pi^{n+2}} \int_{-\frac{L}{\beta}}^{\frac{L}{\beta}} dx_1 \cdots \int_{-\frac{L}{\beta}}^{\frac{L}{\beta}} dx_{n+1} \frac{m_0 m_1 \cdots m_{n+1}}{[m_1^2 + (x_1 - x_2)^2] \cdots [m_n^2 + (x_n - x_{n+1})^2]}$$

$$\times \left[\frac{1}{m_0^2 + \left(\frac{L}{\beta} - x_1\right)^2} \frac{1}{m_{n+1}^2 + \left(\frac{L}{\beta} - x_{n+1}\right)^2} + \frac{1}{m_0^2 + \left(\frac{L}{\beta} + x_1\right)^2} \frac{1}{m_{n+1}^2 + \left(\frac{L}{\beta} + x_{n+1}\right)^2} \right]$$

$$+ \text{cyclic},$$

where we used the obvious relation $\frac{d}{dz} \int_{-z}^{z} f(x)dx = f(z) + f(-z)$. The two factors in the square brackets give the same contribution[5], so that after the shift $x_i \to x_i + L/\beta$, for all the x_i, our limit becomes

$$\lim_{z \to \infty} = \frac{2}{\pi^{n+2}} \int_{0}^{\frac{2L}{\beta}} dx_1 \cdots \int_{0}^{\frac{2L}{\beta}} dx_{n+1} \frac{m_0 m_1 \cdots m_{n+1}}{[m_1^2 + (x_1 - x_2)^2] \cdots [m_n^2 + (x_n - x_{n+1})^2]} \cdot$$

$$\cdot \frac{1}{m_0^2 + x_1^2} \frac{1}{m_{n+1}^2 + x_{n+1}^2} + \text{cyclic}. \tag{2.30}$$

It remains to show that indeed the integrals on the right hand side of (2.28) converge. This can be done by introducing the new variables t_i such that

$$t_i = x_i - x_{i+1}, \quad i = 1, \ldots, n, \quad t_{n+1} = x_{n+1}.$$

---

[5]the second one is obtained by the first one by changing sign to all the integration variables

Then, after rewriting the integral, one sees that the integrand is dominated by $\prod_{i=0}^{n+1} \frac{m_i}{m_i^2 + t_i^2}$.

Now, let us continue our analysis and consider the term

$$\bigcirc(\beta,\beta,\beta) = \bigcirc(3\beta) - \bigcirc(2\beta,\beta) - \bigcirc(\beta,2\beta) + \bigcirc(\beta,\beta,\beta).$$

Using our general formula, find

$$\bigcirc(3\beta) = \frac{2L}{3\pi\beta} + \ldots,$$

$$\bigcirc(2\beta,\beta) = \bigcirc(\beta,2\beta) = \frac{8L}{\beta\pi^2} \int_0^\infty dx \frac{1}{(1+x^2)(4+x^2)} + \ldots,$$

$$= \frac{8L}{3\pi^2\beta} \int_0^\infty dx \left[\frac{1}{1+x^2} - \frac{1}{4+x^2}\right] + \ldots = \frac{2L}{3\pi\beta} + \ldots,$$

$$\bigcirc(\beta,\beta,\beta) = \frac{6L}{\beta\pi^3} \int_0^\infty dx \int_0^\infty dy \frac{1}{(1+x^2)(1+y^2)[1+(x-y)^2]} + \ldots = \frac{2L}{3\pi\beta} + \ldots,$$

so that

$$\lim_{\beta \to 0} \left[\beta \bigcirc(\beta,\beta,\beta) \right] = 0.$$

This is true for any power of K. For example,

$$\mathrm{Tr}K^2 = \bigcirc + \bigcirc + \bigcirc + \ldots$$

and, using the above results, we see that

$$\bigcirc(\beta,\beta,\beta) = \bigcirc(\beta,\beta,\beta) = \bigcirc(\beta,2\beta) - \bigcirc(\beta,\beta,\beta)$$

and then the L/β terms drop out. Indeed, one can prove that any loop integral containing at least a white ball insertion converges in the high-energy limit (see Appendix A.1).

Finally we get

$$\mathrm{Tr}K^n = \bigcirc(n;\beta,\ldots,\beta) + \ldots, \tag{2.31}$$

that is, the leading contribution is given by the loop with exactly n black ball insertions. Now, being the cyclic terms all coincident, we have

$$\bigcirc (n; \beta, \dots, \beta)$$
$$= \frac{2nL}{\beta \pi^n} \int_0^\infty dx_1 \cdots \int_0^\infty dx_{n-1} \frac{1}{(1 + x_1^2)(1 + x_{n-1}^2)[1 + (x_1 - x_2)^2] \cdots [1 + (x_{n-2} - x_{n-1})^2]} + \dots$$
$$= \frac{2nL}{\beta \pi^n} U(n) + \dots$$

As we will see soon, the integral can be computed to give

$$U(n) = \frac{\pi^{n-1}}{n^2},$$

so that

$$\bigcirc (n; \beta, \dots, \beta) = \frac{2L}{n\beta\pi}. \qquad (2.32)$$

Indeed, we can show this as follows. Using the results shown in Appendix A.1, we can add a loop with a white insertion and n black insertions, without changing the divergent term, so that

$$\bigcirc (n; \beta, \dots, \beta) \simeq \bigcirc (n; \beta, \dots, \beta) + \bigcirc (n; \beta, \dots, \beta)$$
$$= \bigcirc (n - 1; 2\beta, \beta, \dots, \beta),$$

where $\simeq$ means equal up to convergent terms. Next we can add the term

$$\bigcirc (n - 1; 2\beta, \beta, \dots, \beta)$$

to obtain

$$\bigcirc (n; \beta, \dots, \beta) \simeq \bigcirc (n - 2; 3\beta, \beta, \dots, \beta).$$

Proceeding in this way, we get

$$\bigcirc (n; \beta, \dots, \beta) \simeq \bigcirc (n\beta), \qquad (2.33)$$

which gives (2.32). Inserting (2.32) in (2.25), we finally get for the entropy

$$S = \frac{2\pi L}{3\beta} + \ldots \tag{2.34}$$

Note that the above result is finite and extensive, no subtraction of infinities needs to be made at any step.

The d-Dimensional Case

The computations detailed out for the one-dimensional case can be extended to any dimension $d \geq 1$. Indeed, using (2.14), one finds again that the loops containing only black insertions dominate so that (2.31) and (2.33) continue to be true. On the other hand,

$$\bigcirc (n\beta) = \frac{V}{(n\beta)^d} \frac{(d-1)!}{2^{d-1}\pi^{\frac{d}{2}}\Gamma(d/2)} + \ldots \tag{2.35}$$

Thus we can easily compute the entropy and find the result

$$S_d = \frac{V}{\beta^d} \frac{(d-1)!}{2^{d-1}\pi^{\frac{d}{2}}\Gamma(d/2)}(d+1)\zeta(d+1) + \ldots \tag{2.36}$$

It can be useful to separate the odd-dimensional cases from the even-dimensional ones. Using the duplication formula for the Gamma function, one finds

$$S_{2k} = \frac{V}{\beta^{2k}} \frac{(2k-1)!}{k!\pi^k 2^{2k+1}}(2k+1)\zeta(2k+1) + \ldots,$$

$$S_{2k+1} = \frac{V}{\beta^{2k+1}} \frac{(k+1)!}{\pi^{k+1}}2\zeta(2k+2) + \ldots$$

For example, for 3 spatial dimensions we find

$$S_3 = \frac{V}{\beta^3} \frac{2\pi^2}{45} + \ldots \tag{2.37}$$

2.4.3   Low-Temperature Limits

In this section, we consider two different low-temperature limits. In the first case we take $\nu \to 0$, with

$$\nu \equiv \frac{V}{(2\pi\beta)^d},$$

for fixed values of the product βm between the inverse temperature and the mass of the field. This can be thought as the small volume limit at fixed values of mass

and temperature. However, we can also interpret it as the low-temperature limit of a massless field; thus the mass plays the role of a IR regulator so that successively the quantity βm must be set to zero.

In the second case, we consider the limit $\beta \to \infty$ for fixed values of the volume V and the mass m, that is the low temperature limit of a massive field.

Small Volumes and Massless Limit

Looking at $\nu \to 0$ as a small volume limit, the result may depend on the shape of P and the way it "shrinks". To avoid this problem, we will suppose for P to shrink down isotropically. This means that for any m-dimensional section of P, having volume V_m, the quantity V_m/β^m must tend to zero when $\nu \to 0$. Note that such condition is automatically satisfied in the low-temperature limit interpretation, as long as P is contained in a compact region. For integrals over regions shrinking down isotropically, we can then use the approximation[6]

$$\int_{\frac{P}{\beta^d}} d^d p f(\vec{p}) = (2\pi)^d \nu f(0) + O(\nu^2). \tag{2.38}$$

To estimate $\mathrm{Tr}K^n$, we must approximate all loop integrals. The simplest one is the tadpole integral:

$$\bigcirc = \int_P d^d p I_\beta(\vec{p} - \vec{p}) \;=\; VI_\beta(0) = \nu \int d^d k e^{-\sqrt{\vec{k}^2 + (\beta m)^2}}.$$

Using (2.38), we see that each integration over P can be simplified giving a factor ν. For example, for the two-point loop we get

$$\bigcirc = \int_{P \times P} d^d p d^d q I_\beta(\vec{p} - \vec{q}) I_\beta(\vec{q} - \vec{p})$$

$$= \frac{1}{(2\pi)^{2d}} \int d^d k d^d k' \int_{\left(\frac{P}{\beta^d}\right)^2} d^d p d^d q e^{-i(\vec{k}-\vec{k}')(\vec{p}-\vec{q})-\left(\sqrt{k^2+(\beta m)^2}+\sqrt{k'^2+(\beta m)^2}\right)}$$

$$= \nu^2 \left(\int d^d k e^{-\sqrt{k^2+(\beta m)^2}} \right)^2 + O(\nu^3).$$

Note that the last integral depends on the temperature only via the fixed product βm, so that the resulting expression is of order ν^2. In the same way we conclude

---

[6]this is the form of the spatial integrals after a substitution $\vec{p} \to \vec{p}/\beta$; the β^d extra factors are reabsorbed by rescaling the momentum variables as $\vec{k} \to \beta\vec{k}$.

that the loop with n full circles is of order v^n. Diagrams with empty circles can be computed using the identity

$$\int_R d^d r = \int d^d x - \int_P d^d p.$$

The integrals over the whole space can be reduced using Eqs. (2.17) and (2.18), whereas each integral over P gives a contribution proportional to v, which is therefore a subleading term with respect to the first one. For example, for the "mixed" two-point loop we get

$$\bigcirc = \int d^d x \int_P d^d p I_\beta(\vec{p} - \vec{x}) I_\beta(\vec{x} - \vec{p}) - \bigcirc$$

$$= \int_P d^d p I_{2\beta}(0) + O(v^2) = v \frac{\Omega_d}{2^d} \int_0^{+\infty} dk k^{d-1} e^{-\sqrt{k^2+(2\beta m)^2}} + O(v^2).$$

In conclusion, to estimate the generic loop integral we can simply remove each empty circle by means of the substitution $\int_R d^d r I_\beta(\vec{p} - \vec{r}) I_{\tilde{\beta}}(\vec{r} - \vec{q}) \to I_{\beta+\tilde{\beta}}(\vec{p} - \vec{q})$, so that the leading order of each diagram is determined by the number of its full balls. By applying this procedure to all terms in (2.26), we find

$$\text{Tr} K = V \sum_{j=1}^{+\infty} I_{j\beta}(0) + O(v^2) = v \Omega_d \sum_{j=1}^{+\infty} \frac{1}{j^d} \int_0^{+\infty} dk k^{d-1} e^{-\sqrt{k^2+(j\beta m)^2}} + O(v^2)$$

$$= v \Omega_d C_d + O(v^2),$$

where C_d is a multiplicative factor that does not depend on v.

The diagrammatic expansion of $\text{Tr} K^n$ contains n full circles in every loop, so that, for the leading term, we get

$$\text{Tr} K^n = \sum_{j_1 \ldots j_n=0}^{+\infty} \int d^d p_1 \ldots d^d p_n I_{j_1\beta}(\vec{p}_1 - \vec{p}_2) \ldots I_{j_n\beta}(\vec{p}_n - \vec{p}_1) + O(v^{n+1})$$

$$= \prod_{l=1}^{n} \left(\sum_{j_l=0}^{+\infty} v I_{j_l\beta}(0) \right) + O(v^{n+1}) = (v \Omega_d C_d)^n + O(v^{n+1}). \tag{2.39}$$

Plugging this result into (2.10) and then into (2.8), we find for the entropy

$$S = -v \Omega_d C_d \ln v + O(v). \tag{2.40}$$

Note that, for $d > 1$, C_d is a finite number. Indeed, it is a function of βm defined by the series

$$C_d = \sum_{j=1}^{+\infty} \frac{1}{j^d} \int_0^{+\infty} dk k^{d-1} e^{-\sqrt{k^2+(j\beta m)^2}}, \tag{2.41}$$

whose terms are positive and bounded by the terms of the converging series $C_d(0)$. Thus

$$C_d(\beta m) \leq C_d(0) = \sum_{j=1}^{+\infty} \frac{1}{j^d} \int_0^{+\infty} dk k^{d-1} e^{-k} = (d-1)! \zeta(d).$$

An IR divergence appears in the one-dimensional massless case. Obviously it could be cured by an IR cut-off that limits the integrations to the external region R. However, a natural regularisation is provided by the mass term. Indeed, we can fix βm at arbitrarily small but positive values, so that the general term in the series (2.41) satisfies

$$\int_0^{+\infty} dk e^{-\sqrt{k^2 + (j\beta m)^2}} = \int_0^{j\beta m} dk e^{-\sqrt{k^2 + (j\beta m)^2}} + \int_{j\beta m}^{+\infty} dk e^{-\sqrt{k^2 + (j\beta m)^2}}$$

$$\leq e^{-j\beta m} j\beta m + \int_{j\beta m}^{+\infty} dk e^{-k} = e^{-j\beta m}(j\beta m + 1),$$

ensuring convergence. For $d > 1$, no divergences occur and in the massless case the entropy (2.40) reads

$$S \sim -X \ln X,$$
$$X = \frac{V}{\beta^d} 2^d \pi^{\frac{d-1}{2}} \Gamma(\frac{d+1}{2}) \zeta(d) \qquad (d > 1, \ \beta m = 0).$$
(2.42)

Again, the above result is finite and no subtractions need to be made.

Low Temperatures for a Massive Field

Let us first consider the one-dimensional case. For $\beta \to \infty$, the two-point function $I_\beta(x)$ behaves as

$$I_\beta(x) \sim \sqrt{\frac{m}{2\pi\beta}} e^{-m\sqrt{\beta^2 + x^2}}.$$

When x falls inside P, the whole expression can be approximated by a constant:

$$I_\beta(p) \sim I_\beta(0) \sim \sqrt{\frac{m}{2\pi\beta}} e^{-m\beta},$$

and each integration over P contributes with a term proportional to the volume, thus we get

$$\bigcirc = \int_{-L}^{L} dp \, I_\beta(p-p) = 2L \, I_\beta(0) \sim 2L \sqrt{\frac{m}{2\pi\beta}} e^{-m\beta},$$

$$\bigcirc (n \text{ points}) \sim \int_{-L}^{L} dp_1 \ldots \int_{-L}^{L} dp_n \left(I_\beta(0) \right)^n \sim \left(2L \sqrt{\frac{m}{2\pi\beta}} e^{-m\beta} \right)^n.$$

It follows that a loop with $n+1$ integrations over P is subleading with respect to one with n integrations and we can use again the usual trick to substitute integrations over R with integrations over the whole space, finding

$$\text{Tr}K \sim L \sum_{n=1}^{+\infty} I_{n\beta}(0) \ .$$

Now, each addend $I_{n\beta}(0)$ is suppressed by a factor $\left(e^{-m\beta}\right)^n$, so that only the first term in the sum is relevant when $\beta \to \infty$. The same argument can be applied to $\text{Tr}K^n$, giving

$$\text{Tr}K^n \sim \left(2L \sqrt{\frac{m}{2\pi\beta}} e^{-m\beta}\right)^n,$$

from which we get the following expression for the entropy

$$S \sim - X \ln X,$$
$$X = 2L \sqrt{\frac{m}{2\pi\beta}} \, e^{-m\beta}. \tag{2.43}$$

This analysis can be easily extended to any dimension. Indeed, the two-point function $I_\beta(p)$ is still suppressed by a factor $e^{-m\beta}$ for $p \in P$, so that all computation work essentially in the same way, providing for the entropy an expression of the form (2.43), where the exponential multiplies a function of β with an at most polynomial growth. We will not enter into more details.

2.5   Interpretation of the Results

In this chapter the problem of computing the entropy of a subsystem confined in a finite region in quantum field theory has been considered. The subsystem under consideration is assumed to be deep inside a much larger system which has reached thermal equilibrium and is therefore described by a thermal Gibbs state. The focus of the present analysis has been the general issue of assigning appropriate quantum degrees of freedom to the considered region. The inside/outside separation is traditionally realised through the usual localisation prescription, which attributes to that region the local relativistic fields therein defined, together with their conjugated momenta. This in fact leads to a tensor product structure (TPS) of the whole Hilbert space. The entropy of a subsystem defined in this way results to be divergent in a way that cannot be renormalised by standard methods from calculations in quantum field theory.

The non-standard regularisation introduced here consists in adopting the NW (Newton-Wigner) localisation scheme to define the TPS of the quantum fields

associated to the division of space into regions. In the NW prescription the vacuum is a product state, thus the divergent, area-dependent contribution to the entropy corresponding to the entanglement across regions never appears in the calculations. The NW operators, unlike the standard local fields, are not relativistically invariant. However, this does not affect the relativistic characterisation of the dynamics. It simply means that localisation, in this picture, is observer-dependent. (After all, a place/region of space is always to be defined on some chosen $t = constant$ hypersurface.) Moreover, Lorentz invariance is naturally broken by thermalisation. The present analysis suggests that the NW prescription for identifying local degrees of freedom should be favoured for a proper treatment of the thermodynamical properties of a quantum field, at least as long as equilibrium states are properly described by Gibbs thermal states. In the next chapter we are going to see that a further justification towards this approach comes from considering limited resolution in describing a state, or coarse-graining. The finiteness of the results obtained in this chapter is by itself a strong indication in this direction: the NW prescription automatically regularises the ultraviolet divergences and directly gives finite results, without the need of additional renormalisation steps or subtractions of infinities. This allowed us to analyse various physical limits.

In the high temperature/large volume limit the calculation gives the expected thermodynamic result: entropy is extensive and, for a massless field, proportional to VT^d, where V is the volume of the region and d the number of spatial dimensions. At leading order in VT^d the results found match the standard calculation of the entropy of a field system with appropriate conditions at its boundary [52]. In other words, in the NW approach, a generic subsystem of a larger thermal system is also approximately thermal and has the same temperature. Again, this seems to suggest that NW localisation is more appropriate for the spatial coarse-graining of microscopic quantities.

At low temperature/small volume, the thermal entropy in our calculation goes to zero but, differently from the standard approach, no unusual subtraction is needed. In the canonical approach [61, 62], thermal entropy is sub-extensive at low temperature, $S_{\text{therm}} \simeq (VT^d)^{(d+1)/d}$, whereas our regularised entropy approaches extensivity from above ($S \simeq -VT^d \ln VT^d$ for small VT^d). Since the calculations in the two approaches follow quite different routes, it is difficult to recognise the technical reason for this discrepancy. Note, however, that at very low temperatures the modes that are typically excited have wavelengths much larger than the size of the subsystem itself. Such modes are not contemplated in the spectrum of the locally defined Hamiltonian, whose lowest non-zero eigenvalues are of order $\sim 1/V^{1/d}$. Those long-wavelength correlations between the internal and the external region dominate in this limit and appear to be the cause of our super-extensive entropy. Note also that $-\epsilon \ln \epsilon$ is the generic asymptotic beha-

viour of the Von Neumann entropy of a density matrix with a parameter ϵ which becomes a pure state in the limit $\epsilon \to 0$.

The "renormalisation" procedure discussed, although unconventional, seems encouraging. The thermodynamical description of quantum field systems is a lively subject, which finds its application beyond the physics of complex systems, especially in contexts involving the interplay between gravitational and quantum effects, as for example in black hole thermodynamics or in the AdS/CFT correspondence. However, many of such interesting applications are affected by the problem of the ultraviolet divergences and, apart from some exceptional cases, many results remain at a qualitative or conjectural level. If holographic entropy bounds (e.g. [72, 73]) and the area-dependent black hole entropy (see [74], and also [75, 76] for entropy renormalisation in that context) are to be taken as meaningful signals of quantum gravity effects, one may want to consistently get rid of the comparable area-dependent contribution that appears already at low energies in flat space. Because of the automatic regularisation, the finiteness of the approach presented seems to provide a powerful and concrete computational method to overcome such technical impasses.

Chapter 3

Classical Entropy in Coarse-Grained Quantum Fields

Summary

The entropy of classical extended systems is typically proportional to the volume occupied by the system. As discussed in the previous chapter, quantum systems show a different behaviour: the entropy of vacuum and thermal states of a sub-region of space is proportional to the area of the region. If classical systems are limiting cases of quantum ones, under which conditions does the transition from area to volume law take place? Here we consider the question within the more general problem of the emergence of classicality in extended continuous variable systems, with particular emphasis on the case of the Klein-Gordon field.

The most general system considered can be represented as a lattice of coupled quantum harmonic oscillators. Two different kinds of measurement imprecision are considered: i) a finite resolution in distinguishing phase-space points of a single oscillator, represented as a *coarse-graining* of the phase space representations of the quantum states, ii) a limited precision in addressing individual lattice sites, resulting in the restriction of possible measurements to measurements of *collective operators*. In the continuum limit, these correspond to i) introducing an error in the measurement of the field observables in specific points of space, ii) introducing a minimal space resolution in distinguishing different points of space. We find that, under a phase space coarse graining larger than the minimal quantum uncertainty, all states become separable and, in the continuum limit, the von Neumann entropy becomes proportional to the volume. The restriction to collective operators, on the other hand, makes all correlations present in vacuum and thermal states vanish, with the resulting effective state being a tensor product of states of the different lattice sites. The entropy obtained from considering collective operators is also proportional to the volume; additionally, it vanishes for small

temperatures, i.e. for the vacuum state, while for large temperatures it converges to the Shannon entropy of a classical system in a thermal state.

An interesting consequence of the result is that it shows how an extended system, in particular a quantum field, can be decomposed into subsystems corresponding to its fine and large structure, the latter representing the degrees of freedom accessible through the measurement of collective operators. The area-scaling correlations are confined in the small-scale subsystem, which has to be traced out when only limited space resolution is possible. In agreement with the results of the previous chapter, it appears that a proper thermodynamic description for quantum fields requires tracing over the appropriate subsystems, which do not correspond to a sharp division of space into subregions.

A manuscript based on the results of this chapter is under preparation.

3.1   Classical Systems as Coarse-Grained Quantum Systems

Quantum mechanics differs radically from classical physics, both in experimental predictions and in the mathematical formulation. The different frameworks in which the two theories are formulated make it difficult to understand if and under what conditions one can be approximated by the other. The coarse-graining approach, outlined in Refs. [18, 19, 20] is promising in this sense, since it provides a way to interpret classical probability distributions as quantum states subject to a large enough experimental error.

In this chapter we are going to see how this approach can be applied to extended quantum systems and, in particular, quantum fields. Consider, as an example, the measurement of a classical electromagnetic field. The electric and magnetic components of the field in a point of space can be measured by observing the response of a charged probe particle located in the chosen position. This measurement is subject to two main sources of imprecision: i) the determination of the field strength (Fig. 3.1a), dependent on how precisely the particle's response can be measured, and ii) the specification of the point at which the measurement is made (Fig. 3.1b), bounded by the limited precision in positioning the probe charge. If we want to map the field in a definite region of space, we have to imagine filling the space with probe charges, the observation will finally consist of a discrete set of points, in each of which a field strength is revealed with some finite accuracy. For a classical field one can think, in principle, to be able to arbitrarily increase the precision of the measurements, for example by using lighter and smaller particles. For large enough precision, however, quantum effects will start
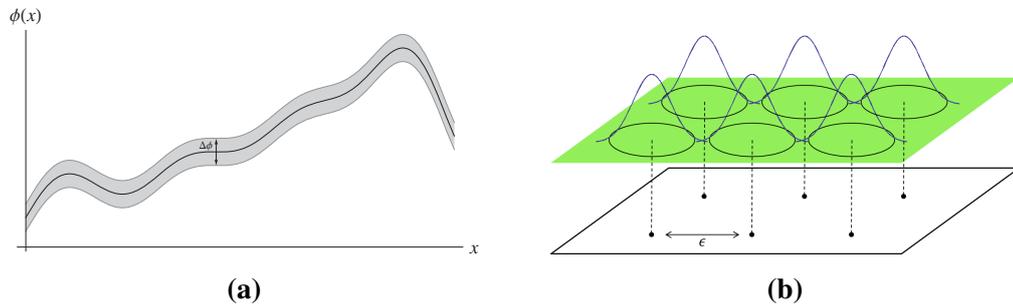
Figure 3.1: Types of imprecisions in the measurement of a field. (a) The value of the field $\phi(x)$ in a point of space x cannot be measured with a precision better than some minimal precision $\Delta\phi$ (and similarly for the conjugate momentum $\pi(x)$). This kind of imprecision is represented as a coarse-graining of phase space variables. (b) The position in space at which a measurement is made can be determined only with limited accuracy, resulting in a minimal distance ϵ between the centres of the sampling regions. This source of error is implemented by restricting the observable degrees of freedom to those accessible via measurement of collective operators.

to become visible.

As already discussed in the previous chapter, the entanglement of the vacuum of quantum fields leads to new interpretational issues absent both in classical physics and non-relativistic quantum mechanics. Of special interest is the divergent, area-scaling entropy associated with a finite region of space: since entropy can be given an operational meaning in terms of the work that can be extracted from a system, how should one interpret its divergent value? Furthermore, the entropy of a classical system can be interpreted as counting the number of microstates compatible with a given probability distribution (macrostate) and is expected to be proportional to the number of degrees of freedom and thus to the volume. If classical states are limiting cases of quantum states, a transition from an area to a volume law should be expected under certain conditions; how does such a transition occur? Such a question extends beyond the realm of quantum field theory, since area laws are known to hold for a large variety of extended systems with local interactions, such as lattices of coupled particles

An important point in the present analysis is the tight connection between entropy, operationally interpreted as a thermodynamic quantity, and the information available about a system[1]. Accordingly, the entropy associated with a system should be linked with the precision achievable when manipulating the system. As outlined above, we are going to model two kinds of measurement imprecision.

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[1]As a simple example, consider a particle in a box. If no information is available about the position of the particle, no work can be extracted from it. However, once position and velocity are known, one can position a piston in the box that will be moved in a desired direction when hit by the particle and produce work. A better knowledge of the particle's state can be used to better position the piston and extract work more efficiently.

The lack of precision in measuring the field's amplitude in a point of space $\vec{x}$ will be modelled as a coarse-graining in the phase space of the corresponding field observables, using methods similar to those introduced in Ref. [19]. The limited resolution in space, on the other hand, corresponds to the measurements of collective operators [78, 79] which, as we are going to see, singles out a subsystem from the global Hilbert space.

3.2   Coarse Graining in Phase Space

3.2.1   Single Particle

We illustrate at first the coarse-graining formalism for the simple case of a single one-dimensional particle. This is formally analogous to a bosonic field measured in a specific point (or in a small region) of space or, more generally, to an arbitrary bosonic field mode. The measurement coarse-graining and the emergence of classicality can be conveniently expressed in the phase-space formalism, which we will now review. (See Ref. [80] for a more extensive introduction.)

Phase Space Formalism   Let $\hat{q}$ and $\hat{p}$ be respectively the position and momentum operators, with canonical commutation relations

$$[\hat{q}, \hat{p}] = i \,. \tag{3.1}$$

We work with dimensionless phase-space variables q, p and units for which $\hbar = c = 1$. An arbitrary operator on the Hilbert space, and in particular a density matrix $\hat{\rho}$, can be fully described by a *characteristic function*. For an arbitrary parameter $s \in [-1, 1]$, this is a function of the real variables r, t defined as

$$\chi_s(r, t) := e^{s \frac{r^2 + t^2}{4}} \operatorname{tr}\left[\hat{\rho} e^{i(r\hat{q} + t\hat{p})} \right]. \tag{3.2}$$

The characteristic functions are the Fourier transforms of *quasiprobability distribution*, phase-space densities which are also faithful representations of quantum states:

$$\rho_s(q, p) := \frac{2}{\pi^2} \int dr dt \chi_s(r, t) e^{-i(rq + tp)}. \tag{3.3}$$

For different values of the parameter s, the definition (3.3) reduces to specific quasiprobability distributions. For $s = 1$, it coincides with the Glauber-Sudarshan P function [81], which provides a diagonal representation of quantum states (or arbitrary operators) on the basis of coherent states:

$$\hat{\rho} = \int d^2\alpha P(\alpha) |\alpha\rangle\langle\alpha| \,, \tag{3.4}$$

where $P(\alpha) \equiv \rho_1(\alpha) = \rho_1(q, p)$, $\alpha := \frac{1}{\sqrt{2}} (q + ip)$, $\int d^2\alpha = \int d\alpha_R d\alpha_I = \frac{1}{2} \int dq dp$ and the coherent states $|\alpha\rangle$ are defined by

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle,$$
$$\hat{a} := \frac{1}{\sqrt{2}} (\hat{q} + i\hat{p}) . \tag{3.5}$$

For $s = -1$, (3.3) corresponds to the definition of the Q function [82]

$$\rho_{-1}(\alpha) \equiv Q(\alpha) := \frac{1}{\pi} \langle \alpha|\hat{\rho}|\alpha \rangle , \tag{3.6}$$

which has the property of being always positive. Finally, for $s = 0$ the definition (3.3) reduces to the Wigner function [83]

$$\rho_0(q, p) \equiv \mathcal{W}_{\hat{\rho}}(q, p) := \frac{1}{\pi} \int dy e^{-2ipy} \langle q - y|\hat{\rho}|q + y \rangle . \tag{3.7}$$

One of the properties of the Wigner function is that expectation values can be calculated as phase-space averages: given a state $\hat{\rho}$ and an observable $\hat{O}$, together with their respective Wigner functions $\mathcal{W}_{\hat{\rho}}(q, p)$ and $\mathcal{W}_{\hat{O}}(q, p)$, the expectation value of the observable $\hat{O}$ given the state $\hat{\rho}$ is given by

$$\langle \hat{O} \rangle_{\hat{\rho}} := \mathrm{Tr}\left(\hat{\rho}\hat{O}\right) = 2\pi \int dq dp \mathcal{W}_{\hat{\rho}}(q, p) \mathcal{W}_{\hat{O}}(q, p). \tag{3.8}$$

Often, the definition used for the Wigner representation of an observable $\hat{O}$ differs by a multiplicative factor from (3.7), which is only used for states. Here we do not make such a distinction and use (3.7) for arbitrary operators, this is the reason for the 2π factor in front of the integral in Eq. (3.8).

A useful property of the quasiprobability distributions (3.3) is that they can all be derived as Gaussian convolutions of the P function:

$$\rho_s(q, p) = \frac{1}{\pi(s-1)} \int dq' dp' e^{\frac{1}{s-1}[(q-q')^2+(p-p')^2]} P(q', p'), \qquad -1 \leq s < 1. \tag{3.9}$$

Note that, despite some similarities, the quasiprobability distributions (3.3), (3.4), (3.6), (3.7) cannot generally be understood as classical probability distributions on phase space. As we are about to see, such an interpretation becomes possible when a sufficiently large experimental error is introduced.

Coarse-Grained Observables and States In classical physics, one assumes that it is possible to measure different points of phase space independently and with arbitrary precision. Observables are functions on phase space $O(q, p)$ and states are positive probability distributions $\rho(q, p)$. The expectation value of an

observable $O(q, p)$ given a state $\rho(q, p)$ can be calculated with the phase-space integral $\int dq dp \rho(q, p) O(q, p)$, analogous to (3.8). A classical probability distribution can be arbitrarily concentrated, with $\rho(q, p) = \delta(q - q_0)\delta(p - p_0)$ representing a pure state. As it is well-known, this picture breaks down in quantum mechanics due to the Heisenberg uncertainty principle, which has consequences on measurements at the scale of phase space areas of the order of the Planck constant $\hbar$. This suggests that, given an experimental error larger than $\hbar$, quantum properties cannot be observed and quantum systems effectively appear as classical. It is possible to formalise such an intuition thanks to the notion of coarse graining of quasiprobability distributions.

Consider an experimental situation in which a quantum particle is observed, but only a limited resolution in phase space is available. This means that, for example, if one tries to perform a projective measurement on a coherent state $|\alpha\rangle$, a different state $|\beta\rangle$ might be addressed instead with some probability[2]. Assuming that the probability of measuring β instead of α is a Gaussian with variance σ^2, a measurement with outcome α corresponds in fact to the measurement of a POVM (projective operator valued measure) element

$$\Pi^\sigma(\alpha) := \frac{1}{\pi\sigma^2} \int d^2\beta\, e^{-\frac{|\alpha-\beta|^2}{\sigma^2}} |\beta\rangle\langle\beta|. \tag{3.10}$$

The variance σ^2 is the *coarse-graining parameter* and it quantifies the minimal measurement error, i.e. the typical distance below which points in phase space cannot be distinguished (since we use $\hbar = c = 1$, σ^2 is measured in units of $\hbar$).

An arbitrary quantum observable $\hat{O}$ can be expanded on a basis of coherent states using its P representation as in Eq. (3.4). This can be thought of as defining the *fine-grained* observable, only measurable with arbitrary phase space resolution. If a minimal error of magnitude σ is present, the best approximation to $\hat{O}$ that can be measured is obtained by formally substituting the coherent states in (3.4) with the POVM elements (3.10). We define therefore the *coarse-grained observable* as

$$\hat{O}^\sigma := \int d^2\alpha\, O_1(\alpha)\Pi^\sigma(\alpha), \tag{3.11}$$

where the function $O_1(\alpha)$ is defined as in (3.3). If we insert Eq. (3.10) in Eq. (3.11) and perform a variable change, we can write the coarse-grained observable again in the form (3.4) as

$$\hat{O}^\sigma = \int d^2\alpha\, O_1^\sigma(\alpha)|\alpha\rangle\langle\alpha|,$$

---

[2]Note that, although different coherent states are not orthogonal, having infinite precision would in principle allow performing a projective measurement on a single coherent state. For example, one could perform a measurement on the projectors $\{|\alpha\rangle\langle\alpha|, \mathbb{1} - |\alpha\rangle\langle\alpha|\}$. A lack in experimental precision prevents identifying the state $|\alpha\rangle$ with arbitrary accuracy and thus performing such a projective measurement.

where the coarse-grained *P* function is defined as the convolution of the original one with a Gaussian:

$$O_1^\sigma(\alpha) := \frac{1}{\pi\sigma^2} \int d^2\beta \, e^{-\frac{|\alpha-\beta|^2}{\sigma^2}} O_1(\beta) \tag{3.12}$$

$$\equiv \frac{1}{2\pi\sigma^2} \int dq' dp' \, e^{-\frac{(q-q')^2+(p-p')^2}{2\sigma^2}} O_1(q',p') \,.$$

The same Gaussian convolution (3.12) can be applied to an arbitrary phase space representation (3.3) of an observable $\hat{O}$, defining the coarse-grained function $(O_s)^\sigma(q,p)$. This is in turn equal to the *s* representation of the coarse-grained operator (3.11), i.e. $(O_s)^\sigma(q,p) = (O^\sigma)_s(q,p)$. To see this, it is sufficient to note that, using the relation (3.9), $(O_s)^\sigma(q,p)$ can be written as a double Gaussian convolution of the *P* representation $O_1(q,p)$. The final result is a consequence of the commutativity of Gaussian convolution, which is apparent from the formula

$$\frac{\sqrt{ab}}{\pi} \int dy e^{-a(q-y)^2} e^{-by^2} = \sqrt{\frac{c}{\pi}} e^{-cq^2}, \quad \frac{1}{c} = \frac{1}{a} + \frac{1}{b} \,. \tag{3.13}$$

In simple words, the phase space coarse graining $\hat{O}^\sigma$ of an observable $\hat{O}$ can be defined by convoluting an arbitrary phase space representation of it with a Gaussian function.

It is convenient to represent the imprecise measurements at the level of states: we want a map $\hat{\rho} \to \hat{\rho}^\sigma$ such that the coarse-grained measurements on arbitrary states can be written as arbitrary measurements on coarse-grained states, namely

$$\langle \hat{O}^\sigma \rangle := \mathrm{Tr}\left(\hat{\rho}\hat{O}^\sigma\right) = \mathrm{Tr}\left(\hat{\rho}^\sigma\hat{O}\right) \equiv \langle \hat{O} \rangle^\sigma. \tag{3.14}$$

We can see that $\hat{\rho}^\sigma$ can be defined by a Gaussian convolution of one of the quasiprobability distributions (3.3) associated with $\hat{\rho}$. The expectation value (3.14) can be evaluated using the Wigner representations of $\hat{\rho}$ and $\hat{O}^\sigma$ through (3.8). It is then straightforward to verify that

$$\int dq dp \, \mathcal{W}_{\hat{O}^\sigma}(q,p) \mathcal{W}_{\hat{\rho}}(q,p) = \int dq dp \, \mathcal{W}_{\hat{O}}^\sigma(q,p) \mathcal{W}_{\hat{\rho}}(q,p)$$

$$= \int dq dp \, \mathcal{W}_{\hat{O}}(q,p) \mathcal{W}_{\hat{\rho}}^\sigma(q,p) \equiv \int dq dp \, \mathcal{W}_{\hat{O}}(q,p) \mathcal{W}_{\hat{\rho}^\sigma}(q,p),$$

where

$$\mathcal{W}_{\hat{\rho}^\sigma}(q,p) := \frac{1}{2\pi\sigma^2} \int dq' dp' \, e^{-\frac{(q-q')^2+(p-p')^2}{2\sigma^2}} \mathcal{W}_{\hat{\rho}}(q',p') \tag{3.15}$$

defines the Wigner function of the coarse-grained state $\hat{\rho}^\sigma$ and $\mathcal{W}^\sigma$ always represents the convolution of the function $\mathcal{W}$ with a Gaussian of variance σ^2, as in Eq. (3.12).

To summarise, the effect of an imprecision σ in distinguishing points in phase space can be represented as a coarse graining of the measured states. The coarse-grained state is defined as a Gaussian convolution of the Wigner function, Eq. (3.15), or of any other quasiprobability distribution (3.3) with arbitrary parameter $-1 \leq s \leq 1$. Note that a classical probability distribution on phase space would be smeared in the same way as (3.15) under the assumption that, in all measurements, an independent, isotropic and homogeneous error of size σ is introduced.

3.2.2   Many Particles

The above definitions and formalism can be directly extended to the case of n distinguishable particles. These may represent the positions of ions within a lattice or a discretised bosonic field. The conjugate position and momentum operators, together with their commutation relations, can be compactly expressed as

$$\hat{\xi} \equiv (\hat{q}_1, \ldots, \hat{q}_n, \hat{p}_1, \ldots, \hat{p}_n), \quad [\hat{\xi}_j, \hat{\xi}_l] = i(\delta_{j+n\,l} - \delta_{j\,l+n}).$$

The phase space formalism can be extended in a straightforward way to the n-particle case. The defining equations for the P, Q and Wigner function are respectively

$$\hat{\rho} = \int d^{2n}\alpha\, P(\vec{\alpha})|\vec{\alpha}\rangle\langle\vec{\alpha}|, \tag{3.16}$$

$$Q(\vec{\alpha}) := \frac{1}{\pi^n}\langle\vec{\alpha}|\hat{\rho}|\vec{\alpha}\rangle, \tag{3.17}$$

$$\mathcal{W}(\vec{q}, \vec{p}) := \frac{1}{\pi^n}\int d^n y\, e^{-2i\vec{p}\cdot\vec{y}}\langle\vec{q} - \vec{y}|\hat{\rho}|\vec{q} + \vec{y}\rangle, \tag{3.18}$$

where $|\vec{\alpha}\rangle \equiv |\alpha_1\rangle\otimes\cdots\otimes|\alpha_n\rangle$ is a tensor product of coherent states, $\alpha_j = \frac{1}{\sqrt{2}}\left(q_j + ip_j\right)$ and $\int d^{2n}\alpha = \int d^n\alpha_R d^n\alpha_I = \frac{1}{2^n}\int d^n q\, d^n p$. The relations between the different quasiprobability distributions still hold. In particular, (3.9) becomes

$$\rho_s(\xi) = \int d^{2n}\xi'\, G_A(\xi - \xi')P(\xi'), \qquad A = \frac{2}{s-1}\mathbb{1}_{2n}, \qquad -1 \leq s < 1, \tag{3.19}$$

where $\rho_s(\xi)$ is the quasiprobability distribution with parameter s associated with $\hat{\rho}$ and we introduced the notation

$$G_A(\vec{x}) := \frac{\sqrt{\det A}}{(2\pi)^{\frac{n}{2}}}e^{-\frac{1}{2}\sum_{ij} x_i A_{ij} x_j} \tag{3.20}$$

for an n-dimensional Gaussian, with A an arbitrary positive definite, symmetric bilinear form on $\mathbb{R}^n$. Useful properties, that have a simple expression in this notation, include

$$\int d^n y\, G_A(\vec{x} - \vec{y})G_B(\vec{y}) = G_C(\vec{x}), \qquad C^{-1} = A^{-1} + B^{-1}, \qquad (3.21)$$

$$G_A(a\vec{x}) = \frac{1}{a^n}G_{a^2 A}(\vec{x}), \qquad\qquad a \in \mathbb{R}^n, \qquad (3.22)$$

$$G_A(\vec{q})G_B(\vec{p}) = G_{A \oplus B}(\vec{q}, \vec{p}), \qquad\qquad (3.23)$$

$$G_A(\vec{x}) \to \delta(\vec{x}) \qquad \text{for} \quad \left\| A^{-1} \right\| \to 0, \qquad (3.24)$$

$$\int \frac{d^n x}{(2\pi)^{n/2}}\, G_A(\vec{x})e^{i\vec{k}\vec{x}} = \sqrt{\det A}\; G_{A^{-1}}(\vec{k}), \qquad\qquad (3.25)$$

$$\int d^n x\, G_A(\vec{x})x_j x_l = (A^{-1})_{jl}. \qquad\qquad (3.26)$$

The coarse graining $\hat{\rho}^\sigma$ of a state $\hat{\rho}$ is defined by

$$\rho_s^\sigma(\xi) := \int d^{2n}\xi'\, G_A(\xi - \xi')\rho_s(\xi'), \qquad\qquad (3.27)$$

with $A = \frac{1}{\sigma^2}\mathbb{1}_{2n}$. (As before, the specific value of s is unimportant, since (3.27) defines the same state $\hat{\rho}^\sigma$ for all $-1 \le s \le 1$.) Notice that expression (3.27) can be immediately generalised to the case where q_j and p_j are subject to different minimal errors Δq and Δp, respectively, simply by setting $A = \frac{\mathbb{1}_n}{\Delta q^2} \oplus \frac{\mathbb{1}_n}{\Delta p^2}$.

The fundamental property of sufficiently large coarse graining in phase space is that it makes quantum correlations unobservable. In fact, the following theorem holds:

Theorem. *The coarse-graining with parameter $\sigma^2 \ge 1$ of any state yields a separable state.*

To prove this, compare (3.19) with (3.27) and notice that the Q function of a state $\hat{\rho}$ coincides with the P function of the coarse-grained state $\hat{\rho}^\sigma$, $\rho_{-1}(\xi) = \rho_1^\sigma(\xi)$, with $\sigma^2 = 1$. Since the Q function is always positive, this means that the P function of a coarse-grained state with $\sigma^2 = 1$ is also positive. Using the expansion (3.16), $\hat{\rho}^\sigma$ can be written as a mixture of products of coherent states, thus it is a separable state. Finally, using (3.21), we can write a coarse-grained P function with $\sigma^2 > 1$ as $P^\sigma(\xi) = \int d^{2n}\xi' G_A(\xi - \xi')P^1(\xi')$, with $A = \frac{1}{\sigma^2-1}\mathbb{1}_{2n}$. Since the Gaussian convolution of a positive function is also positive, the positivity of $P^\sigma(\xi)$ and hence the separability of $\hat{\rho}^\sigma$ for an arbitrary $\sigma^2 \ge 1$ follows.

3.2.3 Coarse-Grained Harmonic Systems

Consider a cubic d-dimensional lattice with N sites per side and one quantum harmonic oscillator per site, for a total of $n = N^d$ oscillators, Fig. 3.2. Each site is labeled by a discrete vector $\vec{j} = (j_1, j_2, \ldots, j_d)$, with every component in the range $j_s = 1, \ldots, N$.
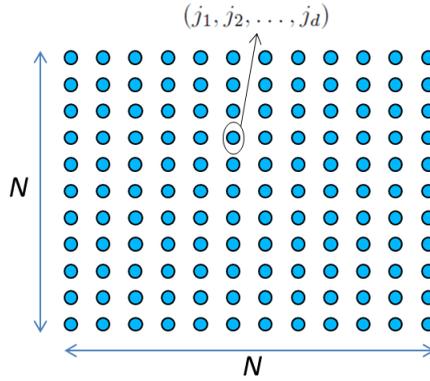
Figure 3.2: A d-dimensional cubic lattice with N sites per side. Each site is identified by a set of integers $\vec{j} = (j_1, j_2, \ldots, j_d)$, each running between 1 and N, and corresponds to the equilibrium position of a quantum harmonic oscillator with Hilbert space $\mathcal{H}_{\vec{j}}$. The full system has thus Hilbert space $\mathcal{H} = \bigotimes_{\vec{j}} \mathcal{H}_{\vec{j}}$. In the picture, $d = 2$.

We assume that the system is in a generic Gaussian state, i.e. a state with a Gaussian Wigner function (or, equivalently, a Gaussian characteristic function), with the additional property $\langle \hat{q}_{\vec{j}} \rangle = \langle \hat{p}_{\vec{l}} \rangle = \langle \hat{q}_{\vec{j}} \hat{p}_{\vec{l}} \rangle = 0$ (this property is not necessary for the argument, but it simplifies the notation and is satisfied for the states under consideration). Such a state is fully characterised by the two-point correlation matrices

$$
\begin{aligned}
g_{\vec{j}\vec{l}} &:= \langle \hat{q}_{\vec{j}} \hat{q}_{\vec{l}} \rangle = \mathrm{Tr}\left[\hat{\rho}\, \hat{q}_{\vec{j}} \hat{q}_{\vec{l}} \right], \\
h_{\vec{j}\vec{l}} &:= \langle \hat{p}_{\vec{j}} \hat{p}_{\vec{l}} \rangle = \mathrm{Tr}\left[\hat{\rho} \hat{p}_{\vec{j}} \hat{p}_{\vec{l}} \right]
\end{aligned}
\tag{3.28}
$$

and the Wigner function reads

$$
\mathcal{W}(\vec{q}, \vec{p}) = G_{g^{-1} \oplus h^{-1}}(\vec{q}, \vec{p}),
\tag{3.29}
$$

as can be directly verified by calculating (3.28) via (3.8) and using (3.26). Additionally, we restrict to the case of translationally invariant states, i.e. such that $g_{\vec{j}\vec{j}+\vec{d}} = g_{\vec{l}\vec{l}+\vec{d}}, h_{\vec{j}\vec{j}+\vec{d}} = h_{\vec{l}\vec{l}+\vec{d}}$ for arbitrary $\vec{j}, \vec{l}, \vec{d}$. In this case, the correlation matrices

are diagonalised by a discrete Fourier transform[3]:

$$
\begin{aligned}
g_{\vec{j}\vec{l}} &= \frac{1}{N^d} \sum_{\vec{k}} g_{\vec{k}} e^{i\frac{2\pi}{N}\vec{k}\cdot(\vec{j}-\vec{l})}, \\
h_{\vec{j}\vec{l}} &= \frac{1}{N^d} \sum_{\vec{k}} h_{\vec{k}} e^{i\frac{2\pi}{N}\vec{k}\cdot(\vec{j}-\vec{l})},
\end{aligned}
\tag{3.30}
$$

where, for brevity, we write $\sum_{\vec{k}} \equiv \sum_{k_1=1}^{N} \cdots \sum_{k_d=1}^{N}$. Ground and thermal states of a harmonic system (such as a non-interacting bosonic field) typically satisfy all the conditions above.

We consider now a situation in which measurements of each $\hat{q}_{\vec{j}}$, $\hat{p}_{\vec{j}}$ are limited by some minimal precision Δq, Δp, respectively. We can calculate the corresponding coarse graining of the Wigner function (3.29) by applying the rule (3.21) for Gaussian convolution, with $A^{-1} = g \oplus h$ and $B^{-1} = \left(\Delta q^2 \, \mathbb{1}_n\right) \oplus \left(\Delta p^2 \, \mathbb{1}_n\right)$. The resulting state is again Gaussian and is characterised by the coarse-grained two-point correlation matrices

$$
\begin{aligned}
g^{\sigma} &= g + \Delta q^2 \, \mathbb{1}_{N^d} = g + \frac{\sigma^2}{m^2} \, \mathbb{1}_{N^d}, \\
h^{\sigma} &= h + \Delta p^2 \, \mathbb{1}_{N^d} = h + m^2 \sigma^2 \, \mathbb{1}_{N^d},
\end{aligned}
\tag{3.31}
$$

where $m := \sqrt{\frac{\Delta p}{\Delta q}}$ is the parameter that specifies the ratio between the errors in the conjugate observables $\hat{q}_{\vec{j}}$, $\hat{p}_{\vec{j}}$ and is assumed to be fixed, while $\sigma := \sqrt{\Delta q \Delta p}$ is the coarse-graining parameter, with $\sigma^2 \gg \hbar$ defining the classical limit. Note that the matrices (3.31) are still diagonal in the Fourier basis: the coarse graining has the effect of adding a constant to their eigenvalues $g_{\vec{k}} \to g_{\vec{k}} + \frac{\sigma^2}{m}$, $h_{\vec{k}} \to h_{\vec{k}} + m\sigma^2$.

The Von Neumann entropy of a Gaussian state was first calculated in Ref. [55]; it is possible to express it as function of the matrix $C := \sqrt{g \cdot h}$ (see, e.g., Ref. [59]):

$$
\begin{aligned}
S &= \mathrm{Tr}\left[s\left(C\right)\right], \\
s(x) &:= \left(x + \frac{1}{2}\right) \log\left(x + \frac{1}{2}\right) - \left(x - \frac{1}{2}\right) \log\left(x - \frac{1}{2}\right).
\end{aligned}
\tag{3.32}
$$

Note that one always has $C \geq \frac{1}{2}$ (generalised Heisenberg uncertainty relations), which means $g_{\vec{k}} h_{\vec{k}} \geq \frac{1}{4}$. When applied to a coarse-grained, translationally-invariant state, the expression (3.32) gives $S^{\sigma} = \sum_{\vec{k}} s\left(c_{\vec{k}}^{\sigma}\right)$, with $c_{\vec{k}}^{\sigma} = \sqrt{\left(g_{\vec{k}} + \frac{\sigma^2}{m^2}\right)\left(h_{\vec{k}} + m^2\sigma^2\right)}$. For any $\sigma > 0$ we have $c_{\vec{k}}^{\sigma} > \frac{1}{2} + \delta$ for some $\delta > 0$ independent of $\vec{k}$. This gives

---

[3]The discrete Fourier transform of a matrix $A_{\vec{j}\vec{l}}$ is $\widetilde{A}_{\vec{k}\vec{k}'} = \frac{1}{N^d} \sum_{\vec{j}\vec{l}} e^{i\frac{2\pi}{N}\left(\vec{j}\cdot\vec{k}-\vec{l}\cdot\vec{k}'\right)} A_{\vec{j}\vec{l}}$. If A is translationally invariant, i.e. $A_{\vec{j}\vec{j}+\vec{d}} = A_{\vec{d}}$ for all $\vec{j}$, then $\widetilde{A}_{\vec{k}\vec{k}'} = \frac{1}{N^d} \sum_{\vec{j}\vec{d}} e^{i\frac{2\pi}{N}\vec{j}\cdot\left(\vec{k}-\vec{k}'\right)} e^{i\frac{2\pi}{N}\vec{d}\cdot\vec{k}'} A_{\vec{j}\vec{j}+\vec{d}} = \delta_{\vec{k}\vec{k}'} \sum_{\vec{d}} e^{i\frac{2\pi}{N}\vec{d}\cdot\vec{k}'} A_{\vec{d}}$.

$S > N^d s(\frac{1}{2} + \delta)$, which means that, for N sufficiently large[4], the Von Neumann entropy scales as the total number of lattice points, i.e. as the volume of the system.

It is simple to prove that, if the entropy of the whole system scales as the number of lattice sites, so does the entropy of any sub-region. Consider first the half-space case: divide the lattice in two identical sub-lattices A and B, containing $\frac{N^d}{2}$ sites each. For symmetry reasons, the reduced states over the two half-chains have the same entropy, $S_A = S_B$. We also have that the entropy of all the space is bounded by the sum of the two reduced entropies, $S_{AB} \leq S_A + S_B$, from which follows $S_A = S_B \geq \frac{1}{2} S_{AB} \propto \frac{N^d}{2}$. The same argument can be used for divisions of the lattice into an arbitrary number of equal sub-lattices; thus, for every subsystems containing l sites, we have a bound $S_l \geq bl$ for some positive constant b. We have thus shown that a coarse-graining of a translationally invariant state of the form (3.29) results in a volume law for the entropy of an arbitrary sub-lattice. Note that, in the limit $N \to \infty$ (in particular in the continuum limit defining a quantum field), any finite, no matter how small, coarse-graining, gives a volume scaling for the entropy.

3.3   Collective Field Operators

Quantum fields, unlike the systems considered so far, possess infinitely many degrees of freedom. However, in practical situations it is impossible to resolve points in space with arbitrary precision: a measurement of a field must necessarily consist of a sample of a finite number of points, where each point corresponds in fact to a finite region of space. In this section we consider the effects of such a limited space resolution on the correlations and entropy of quantum fields.

3.3.1   General Profiles

We consider a bosonic, scalar field in d space dimensions, with conjugate operators $\hat{\phi}(\vec{x})$, $\hat{\pi}(\vec{x})$ satisfying the canonical commutation relations

$$[\hat{\phi}(\vec{x}), \hat{\pi}(\vec{y})] = i\,\delta(\vec{x} - \vec{y}). \tag{3.33}$$

The d-dimensional space is sampled in a discrete set of points $\vec{j} \in \mathbb{Z}^d$. Each discrete point represents the position of the centre of an idealised detector described by a real, positive function $f_{\vec{j}}(\vec{x})$ (the *detection profile*), which determines how much the field in the point $\vec{x}$ contributes to the measurement outcome of the $\vec{j}$-th

---

[4]The entropy might have other contributions proportional to different powers of N, such as an area term of the form cN^{d-1}, with c is a constant of order one. However, the volume scaling overtakes as soon as $N > \frac{c}{s(\frac{1}{2}+\delta)}$.

detector. Assuming that the detection profile does not depend on the observable measured, the algebra of accessible observables is generated by the collective field operators

$$
\begin{aligned}
\hat{q}_{\vec{j}} &:= \int d^d x f_{\vec{j}}(\vec{x}) \hat{\phi}(\vec{x}), \\
\hat{p}_{\vec{j}} &:= \int d^d x f_{\vec{j}}(\vec{x}) \hat{\pi}(\vec{x}).
\end{aligned}
\tag{3.34}
$$

If the functioning of the detector does not depend on its position, a single profile can be used for all points in space:

$$
f_{\vec{j}}(\vec{x}) \equiv f(\vec{x} - \vec{j}D),
\tag{3.35}
$$

where D is the distance between the sampling points. The collective operators (3.34) satisfy canonical commutation relations if $\int d^d x f_{\vec{j}}(\vec{x}) f_{\vec{l}}(\vec{x}) = \delta_{\vec{j}\vec{l}}$. The vanishing of the commutator between operators in different points guarantees that they define different subsystems [65]. The collective operators thus define a discrete harmonic lattice, analogous to the system considered in the previous section, which represents a subsystem of the continuous filed. In this picture, the whole system factorises in two subsystems

$$
\mathcal{H} = \mathcal{H}_{coll} \otimes \mathcal{H}_{fine},
\tag{3.36}
$$

where $\mathcal{H}_{coll} = \bigotimes_{\vec{j}} \mathcal{H}_{\vec{j}}$ is the subsystem generated by the algebra of collective operators, each $\mathcal{H}_{\vec{j}}$ being the Hilbert space identified by the conjugate operators $\hat{q}_{\vec{j}}$, $\hat{p}_{\vec{j}}$, while $\mathcal{H}_{fine}$ represents the fine-grained, unobservable degrees of freedom. We will assume, for the general discussion, that the detection profile f has a compact support contained in a region of size D (thus different profiles do not overlap).

As for the discrete case, we consider a Gaussian, translationally invariant state with $\langle \hat{\phi}(\vec{x}) \rangle = \langle \hat{\pi}(\vec{x}) \rangle = \langle \hat{\phi}(\vec{x})\hat{\pi}(\vec{y}) \rangle = 0$, completely specified by the two-point correlation functions

$$
\begin{aligned}
\langle \hat{\phi}(\vec{x})\hat{\phi}(\vec{y}) \rangle &= \int \frac{d^d k}{(2\pi)^d} e^{i\vec{k}\cdot(\vec{x}-\vec{y})} g(\vec{k}), \\
\langle \hat{\pi}(\vec{x})\hat{\pi}(\vec{y}) \rangle &= \int \frac{d^d k}{(2\pi)^d} e^{i\vec{k}\cdot(\vec{x}-\vec{y})} h(\vec{k}),
\end{aligned}
\tag{3.37}
$$

analogously to (3.30). The effective state, as it appears by measuring the observables generated by the collective operators (3.34), is obtained from the original one by tracing over the subsystem $\mathcal{H}_{fine}$. Since tracing is a linear operation, the resulting state is again Gaussian. The corresponding correlation matrices, defined as in Eq. (3.28), are given by

$$
\begin{aligned}
g_{\vec{j}\vec{l}} &= \int d^d x d^d y f_{\vec{j}}(\vec{x}) f_{\vec{l}}(\vec{y}) \langle \hat{\phi}(\vec{x})\hat{\phi}(\vec{y}) \rangle = \int d^d k \tilde{f}_{\vec{j}}(\vec{k}) \tilde{f}_{\vec{l}}^*(\vec{k}) g(\vec{k}), \\
h_{\vec{j}\vec{l}} &= \int d^d x d^d y f_{\vec{j}}(\vec{x}) f_{\vec{l}}(\vec{y}) \langle \hat{\pi}(\vec{x})\hat{\pi}(\vec{y}) \rangle = \int d^d k \tilde{f}_{\vec{j}}(\vec{k}) \tilde{f}_{\vec{l}}^*(\vec{k}) h(\vec{k}),
\end{aligned}
\tag{3.38}
$$

where $\tilde{f}_{\vec{j}}(\vec{k}) := \int \frac{d^d k}{(2\pi)^{d/2}} f_{\vec{j}}(\vec{x}) e^{i\vec{k}\cdot\vec{x}}$ is the Fourier transform of the detection profile. Using (3.35), we have $\tilde{f}_{\vec{j}}(\vec{k}) = \tilde{f}(\vec{k}) e^{i\vec{k}\cdot\vec{j}D}$ and the correlation matrices can be written as

$$
\begin{aligned}
g_{\vec{j}\vec{l}} &= \int d^d k |\tilde{f}(\vec{k})|^2 e^{iD\vec{k}\cdot(\vec{j}-\vec{l})} g(\vec{k}) = \left(\frac{D}{2\pi}\right)^d \int_{[0,\frac{2\pi}{D}]^d} d^d k \; e^{iD\vec{k}\cdot(\vec{j}-\vec{l})} g_D(\vec{k}), \\
h_{\vec{j}\vec{l}} &= \int d^d k |\tilde{f}(\vec{k})|^2 e^{iD\vec{k}\cdot(\vec{j}-\vec{l})} h(\vec{k}) = \left(\frac{D}{2\pi}\right)^d \int_{[0,\frac{2\pi}{D}]^d} d^d k \; e^{iD\vec{k}\cdot(\vec{j}-\vec{l})} h_D(\vec{k}),
\end{aligned}
\tag{3.39}
$$

where

$$
\begin{aligned}
g_D(\vec{k}) &:= \left(\frac{2\pi}{D}\right)^d \sum_{\vec{l}\in\mathbb{Z}^d} |\tilde{f}(\vec{k} + \frac{2\pi}{D}\vec{l})|^2 g(\vec{k} + \frac{2\pi}{D}\vec{l}), \\
h_D(\vec{k}) &:= \left(\frac{2\pi}{D}\right)^d \sum_{\vec{l}\in\mathbb{Z}^d} |\tilde{f}(\vec{k} + \frac{2\pi}{D}\vec{l})|^2 h(\vec{k} + \frac{2\pi}{D}\vec{l})
\end{aligned}
\tag{3.40}
$$

are the eigenvalues of the correlation matrices. Note that the momentum integrals are now bounded by the finite value $\frac{2\pi}{D}$, which therefore plays the role of an ultraviolet regulator.

The von Neumann entropy of the reduced state can be evaluated using Eq. (3.32). The matrix $(C^2)_{\vec{j}\vec{l}} = \sum_{\vec{i}} g_{\vec{j}\vec{i}} h_{\vec{i}\vec{l}}$ is obtained by multiplying the diagonal elements (3.40) of the correlation matrices, as they are all diagonal in the same basis. We find

$$
\begin{aligned}
C_{\vec{j}\vec{l}} &= \left(\frac{D}{2\pi}\right)^d \int_{[0,\frac{2\pi}{D}]^d} d^d k \; e^{iD\vec{k}\cdot(\vec{j}-\vec{l})} c_D(\vec{k}), \\
c_D(\vec{k}) &:= \sqrt{g_D(\vec{k}) h_D(\vec{k})}.
\end{aligned}
\tag{3.41}
$$

The entropy is finally given by

$$
S_D = \sum_{\vec{j}} s(C)_{\vec{j}\vec{j}} = \left(\sum_{\vec{j}} 1\right) \left(\frac{D}{2\pi}\right)^d \int_{[0,\frac{2\pi}{D}]^d} d^d k \; s(c_D(\vec{k})),
\tag{3.42}
$$

where s is the function defined in (3.32). The expression (3.39), with the infinite sum $\sum_{\vec{j}} 1$, is only divergent if we consider the fields (3.33) extended to all $\mathbb{R}^d$. If we restrict the fields to a finite region of size L, the indices $j_1,\ldots,j_d$ of the matrices (3.39) run from 1 to $N = \frac{L}{D}$, so that $\sum_{\vec{j}} 1 = N^d = \frac{L^d}{D^d}$.

For systems with an energy gap (i.e. systems, such as massive fields, where the energy difference between ground and first excited state does not vanish in the continuum limit), the correlation functions typically decay exponentially at distances larger than some correlation length λ [84]. In such a case, the space integrals in Eq. (3.39), defining the correlation matrices of the collective operators, have to be evaluated only for $\|\vec{x} - \vec{y}\| \lesssim \lambda$. Since in this region, for $D \gg \lambda$, the integrand $f_{\vec{j}}(\vec{x}) f_{\vec{l}}(\vec{y}) = f(\vec{x} - \vec{j}D) f(\vec{y} - \vec{l}D)$ would vanish unless $\vec{j} = \vec{l}$. In this case

one gets

$$g_{\vec{j}\vec{l}} \sim g_D \delta_{\vec{j}\vec{l}}, \qquad\qquad h_{\vec{j}\vec{l}} \sim g_D \delta_{\vec{j}\vec{l}}, \tag{3.43}$$

$$g_D := \int d^d k |\tilde{f}(\vec{k})|^2 g(\vec{k}), \qquad\qquad h_D := \int d^d k |\tilde{f}(\vec{k})|^2 h(\vec{k}). \tag{3.44}$$

In other words, if the resolution D in space is larger than the correlation length of the system, no correlations are observable between collective operators at different points. The state can therefore be written as a product state over the different points of space[5], $\rho = \bigotimes_{\vec{j}} \rho_{\vec{j}}$. Consequently, the von Neumann entropy is additive and proportional to the volume:

$$S = -\sum_{\vec{j}} \mathrm{Tr} \rho_{\vec{j}} \ln \rho_{\vec{j}} = \left(\frac{L}{D}\right)^d s(\sqrt{g_D h_D}). \tag{3.45}$$

The same result holds also for any subregion, because the reduced state in a subregion A is simply $\rho_A = \bigotimes_{j \in A} \rho_j$.

3.3.2 Gaussian Profiles

It is possible to prove the vanishing of the correlations, and the result (3.45), for the specific case of Gaussian detection profiles:

$$f_\epsilon(\vec{x}) := \frac{1}{(2\pi\epsilon^2)^{d/4}} e^{-\frac{\|\vec{x}\|^2}{4\epsilon^2}} = \left(8\pi\epsilon^2\right)^{d/4} G_{\frac{1}{2\epsilon^2}}(\vec{x}),$$

$$\left|f_\epsilon(\vec{x})\right|^2 = G_{\frac{1}{\epsilon^2}}(\vec{x}), \qquad\qquad \left|\tilde{f}_\epsilon(\vec{k})\right|^2 = G_{4\epsilon^2}(\vec{k}),$$

where we omit the identity matrix when using the notation (3.20), as for example $G_{4\epsilon^2} \equiv G_{4\epsilon^2 \mathbb{1}_d}$. This choice of profile is natural if we interpret the smearing (3.34) as arising from a random error in the identification of a point in space. To guarantee that measurements in different points are independent, and that different collective operators effectively identify different subsystems, we need the overlap between neighbouring profiles to be small, i.e. $\epsilon \ll D$. In this limit, the Gaussian profiles can be treated as compact-support profiles and the general results of Sec. 3.3.1 apply.

---

[5]This only true for Gaussian states, because they are fully determined by their two-point correlations (note that $\langle \hat{q}_{\vec{j}} \rangle = \langle \hat{p}_{\vec{l}} \rangle = \langle \hat{q}_{\vec{j}} \hat{p}_{\vec{l}} \rangle = 0$ is always assumed.)

The correlation matrices for collective operators read

$$g_{\vec{j}\vec{l}} = \left(8\pi\epsilon^2\right)^{d/2} \int d^d x d^d y \; G_{\frac{1}{2\epsilon^2}}(\vec{x} - \vec{j}D) G_{\frac{1}{2\epsilon^2}}(\vec{y} - \vec{l}D) \langle \hat{\phi}(\vec{x})\hat{\phi}(\vec{y})\rangle$$

$$= \left(8\pi\epsilon^2\right)^{d/2} \int d^d y \; G_{\frac{1}{4\epsilon^2}}((\vec{j} - \vec{l})D - \vec{y}) \langle \hat{\phi}(\vec{y})\hat{\phi}(0)\rangle, \tag{3.46}$$

$$h_{\vec{j}\vec{l}} = \left(8\pi\epsilon^2\right)^{d/2} \int d^d y \; G_{\frac{1}{4\epsilon^2}}((\vec{j} - \vec{l})D - \vec{y}) \langle \hat{\pi}(\vec{y})\hat{\pi}(0)\rangle,$$

where property (3.21) and the translational invariance of the correlation functions have been used. We want to find the limit for which condition (3.43) holds. This occurs when the integrals (3.46) vanish for $\vec{j} \neq \vec{l}$. In Appendix B.1 it is shown that, for any positive, bounded, asymptotically monotonically decreasing function φ, we have

$$\int d^d y \; G_{\frac{1}{4\epsilon^2}}(\vec{a} - \vec{y}) \varphi(\|\vec{y}\|) \rightarrow \varphi(\|\vec{a}\|) \tag{3.47}$$

for $\frac{\|\vec{a}\|}{\epsilon} \rightarrow \infty$. Assuming that $\langle \hat{\pi}(\vec{y})\hat{\pi}(0)\rangle$ and $\langle \hat{\pi}(\vec{y})\hat{\pi}(0)\rangle$ vanish at infinity (as is typically the case), by applying (3.47) to (3.46) we find that, for $D \gg \epsilon$,

$$g_{\vec{j}\vec{l}} \simeq \left(8\pi\epsilon^2\right)^{d/2} \langle \hat{\phi}((\vec{j} - \vec{l})D)\hat{\phi}(0)\rangle$$

$$h_{\vec{j}\vec{l}} \simeq \left(8\pi\epsilon^2\right)^{d/2} \langle \hat{\pi}((\vec{j} - \vec{l})D)\hat{\pi}(0)\rangle$$

for $\vec{j} \neq \vec{l}$. Thus the approximation (3.43) holds when D is large with respect to ϵ and when both $\epsilon^d \langle \hat{\phi}(D)\hat{\phi}(0)\rangle$ and $\epsilon^d \langle \hat{\pi}(D)\hat{\pi}(0)\rangle$ tend to zero[6].

For example, in the vacuum state of a Klein-Gordon field of mass M the correlation functions decay exponentially with M, so we can plug $\varphi(\|\vec{x}\|) \sim e^{-M\|\vec{x}\|}$ in (3.47), which gives the exponential decay e^{-MD} for the off-diagonal elements of the correlation matrices. This means that, in this case, no correlations between collective operators can be found for $DM \rightarrow \infty$, i.e. for spacing between the sampling points much larger than the Compton wavelength $\frac{1}{M}$ in the adopted units.

3.3.3 Vacuum and Thermal States of the Klein-Gordon Field

The thermal state of a Klein-Gordon field is a Gaussian state. For an inverse temperature β, it is characterised by

$$\begin{aligned} g(\vec{k}) &= \frac{1}{2\omega_k} \coth(\frac{\beta\omega_k}{2}), \quad h(\vec{k}) = \frac{\omega_k}{2} \coth(\frac{\beta\omega_k}{2}), \\ \omega_k &= \sqrt{k^2 + M^2}, \qquad k = \|\vec{k}\|. \end{aligned} \tag{3.48}$$

---

[6]Note that, in order to derive Eq. (3.47), it is not sufficient to use $G_{\frac{1}{4\epsilon^2}}(\vec{x}) \rightarrow \delta(\vec{x})$ for $\epsilon \rightarrow 0$, since ϵ is not dimensionless and has to be compared with a quantity of the same dimension. Furthermore, the expression (3.47) does not necessarily converge in the limit $\frac{\|\vec{a}\|}{\epsilon} \gg 1$ (e.g. for a periodic φ), for this reason the monotonicity condition is used (although weaker conditions could also be used).

(See Ref. [85].) In the limit $D \gg \epsilon \gg \frac{1}{M}$, the entropy takes the form (3.45). Additionally, we have $\left|\tilde{f}_\epsilon(\vec{k})\right|^2 \to \delta(\vec{k})$, whenever the Gaussian $\left|\tilde{f}_\epsilon(\vec{k})\right|^2$ is integrated with functions $g(\vec{k})$, $h(\vec{k})$ that have small derivative compared to ϵ. This is the case when $\epsilon \gg \frac{1}{M}$ and $\epsilon \gg \beta$ (independently of the relation between β and M). Using this approximation into Eq. (3.44), one finds $g_D \to g(0) = \frac{1}{2M} \coth(\frac{\beta M}{2})$, $h_D \to h(0) = \frac{M}{2} \coth(\frac{\beta M}{2})$. The entropy is thus given by

$$S = \left(\frac{L}{D}\right)^d s\left(\frac{1}{2}\coth(\frac{\beta M}{2})\right), \tag{3.49}$$

where the function s is defined in Eq. (3.32).

Vacuum State   In the low-temperature limit, $\beta M \to \infty$, we have $\coth(\frac{\beta M}{2}) \to 1$. Since $s(1/2) = 0$, we find that $S \to 0$. Thus the entropy of the vacuum state is zero when all available measurements have a minimal precision larger than the Compton wavelength. This implies that the corresponding state, which was defined as the vacuum state reduced over the subsystem $\mathcal{H}_{coll}$, is pure. We conclude that the vacuum state $|0\rangle$ of the Klein-Gordon field is a product state in the division in subsystems (3.36):

$$|0\rangle \sim |\Omega\rangle_{coll} \otimes |\omega\rangle_{fine}, \tag{3.50}$$

where $|\Omega\rangle_{coll}$ is the effective state that can be measured with the limited space resolution and $|\omega\rangle_{fine}$ is the reduced state of the remaining subsystem $\mathcal{H}_{fine}$, which would require a higher precision to be measured[7]. Additionally, since the condition (3.43) holds, no correlations are left among the spaces $\mathcal{H}_{\vec{j}}$, which means that the reduced state is a product $|\Omega\rangle = \bigotimes_j |\Omega_j\rangle$.

What we have found is that, under the restriction of measurements with a minimal precision larger than the Compton wavelength, the vacuum state of the Klein-Gordon field appears effectively as a pure product state. This is also how the vacuum appears in the Newton-Wigner localisation, discussed in Chapter 2. This suggests that the Newton-Wigner localisation naturally emerges when short-distance correlations are unobservable.

High Temperature   The high-temperature limit, in the regime of poor spatial resolution, is defined as the limit $D \gg \epsilon \gg \frac{1}{M} \gg \beta$. By Inserting (3.48) into

---

[7]The factorisation (3.50) is approximate because the Gaussian profile only approximatively define different subsystems.

(3.44) with a Gaussian profile we have

$$
\begin{aligned}
g_D &= \int d^d k \, G_{4\epsilon^2}(\vec{k}) \frac{\coth(\frac{\beta\omega_k}{2})}{2\omega_k} \\
&= \int \frac{d^d k}{\beta^d} G_{4\epsilon^2}\left(\vec{k}/\beta\right) \coth\left(\frac{\sqrt{\|\vec{k}\|^2 + \beta^2 M^2}}{2}\right) \frac{\beta}{2\sqrt{\|\vec{k}\| + \beta^2 M^2}} \\
&= \frac{\beta}{2} \int d^d k \, G_{4\frac{\epsilon^2}{\beta^2}}\left(\vec{k}\right) \frac{\coth\left(\frac{\sqrt{\|\vec{k}\| + \beta^2 M^2}}{2}\right)}{\sqrt{\|\vec{k}\| + \beta^2 M^2}},
\end{aligned}
$$

where the property (3.22) has been used. Since we are considering the limit $\beta M \to 0$, we can make the simplification $\sqrt{\|\vec{k}\|^2 + \beta^2 M^2} \to \|\vec{k}\|$. Furthermore, the integrand falls off exponentially for $\|\vec{k}\| > \frac{\beta}{\epsilon} \to 0$, so we can use the expansion $\coth(\|\vec{k}\|) \sim \frac{1}{\|\vec{k}\|}$ for $\|\vec{k}\| \to 0$. We find[8]

$$
\begin{aligned}
g_D &\sim \beta \int d^d k \, G_{4\frac{\epsilon^2}{\beta^2}}\left(\vec{k}\right) \frac{\coth\left(\frac{\|\vec{k}\|}{2}\right)}{2\|\vec{k}\|} \sim \beta \int d^d k \, G_{4\frac{\epsilon^2}{\beta^2}}\left(\vec{k}\right) \frac{1}{\|\vec{k}\|^2} \\
&= \beta \left(\frac{2\epsilon}{\beta\sqrt{2\pi}}\right)^d \gamma_d \int_0^\infty dk \, k^{d-1} \frac{1}{k^2} e^{-2\frac{\epsilon^2}{\beta^2}k^2} \\
&= \frac{\gamma_d}{\pi^{d/2}} \Gamma(\frac{d}{2} - 1) \frac{\epsilon^2}{\beta} = \frac{4}{d-2} \frac{\epsilon^2}{\beta},
\end{aligned}
$$

with $\gamma_d = \frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})}$. With similar steps one finds $h_D \sim \frac{1}{\beta}$, so that

$$
c_D = \sqrt{g_D h_D} \sim t_d \frac{\epsilon}{\beta},
$$

with $t_d = \sqrt{\frac{4}{d-2}}$. Using Eq. (3.45), we find for the entropy in the high-temperature limit

$$
S \sim \left(\frac{L}{D}\right)^d s(t_d \frac{\epsilon}{\beta}) \sim \left(\frac{L}{D}\right)^d \log(\frac{\epsilon}{\beta}). \tag{3.51}
$$

---

[8]For $d \leq 2$ the integral does not converge. This is an artifact of applying the substitution $\frac{1}{k^2 + \beta^2 M^2} \to \frac{1}{k^2}$ to small values of k. Keeping the original form of the integrand would result in a different numerical factor in the result, but the scaling with the parameters ϵ and β would remain the same.

The last approximation is obtained by applying the asymptotic behaviour

$$
\begin{aligned}
s(x) &= x \log\left(1 + \frac{1}{x} + o(\frac{1}{x})\right) + \log(x + o(x)) \\
&= \log x + o(\log x), \qquad x \to \infty,
\end{aligned}
\tag{3.52}
$$

and neglecting the constant term $\log(t_d)$. As we are going to see in the next section, the result (3.51) can be interpreted as the entropy of a classical system.

3.4 Emergence of Classical Entropy

To conclude the analysis we compare the results obtained with the entropy of classical systems. The classical Shannon entropy for a continuous random variable $\vec{x} \in \mathbb{R}^n$ with probability density $p(\vec{x})$ is defined as

$$
S(p) := -\int d^n x \, p(\vec{x}) \log p(\vec{x}).
\tag{3.53}
$$

This is not always positive and approaches $-\infty$ as $p(\vec{x})$ approaches a delta function. It is indeed impossible to define a classical entropy as a positive and finite quantity, the reason being that an infinite amount of information is required to specify a pure state (i.e. a single point in $\mathbb{R}^n$). However, as long as one is only concerned with entropy differences, (3.53) provides a proper definition up to an additive term proportional to the number of degrees of freedom n. A common procedure for defining a finite entropy, often used in classical statistical mechanics, is to split the volume in cubic cells of side h, with $h > 0$ being some arbitrary constant. One can then identify a discrete probability distribution by averaging the probability density $p(\vec{x})$ over each cell, $p_j := \int_{\text{Cell}_j} p(\vec{x}) \, d^n x$ and use the discrete version of the Shannon entropy

$$
S_h := -\sum_j p_j \log p_j,
\tag{3.54}
$$

which is always positive. The two definitions are equivalent, up to a constant, as long as only probability distributions are considered that are approximatively constant within each cell, which can always be achieved by taking h arbitrarily small.

Shannon Entropy from Phase Space Coarse Graining   Since the classical entropy for continuous variables is well-defined only by assuming some kind of "coarse graining" (i.e. assuming a minimal resolution, which can in principle be

as small as possible), it is natural to expect that the introduction of coarse graining at the level of quantum states can link the quantum with the classical notion of entropy. This can be seen explicitly for Gaussian states subject to phase space coarse-graining, as defined in Sec. 3.2.

Recall that the von Neumann entropy of a state with Wigner function $\mathcal{W}(\vec{q}, \vec{p}) = G_{g^{-1}}(\vec{q})G_{h^{-1}}(\vec{p})$ is given by Eq. (3.32) and that the generalised Heisenberg uncertainty can be expressed as $C \geq \frac{1}{2}$, with $C = \sqrt{g \cdot h}$. The limit of large variance is then given by $C \gg \frac{1}{2}$ (i.e. all eigenvalues of C are much larger than $\frac{1}{2}$). In this limit, applying the approximation (3.52), the entropy becomes

$$S = \mathrm{Tr}\,s(C) \sim \mathrm{Tr}\log C = \log\det C = \frac{1}{2}\log\left(\det g \det h\right). \qquad (3.55)$$

This can be directly compared with the Shannon entropy of a general Gaussian probability distribution $p(\vec{x}) = G_A(\vec{x})$, which can be easily calculated from Eq. (3.53) and is given by

$$S(G_A) = \frac{1}{2}\log\left(\det A^{-1}\right) + n\,\mathrm{const}. \qquad (3.56)$$

For $\vec{x} \in \mathbb{R}^{2n}$ and $A = g^{-1} \oplus h^{-1}$ this is equal to Eq. (3.55), up to the aforementioned volume-proportional constant intrinsic in the definition of classical entropy. Since the Wigner function of a coarse-grained Gaussian state is determined by $C = \sqrt{\left(g + \frac{\sigma^2}{m^2}\right) \cdot (h + m^2\sigma^2)}$, a large coarse-grain parameter $\sigma^2 \gg 1$ immediately leads to the approximation (3.55) and thus to the equivalence of classical and quantum entropy[9].

Classical Thermal Entropy from Collective Operators   The thermodynamics of a classical field is notoriously problematic, suffering of ultraviolet divergences that are eventually cured only within the quantum formalism. It is however sensible to consider thermal states for classical harmonic systems on a lattice, formally analogous to classical fields measured with a minimal space resolution, and compare them with the corresponding thermal states of quantum systems.

For a Klein-Gordon field in a d-dimensional box of size L we introduce a short-distance cut-off $\epsilon := \frac{L}{N}$, with N a natural number, and the discretised canonical

---

[9]Notice that for specific states (e.g. the ground state of a harmonic oscillator) the large coarse-grain limit implies $C \sim \sigma$, which means that the measurement error completely washes away the features of the original states. In this case the entropy is given by $S \sim n\log\sigma$, i.e. it only contains the constant factor that can be absorbed in the definition of the classical entropy. However, there exist states for which the condition $C \gg \frac{1}{2}$ applies independently of the coarse graining. If $\det C \gg \sigma$, one is in the regime of classical states, for which the coarse-graining does not affect the measurement statistics in an appreciable way. The point is that the condition $\sigma^2 \gg 1$ makes it possible to interpret *any* state as a classical one.

variables $q_{\vec{j}} := \sqrt{E}\epsilon^{d/2}\phi(\vec{j}\epsilon)$, $p_{\vec{j}} := \frac{\epsilon^{d/2}}{\sqrt{E}}\pi(\vec{j}\epsilon)$, with $E := \frac{1}{\epsilon}\sqrt{M^2\epsilon^2 + 2d}$. The Hamiltonian of the discretised Klein-Gordon field can be written as

$$H(\vec{q}, \vec{p}) = \frac{E}{2}\sum_{j_1,\dots,j_d=1}^{n}\left[q_{\vec{j}}^2 + p_{\vec{j}}^2 - \alpha\sum_s q_{\vec{j}}q_{\vec{j}+\vec{u}_s}\right], \tag{3.57}$$

where $\alpha := \frac{2}{E^2\epsilon^2}$, $\vec{u}_s$ are the d-dimensional unit vectors $\vec{u}_1 = (1, 0, \dots, 0)$, $\dots$, $\vec{u}_d = (0, \dots, 0, 1)$, and we assume periodic boundary conditions $j_s + N \equiv j_s$ for $s = 1, \dots, d$. The continuum limit is found for $N \to \infty$ (see Appendix B.2)[10]. We can consider Hamiltonians of the more general form

$$H(\vec{q}, \vec{p}) = \frac{1}{2}\sum_{j_1\dots j_d=1}^{N}\left[X_{\vec{j}\vec{l}}q_{\vec{j}}q_{\vec{l}} + P_{\vec{j}\vec{l}}p_{\vec{j}}p_{\vec{l}}\right], \tag{3.58}$$

where X and P are real, symmetric, translationally invariant matrices. The state of the system in thermal equilibrium is represented by the Gibbs probability distribution

$$\rho_\beta(\vec{q}, \vec{p}) = \frac{e^{-\beta H(\vec{q},\vec{p})}}{Z_\beta}, \tag{3.59}$$

where β is the inverse temperature and

$$Z_\beta := \int d^{N^d}q\, d^{N^d}p\; e^{-\beta H(\vec{q},\vec{p})} \tag{3.60}$$

is the classical partition function. The entropy of the thermal state can be either calculated with Eq. (3.56) or using the formula

$$S = \left(-\beta\frac{\partial}{\partial\beta} + 1\right)\log Z_\beta = -\frac{1}{2}\log\left[\det\left(\beta X\right)\det\left(\beta P\right)\right] + N^d\log\left(2\pi e\right). \tag{3.61}$$

In the continuum limit, $N \to \infty$, we have $E \sim \frac{1}{\epsilon}$, $\alpha \sim \frac{1}{d}$ and the Hamiltonian (3.57) can be written in the form (3.58) using the matrices

$$X_{\vec{j}\vec{l}} \sim \frac{1}{\epsilon}\left[\delta_{\vec{j}\vec{l}} - \frac{1}{2d}\sum_s\left(\delta_{\vec{j}\,\vec{l}+\vec{u}_s} + \delta_{\vec{j}+\vec{u}_s\,\vec{l}}\right)\right], \qquad\qquad P_{\vec{j}\vec{l}} \sim \frac{1}{\epsilon}\delta_{\vec{j}\vec{l}}.$$

These matrices have eigenvalues $x_{\vec{k}} = \frac{1}{\epsilon}\left[1 - \frac{1}{d}\sum_s\cos\left(\frac{2\pi}{N}k_s\right)\right]$ and $p_{\vec{k}} = \frac{1}{\epsilon}$ respectively. For $N \to \infty$ we also have $x_{\vec{k}} \sim \frac{1}{\epsilon}$. Finally, from (3.61) we can derive

$$S \sim N^d\log\left(\frac{\epsilon}{\beta}\right) + N^d\text{const.} \tag{3.62}$$

---

[10]The discretised Klein-Gordon Field introduced here is equivalent to the system defined by collective operators with Gaussian profiles, as introduced in Section 3.3.2, in the limit $\frac{1}{M} \gg D \gg \epsilon$.

Up to the usual volume-proportional term, the expression (3.62) corresponds to Eq. (3.51). This means that, for poor space resolution and high temperature, the entropy of a quantum field in a thermal state can be interpreted as the entropy of a classical, discretised field, also in a thermal state.

Chapter 4

Observing Quantum Effects with Bounded Reference Frames

Summary

Quantum experiments usually assume the existence of perfect, classical reference frames, which allow for the specification of measurement settings (e.g. orientation of the Stern-Gerlach magnet in spin measurements) with arbitrary precision. If the reference frames are themselves quantum systems with finite quantum numbers (i.e. the reference frames are "bounded"), the precision with which the measurement settings can be defined is limited, providing a limitation on the possibility of observing quantum effects. In this chapter we consider the requirements on reference frame necessary for the violation of local realism in entangled spin systems. As bounded reference frames for directions, spin coherent states are considered. We find that, for composite systems of an arbitrary number of spin-$\frac{1}{2}$ particles, reference frames of very small size are sufficient for the violation of Bell-like inequalities. In contrast, we find numerically that, in order to observe an analogous violation for macroscopic entangled spins, the size of the reference frame must be at least quadratically larger than that of the entangled spins. This suggests that the non-observance of quantum phenomena at the macroscopic scale might be related to the lack of sufficiently powerful reference frames.

This chapter is based on and contains material from the publication

4.1   Reference Frames in Quantum Mechanics

The Kochen-Specker test of contextuality [86] and Bell's test of local realism [1] provide theory-independent tests of the "classicality" of a system. In the latter, correlations between space-like separated parts of a composite system are measured for different choices of measurement settings. Certain combinations of these correlations constitute "test quantities" (Bell's inequalities) that are bounded in all classical (local realistic) theories. Violation of these bounds imply that the tested state has no local realistic explanation. Typically, the choices of the settings correspond to different orientations of the measuring apparatuses (like a polariser or the Stern-Gerlach magnet). This implicitly assumes the existence of an external (classical) reference frame (RF), which allows one to specify with arbitrary precision the directions chosen. But, what if no RF is available? The impossibility of specifying measurement settings precisely, in the absence of a perfect RF, leads to a kind of "intrinsic decoherence" [87, 88, 89] that might wash out all quantum features. *What are the minimal RF resources such that quantum features of a given system can still be observed?*

If we adopt the natural assumption that physical resources in the Universe are finite, we will always be confronted with bounded RFs. Physically, this means that our measurements will always be imprecise. It is of fundamental interest to determine the minimal measurement precision required such that one can still observe genuine quantum features, such as violation of local realism or non-contextuality (see, for example, [90, 18]). In addition to these foundational reasons, the questions given above are relevant for developing methods to contend with bounded RFs using relational encodings, particularly in the context of computation, cryptography, and communication [91, 92, 93, 94, 95, 96]. For certain tasks, such as quantum key distribution [97] or quantum communication complexity [98], entangled states are useful only to the extent that they violate Bell's inequalities. It is thus important to quantify the costs in RF resources for the violation.

To introduce the idea of measuring relative degrees of freedom in the situation of lacking an external RF consider the problem of determining the direction towards which a spin-1/2 particle points. In general the direction can be defined as a relative angle to some macroscopic pointer (e.g. the Stern-Gerlach magnet), which serves as an external RF. Performing many repetitions of the Stern-Gerlach experiment with the same spin state, we can infer this angle. If we are given two spin-1/2 particles, one can determine the relative angle between them, by first measuring the angles between each of the spins and the external RF and from these computing the relative angle. Now suppose that the experimenter has no access to such an external Cartesian RF; operationally, this means that she has no information about her orientation with respect to the rest of the world (but she can

still control all the devices in her laboratory). In particular, the angles between her instruments and those used to prepare the particles are not known and may change in every repetition of the experiment. Nonetheless, the relative orientation between the two spins can be measured in a manner which is invariant under rotations. If she measures the total spin of the two particles, this can take the values 0 and 1. Now we are tempted to say that the two spins add when they are aligned and subtract when they are anti-aligned, and so we can interpret this as the measurement of the projection of the first spin along the direction of the second. This procedure leads unavoidably to errors: e.g. if the spins were initially in the state $|\psi^+\rangle = \frac{1}{\sqrt{2}}(|z+\rangle|z-\rangle + |z-\rangle|z+\rangle)$, then a measurement on each particle with respect to an external RF along z would imply that they are anti-aligned along this direction. However, the measurement of total spin is interpreted as if they were aligned, because the total spin of $|\psi^+\rangle$ is 1. As this procedure is proven to be optimal [99], there is a fundamental restriction in the determination of the relative angle between two (finite) spins that the experimenter can achieve in absence of an external reference frame. One can apply the same procedure using a spin-j coherent state as the RF; as j becomes larger, the errors introduced decrease and, eventually, for $j \to \infty$ (unbounded RF) the measurement with the classical RF is exactly reproduced[1].

The question we are interested in is how "strong" the RFs need to be to allow violation of Bell's inequalities, if in the Bell test the observers are given bounded RFs. Since we are interested in violations of local realism in the transition from quantum to classical RFs, we use the spin coherent states to represent quantum RFs as they are closest to the notion of a classical direction. As we are going to see, a pair of spin-1/2 particles exhibits violation of Clauser-Horne-Shimony-Holt (CHSH) inequality already for $j_{RF} > \frac{5}{2}$. In the case of multi-particle Mermin [100] inequalities, even if half of the RFs are of minimal size $j_{RF} = 1/2$, and the other half "unbounded" (classical), the ratio between the quantum and local realistic bound remains exponential in the number of entangled spins. Finally, for the case of two macroscopic spins exhibiting violations of a Bell inequality when classical RFs are available, we find that the violation is possible with bounded RFs only if their size is *quadratically* larger than the size of the spins. Since our everyday RFs do not meet this requirement of macroscopically large spins, this suggests an explanation as to why we do not see such violations in everyday life. All the results are derived for violations of local realism, but they can straightforwardly

---

[1]In order to physically implement measurements of total spin, one must be able to entangle the two particles. In practice, information about the alignment of the beams containing the particles with respect to the lab would need to be available. However, typically this information about beam alignment does not contain any information about the particle spins - i.e. the internal degrees of freedom of the two particles. Therefore, one can lack RF for internal degrees of freedom and still be able to perform the required measurements in the lab.

be extended to contextuality proofs as well.

4.2   Measurement of Relative Degrees of Freedom.

Here we only consider directional RFs. Given a classical, external RF, one can measure the projection of a spin-j_S particle along a specific direction, where the $2j_S + 1$ possible outcomes $m = -j_S, \ldots, j_S$, correspond to the projectors $\Pi_m = |j_S, m\rangle\langle j_S, m|$. Given an initial state $|\psi\rangle$, the probability of detecting the outcome m is

$$p_m = \langle\psi|\Pi_m|\psi\rangle = |\langle j_s, m|\psi\rangle|^2.$$

Assuming experimental conditions in which the resources available are limited, we consider bounded RFs by replacing the classical RF with a quantum RF in the form of a coherent state of spin j_{RF}.

Without an external RF, the experimenter can only measure relational degrees of freedom of the particle and the coherent state $|j_{RF}\rangle$. The task is thus to estimate the relative angle between them using only rotationally invariant operations. An optimal procedure consists in performing the projective measurement onto the subspaces of total spin j of two spins [91], which can take the values $j = |j_{RF} - j_S|, \ldots, j_{RF} + j_S$. When the outcome $j = j_{RF} + m$ of total spin is observed, we associate the spin component m along the direction of the bounded RF to the system. In this way the spin projection measurement relative to a bounded RF simulates the one relative to an unbounded RF. The projectors associated to subspaces of total spin are

$$\hat{\Pi}_{j_{RF}+m} = \sum_{m'=-j_{RF}-m}^{j_{RF}+m} |j_{RF} + m, m'\rangle\langle j_{RF} + m, m'| .$$

The effective measurement on the system alone is represented by the POVM elements

$$\hat{P}_{j_S\, m}^{j_{RF}} = \langle j_{RF}|\hat{\Pi}_{j_{RF}+m}|j_{RF}\rangle. \tag{4.1}$$

These can be expressed in terms of the Clebsch-Gordan coefficients $C^{\ j_1\ \ j_2\ \ j}_{\ m_1\ m_2\ m} := \langle j, m \| j_1, m_1\rangle|j_2, m_2\rangle$ and are given by

$$\hat{P}_{j_S\, m}^{j_{RF}} = \sum_{m_S\, n_S} C^{\ j_{RF}\ \ j_S\ \ j_{RF}+m}_{\ j_{RF}\ m_S\ j_{RF}+m_S}\ C^{\ j_{RF}\ \ j_S\ \ j_{RF}+m}_{\ j_{RF}\ n_S\ j_{RF}+n_S}\ |j_S, m_S\rangle\langle j_S, n_S|.$$

Using the asymptotic properties of the Clebsch-Gordan coefficients [101], one has $C^{j_r\ j_s\ j_r+m}_{j_r m_s\, j_r+m_s} \rightarrow \delta_{m m_s}$ for $j_r \rightarrow \infty$ and it can be easily seen that $\hat{P}_{j_S\, m}^{j_{RF}} \rightarrow$

$|j_S, m\rangle\langle j_S, m| \equiv \hat{\Pi}_m$ when $j_{RF} \to \infty$. This shows that the relational measurement with increasingly larger bounded RF tends to the measurement with unbounded RF.

In the Bell experiment each of the observers chooses between two or more measurement settings, corresponding, for example, to measurements of spin components along different directions $\vec{\alpha}_1, \vec{\alpha}_2,...$ In our scenario this choice corresponds to the use of coherent states $|\vec{\alpha}_1\rangle, |\vec{\alpha}_2\rangle,...$ pointing to different directions as RFs. Here $|\vec{\alpha}_i\rangle$ is the eigenstate with the maximal eigenvalue of the spin component along the direction $\vec{\alpha}_i$. One possible way to prepare such states is to apply an appropriate rotation to the given coherent state $|j_{RF}\rangle$ pointing towards z axis. Since, however, Alice and Bob are assumed to have no RF, we consider the following operational realisation. In every experimental run a third party (Charlie) sends to both Alice and Bob one coherent state for each possible setting, together with the entangled pair to be measured. Each coherent state is prepared along the direction which would be chosen when classical RF were used. Having no RF for directions, Alice cannot know the angles of the different coherent states, but she can still distinguish between them (for example, Charlie can send them with a short, agreed, time delay), then Alice can decide which one to use as a RF, allowing the freedom of choice necessary in a Bell experiment. It is here assumed that the channel between Charlie and the observers is subject to a collective noise, that is to say, all the particles sent to one observer undergo the same unknown rotation (but a different rotation occurs in different runs and for the different observers), this is important since we want to exploit relative degrees of freedom. Such an assumption could be reasonable in some quantum communication schemes.

4.3 Violation of Bell's Inequalities.

As a first example we consider a Bell experiment on an entangled pair of spin-1/2 particles with bounded RFs. We will determine the minimal size for the spin RFs such that the outcomes can still violate Bell's inequalities.

We consider the CHSH inequality [102]

$$S := \left| E(\vec{\alpha}_1, \vec{\beta}_1) + E(\vec{\alpha}_1, \vec{\beta}_2) + E(\vec{\alpha}_2, \vec{\beta}_1) - E(\vec{\alpha}_2, \vec{\beta}_2) \right| \leq 2, \qquad (4.2)$$

where $E(\vec{\alpha}_i, \vec{\beta}_j)$ is the correlation function for the measurement $\vec{\alpha}_i$ at one laboratory and $\vec{\beta}_j$ at the other laboratory. In quantum mechanics, for a given state $\hat{\rho}$ of the pair, if the first spin is measured along direction $\vec{\alpha}_i$ and the second along $\vec{\beta}_j$, the correlation function reads $E(\vec{\alpha}_i, \vec{\beta}_j) = \text{Tr}\left[\hat{\rho} (\vec{\alpha}_i \cdot \vec{\sigma}) (\vec{\beta}_j \cdot \vec{\sigma})\right]$.

In contrast to the standard Bell experiment in which two distant observers possess unbounded RFs, we assume that they can only use their coherent states

($|j_1\rangle$ and $|j_2\rangle$) with respect to which entangled spins can be measured. How large must j_1 and j_2 be, such that the CHSH inequality is still violated?

We assume that the pair is in the singlet state $|\psi^-\rangle = \frac{1}{\sqrt{2}}(|z+\rangle|z-\rangle - |z-\rangle|z+\rangle)$. The two observers can choose between two measurement settings each, the setting being defined by the direction towards which the RF coherent state is pointing. As $|\psi^-\rangle$ is a rotationally invariant state, the only relevant parameter in the correlation function is the relative angle between the two pointers. It is more mathematically convenient (but operationally equivalent) to write the state with fixed measurement settings and then to apply a rotation of an angle ϑ to one of the particles. The corresponding rotated singlet state is

$$|\psi^-(\vartheta)\rangle = \frac{1}{\sqrt{2}}\left[\sin\frac{\vartheta}{2}\left(|z+\rangle|z+\rangle + |z-\rangle|z-\rangle\right) + \cos\frac{\vartheta}{2}\left(|z+\rangle|z-\rangle - |z-\rangle|z+\rangle\right)\right].$$

If one measures the total spin of the joint particle-RF system at the two laboratories, the outcome probabilities are given by

$$p_{mn}(\vartheta) = \sum_{m_1 m_2}|\langle j_1|\langle j_2|\langle\psi(\vartheta)\|j_1 + m, j_1 + m_1\rangle|j_2 + n, j_1 + m_2\rangle|^2, \qquad (4.3)$$

where $m, n = -\frac{1}{2}, \frac{1}{2}$. (i.e. $p_{\frac{1}{2}\frac{1}{2}}(\vartheta)$ is the probability of finding the two particles aligned along $|j_1\rangle$ and $|j_2\rangle$ respectively, $p_{-\frac{1}{2}-\frac{1}{2}}(\vartheta)$ is the probability of finding both anti-aligned, etc). To calculate the probabilities (4.3) one needs the coefficients

$$\langle j|\langle z+\|j+m, j+n\rangle = \delta_{n,\frac{1}{2}}\delta_{m,\frac{1}{2}},$$
$$\langle j|\langle z-\|j+m, j+n\rangle = \frac{\delta_{n,-\frac{1}{2}}}{\sqrt{2j+1}}\left(\delta_{m,\frac{1}{2}} + \sqrt{2j}\delta_{m,-\frac{1}{2}}\right), \qquad (4.4)$$

from which one gets

$$\begin{aligned}
p_{mn}(\vartheta) = \frac{1}{2}\sum_{m_1 m_2}\Bigg| & \sin\frac{\vartheta}{2}\Bigg[\delta_{m_1\frac{1}{2}}\delta_{m\frac{1}{2}}\delta_{m_2\frac{1}{2}}\delta_{n\frac{1}{2}} \\
& + \frac{\delta_{m_1-\frac{1}{2}}\delta_{m_2-\frac{1}{2}}}{\sqrt{(2j_1+1)(2j_2+1)}}\left(\delta_{m\frac{1}{2}} + \sqrt{2j_1}\delta_{m-\frac{1}{2}}\right)\left(\delta_{n\frac{1}{2}} + \sqrt{2j_2}\delta_{n-\frac{1}{2}}\right)\Bigg] \\
& + \cos\frac{\vartheta}{2}\Bigg[\delta_{m_1\frac{1}{2}}\delta_{m\frac{1}{2}}\frac{\delta_{m_2-\frac{1}{2}}}{\sqrt{2j_2+1}}\left(\delta_{n\frac{1}{2}} + \sqrt{2j_2}\delta_{n-\frac{1}{2}}\right) \\
& - \frac{\delta_{m_1-\frac{1}{2}}}{\sqrt{2j_1+1}}\left(\delta_{m\frac{1}{2}} + \sqrt{2j_1}\delta_{m-\frac{1}{2}}\right)\delta_{m_2\frac{1}{2}}\delta_{n\frac{1}{2}}\Bigg]\Bigg|^2
\end{aligned}$$

and thus

$$p_{mn}(\vartheta) = \frac{1}{2} \sin^2 \frac{\vartheta}{2} \left[\delta_{m\frac{1}{2}} \delta_{n\frac{1}{2}} + \frac{\left(\delta_{m\frac{1}{2}} + 2j_1 \delta_{m-\frac{1}{2}} \right) \left(\delta_{n\frac{1}{2}} + 2j_2 \delta_{n-\frac{1}{2}} \right)}{(2j_1 + 1)(2j_2 + 1)} \right]$$
$$+ \frac{1}{2} \cos^2 \frac{\vartheta}{2} \left[\frac{\delta_{m\frac{1}{2}}}{2j_2 + 1} \left(\delta_{n\frac{1}{2}} + 2j_2 \delta_{n-\frac{1}{2}} \right) + \frac{\delta_{n\frac{1}{2}}}{2j_1 + 1} \left(\delta_{m\frac{1}{2}} + 2j_1 \delta_{m-\frac{1}{2}} \right) \right].$$

Inserting this into the definition of the correlation function

$$E^{j_1 j_2}(\vartheta) := - \sum_{mn=-\frac{1}{2}}^{\frac{1}{2}} (-1)^{m+n} p_{mn}(\vartheta)$$

one obtains

$$E^{j_1 j_2}(\vartheta) = \frac{1}{2} \left[\sin^2 \frac{\vartheta}{2} \left(1 + \frac{1 + 4j_1 j_2 - 2j_1 - 2j_2}{(2j_1 + 1)(2j_2 + 1)} \right) + \cos^2 \frac{\vartheta}{2} \left(\frac{1 - 2j_1}{2j_1 + 1} + \frac{1 - 2j_2}{2j_2 + 1} \right) \right]$$
$$= \left[\sin^2 \frac{\vartheta}{2} \frac{1 + 4j_1 j_2}{(2j_1 + 1)(2j_2 + 1)} + \cos^2 \frac{\vartheta}{2} \frac{1 - 4j_1 j_2}{(2j_1 + 1)(2j_2 + 1)} \right] \qquad (4.5)$$

and finally

$$E^{j_1 j_2}(\vartheta) = \frac{1 - 4j_1 j_2 \cos \vartheta}{(2j_1 + 1)(2j_2 + 1)}. \qquad (4.6)$$

In the limit of large j_1 and j_2, Eq. (4.6) becomes the familiar expression $E(\vartheta) = -\cos \vartheta$ for the singlet correlations with classical RFs.

The CHSH expression (4.2), applied to the correlation (4.6), is maximised when the relative angle between all pairs of measurement settings is $\frac{3}{4}\pi$, except for the pair $\vec{\alpha}_2, \vec{\beta}_2$, for which the angle $\frac{\pi}{4}$ has to be chosen[2]. This choice of measurement settings can be arranged on a plane as shown in Fig. 4.1. Plugging (4.6) into (4.2) with this choice of settings, the RF-dependent CHSH expression becomes

$$S(j_1, j_2) = 2 \left| \frac{1 + 4\sqrt{2} j_1 j_2}{(2j_1 + 1)(2j_2 + 1)} \right|. \qquad (4.7)$$

This expression exceeds the local realistic bound of 2 if $j_1 > \frac{j_2}{2(\sqrt{2}-1)j_2-1}$. Therefore, for equal RFs, one needs at least

$$j_1 = j_2 = \frac{5}{2}. \qquad (4.8)$$

This is the minimal size of coherent-state reference frames necessary in order to observe a violation of the Bell-CHSH inequality

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[2]Note that, in the correlation (4.6), the term $\cos \vartheta$ is "shifted" by a constant, so that, unlike the case with classical RFs, the CHSH expression (4.2) is not invariant for $\vartheta \to \vartheta + \pi$. For this reason the optimal measurement settings do not coincide with those traditionally adopted for the violation of the Bell-CHSH inequality
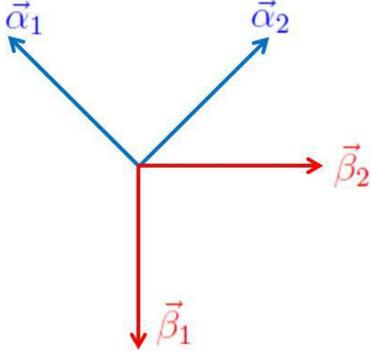
Figure 4.1: Measurement settings necessary for the maximal violation of the Bell-CHSH inequality.

4.4   Mermin Inequalities.

We study now the requirements for the violation of multi-particle Bell's inequalities with bounded RFs. Consider N spin-1/2 particles (systems $S_1, ..., S_N$), that are measured along directions $\vec{\alpha}_1, \dots, \vec{\alpha}_N$. Each individual measurement can give $\pm\frac{1}{2}$ as result; a specific outcome is thus labelled by a string $\{\mu_1, \dots, \mu_N\}$, where $\mu_k = 1$ stands for the k-th spin detected aligned with $\vec{\alpha}_k$, while $\mu_k = -1$ represents the spin anti-aligned with $\vec{\alpha}_k$. The multi-particle correlations are defined as

$$E(\vec{\alpha}_1, \dots, \vec{\alpha}_N) = \sum_{\mu_1, \dots, \mu_N = \pm 1} \prod_{k=1}^{N} \mu_k p(\mu_1, \dots, \mu_N \,|\, \vec{\alpha}_1, \dots, \vec{\alpha}_N),$$

where $p(\mu_1, \dots, \mu_N \,|\, \vec{\alpha}_1, \dots, \vec{\alpha}_N)$ is the probability for observing the outcomes $\mu_1, \dots, \mu_N$ given the settings $\vec{\alpha}_1, \dots, \vec{\alpha}_N$.

The Mermin inequality is given by [100, 103]

$$M := \left| \sum_{x_1, \dots, x_N = 0, 1} \cos[\frac{\pi}{2}(x_1 + \cdots + x_N)] E(\vec{\alpha}_{x_1}, \dots, \vec{\alpha}_{x_N}) \right| \leq 2^{\frac{N-1}{2}}. \qquad (4.9)$$

Using classical RFs, the Mermin expression reaches its maximal value of $M = 2^{N-1}$ for the Greenberger-Horne-Zeilinger (GHZ) state

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(\otimes_{k=1}^{N} |z+\rangle_{S_k} + \otimes_{k=1}^{N} |z-\rangle_{S_k} \right)$$

and measurement settings $\vec{\alpha}_0 = X \equiv (\frac{\pi}{2}, 0)$ and $\vec{\alpha}_1 = Y \equiv (\frac{\pi}{2}, \frac{\pi}{2})$ for every particle. Note that the ratio between maximal quantum and local realistic bound increases exponentially with the number of particles: $M_Q/M_{LR} = 2^{\frac{N-1}{2}}$.

Again, we assume that the k-th observer, $k = 1, ..., N$, is given a bounded RF in the form of a coherent state $|j_k\rangle$. Each of the observers has to measure along directions $\vec{\alpha}_0 \equiv (\vartheta_0, \varphi_0)$ and $\vec{\alpha}_1 \equiv (\vartheta_1, \varphi_1)$. As for the two-particle case, such measurements are reproduced by aligning each coherent state $|j_k\rangle$ along the prescribed angle and then measuring the total spin of the joint system k-th particle + k-th coherent state, interpreting the outcome as the projection of the particle's spin along the coherent state's direction. Since the total-spin projectors are rotationally invariant, this procedure is equivalent to applying an opposite rotation on each particle S_k. The inverse rotation acts on each spin-$1/2$ system as

$$R^{-1}(\vec{\alpha}_k)|z+\rangle = \cos\frac{\vartheta_k}{2}|z+\rangle - \sin\frac{\vartheta_k}{2}|z-\rangle \equiv |\vec{\alpha}_k+\rangle$$

$$R^{-1}(\vec{\alpha}_k)|z-\rangle = e^{-i\varphi_k}\left(\sin\frac{\vartheta_k}{2}|z+\rangle + \cos\frac{\vartheta}{2}|z-\rangle\right) \equiv |\vec{\alpha}_k-\rangle.$$

After rotating all spins, the GHZ state becomes

$$|\psi(\vec{\alpha}_1, \ldots, \vec{\alpha}_N)\rangle = \frac{1}{\sqrt{2}}\left(\otimes_{k=1}^{N}|\vec{\alpha}_k+\rangle_{S_k} + \otimes_{k=1}^{N}|\vec{\alpha}_k-\rangle_{S_k}\right). \tag{4.10}$$

The total-spin projector for the k-th system-RF pair is given by

$$\Pi_{j_k+\frac{\mu_k}{2}} = \sum_{m_k=-(j_k+\frac{\mu_k}{2})}^{j_k+\frac{\mu_k}{2}} |j_k + \frac{\mu_k}{2}, m_k\rangle\langle j_k + \frac{\mu_k}{2}, m_k|, \quad \mu_k = \pm 1. \tag{4.11}$$

The probability for a specific set of outcomes is found by tracing the state (4.10) with the projectors (4.11):

$$p(\vec{\alpha}_1, \ldots, \vec{\alpha}_N | \mu_1, \ldots, \mu_N) = \text{Tr}\left[\otimes_{k=1}^{N}\Pi_{j_k+\frac{\mu_k}{2}}|\text{Ref}\rangle\langle\text{Ref}| \otimes |\psi(\vec{\alpha}_1, \ldots, \vec{\alpha}_N)\rangle\langle\psi(\vec{\alpha}_1, \ldots, \vec{\alpha}_N)|\right],$$

where $|\text{Ref}\rangle = \otimes_{k=1}^{N}|j_k\rangle$. After a somewhat lengthy but straightforward calculation, one obtains the following expression for the multi-particle correlations:

$$E(\vec{\alpha}_1, \ldots, \vec{\alpha}_N | j_1, \ldots j_N) = \frac{1}{\prod_{k=1}^{N} d_k}\left\{\frac{1}{2}\left[\prod_{k=1}^{N}(1 + 2j_k\cos\vartheta_k)\right.\right.$$

$$\left.\left. + \prod_{k=1}^{N}(1 - 2j_k\cos\vartheta_k)\right] + \cos(\sum_{k=1}^{N}\varphi_k)\prod_{k=1}^{N}2j_k\sin\vartheta_k\right\}, \tag{4.12}$$

where $d_k = 2j_k + 1$.

Inserting the correlation function (4.12) into the left-hand side of the inequality (4.9) we find for the Mermin expression:

$$M(j_1, \ldots, j_k) = \frac{1}{\prod_{k=1}^{N} d_k}\left|\sqrt{2}\cos(N\frac{\pi}{4}) + 2^{N-1}\prod_{k=1}^{N}(2j_k)\right|. \tag{4.13}$$

For $j_k \to \infty$, this approaches the value 2^{N-1} when unbounded RFs are used. In the limit of large number of particles, the Mermin expression becomes

$$M = 2^{N-1} \prod_{k=1}^{N} \frac{j_k}{j_k + \frac{1}{2}} + O(1), \; N \to \infty. \tag{4.14}$$

If all the RFs are of the same size, $j_k = j \; \forall \, k$, the minimal size of RFs that leads to violation is $j = 3/2$. One can use, however, even fewer resources if one allows spins of different lengths for RFs. If one takes N_1 spins of size j_1 and N_2 of size j_2, expression (4.14) becomes $M \approx 2^{N-1} \left(\frac{j_1}{j_1 + \frac{1}{2}} \right)^{N_1} \left(\frac{j_2}{j_2 + \frac{1}{2}} \right)^{N_2}$. In this case the Mermin inequality is violated if

$$\left(\sqrt{2} \frac{j_1}{j_1 + \frac{1}{2}} \right)^{N_1} \left(\sqrt{2} \frac{j_2}{j_2 + \frac{1}{2}} \right)^{N_2} > \sqrt{2}. \tag{4.15}$$

As both factors are positive, (4.15) can hold only if at least one of the two is larger than 1, which is equivalent to $j_i > \frac{1}{2(\sqrt{2}-1)} = 1.21$. This implies that some of the RFs must have spin size equal to or larger than $\frac{3}{2}$. If the parties have N_1 spin-$\frac{3}{2}$ RFs and $N_2 = N - N_1$ spin-$\frac{1}{2}$ RFs, the minimal ratio is $\frac{N_1}{N} \cong 0.85$ for seeing violation. Therefore the minimal resources needed is 85% of spin-$\frac{3}{2}$ and 15% of spin-$\frac{1}{2}$ reference frames.

Another interesting case is when a fraction of the RFs is unbounded, which is equivalent to taking the limit $j_2 \to \infty$ in the inequality (4.15). For N_1 RFs of size j_1 and N_2 unbounded RFs, it becomes $\left(\sqrt{2} \frac{j_1}{j_1 + \frac{1}{2}} \right)^{N_1} > 2^{\frac{1-N_2}{2}}$. For $j_1 = 1/2$, this is satisfied when $N_2 > N_1 + 1$, which means that when half of the RFs are unbounded and half are as small as spin-$\frac{1}{2}$, violation of the Mermin inequality is still possible.

Note that in all cases considered – even when using small quantum RFs – the ratio between the quantum and local realistic bound is still exponential, as can be easily seen by inserting the results found into the expression (4.14). However, if a single measurement is replaced with a random guess (corresponding mathematically to $j_1 = 0$), the inequality is satisfied. Thus a non-trivial RF is required for every observer in order to see nonclassicality.

4.5   Higher Spins and the Classical Limit.

It was shown in [90] that violation of Bell's inequalities with entangled systems of arbitrarily large dimension is possible. This shows that the view that large quantum numbers are associated with the classical limit is, in general, erroneous.

We will show that to observe violations of local realism for large spins it is necessary to use the RFs of size sufficiently large compared to the size of the spins. The scaling of the two sizes is the issue we are interested in.

Following Peres [90], we consider a pair of spin-j_S particles in the generalised singlet state:

$$|\Psi_{j_S}^-\rangle := \frac{1}{\sqrt{2j_S + 1}} \sum_{m=-j_S}^{j_S} (-1)^{j_S-m}|j_S, m\rangle|j_S, -m\rangle. \tag{4.16}$$

and define the parity measurement

$$\hat{P}^c = \sum_{m=-j_S}^{j_S} (-1)^{j_S-m}\hat{\Pi}_m , \tag{4.17}$$

with $\hat{\Pi}_m = |j_s, m\rangle\langle j_s, m|$ the projectors onto subspaces of the spin component along the z axis. The parity measurement takes the value $+1$ for all even m, and -1 for all odd m. When the parity operator is defined with respect to spin projection along some other direction $\vec{\alpha}$, we will speak about parity measurement $P^c(\vec{\alpha})$ along this direction. For Alice's measurement along the direction $\vec{\alpha}$ and Bob's along $\vec{\beta}$, the correlation function is defined as $E(\vec{\alpha}, \vec{\beta}) = \langle\Psi_{j_S}^-|\hat{P}^c(\vec{\alpha}) \otimes \hat{P}^c(\vec{\beta})|\Psi_{j_S}^-\rangle$. The CHSH inequality (4.2) is violated for parity measurements in the singlet state for arbitrarily large spins [90, 15].

To consider violation of the inequality with bounded RFs we introduce a coherent state of length j_{RF} for each observer, and replace the projectors $\hat{\Pi}_m$ in (4.17) with the POVM from Eq. (4.1). When the measurement setting $\vec{\alpha} = (\vartheta, \varphi)$ is chosen, the coherent state $|\vec{\alpha}\rangle$ aligned in that direction is used. In the basis of the spin projection along the z axis, it reads

$$|\vec{\alpha}\rangle \equiv |\vartheta, \varphi\rangle = \sum_{m=-j_{RF}}^{j_{RF}} |m\rangle\binom{2j_{RF}}{j_{RF} + m}^{1/2} \cos^{j_{RF}+m}(\frac{\vartheta}{2}) \sin^{j_{RF}-m}(\frac{\vartheta}{2})e^{-im\varphi}.$$

The rotated POVM is given by $\hat{P}_{j_S\,m}^{j_{RF}}(\vec{\alpha}) = \langle\vec{\alpha}|\hat{\Pi}_{j_{RF}+m}|\vec{\alpha}\rangle$ and the corresponding parity operator by $\hat{P}_{j_S}^{j_{RF}}(\vec{\alpha}) = \sum_{m=-j_S}^{j_S} (-1)^{j_S-m}\hat{P}_{j_S\,m}^{j_{RF}}(\vec{\alpha})$. Finally, the RF-dependent correlations read

$$E_{j_{RF}}(\vec{\alpha}, \vec{\beta}) = \langle\Psi_{j_S}^-|\hat{P}_{j_S}^{j_{RF}}(\vec{\alpha}) \otimes \hat{P}_{j_S}^{j_{RF}}(\vec{\beta})|\Psi_{j_S}^-\rangle. \tag{4.18}$$

We consider the situation where all the measurement angles are chosen in the same plane ($\varphi = 0$), with the first observer choosing between settings ϑ_1 and ϑ_3 and the second between ϑ_2 and ϑ_4. Taking $\vartheta_1 - \vartheta_2 = \vartheta_2 - \vartheta_3 = \vartheta_3 - \vartheta_4 \equiv \Delta\vartheta$, the CHSH inequality reads

$$S_{j_{RF}} = \left|3E_{j_{RF}}(\Delta\vartheta) - E_{j_{RF}}(3\Delta\vartheta)\right| \leq 2.$$

$j_S =$	1/2	1	3/2	2	5/2	3	7/2	4	9/2	5	11/2	6
$j_{RF} \geq$	7/2	23/2	45/2	73/2	107/2	147/2	193/2	123	152	369/2	220	259

Table 4.1: Minimal size of the spin reference frame j_{RF} necessary to observe violation of local realism in a pair of maximally-entangled spin-j_S particles (numerical calculation). The data are plotted in Fig. 4.2.

For classical reference frames, the angle difference which maximises S in the limit of large spin j_S is $\Delta\vartheta = \frac{x}{2j_S+1}$, with $x = 1.054$. Note that the angle difference is inversely proportional to the spin size. In the case of bounded RFs of finite size j_{RF}, the correlation (4.18) is hard to compute analytically, primarily due to the presence of a large number of non-trivial Clebsch-Gordan coefficients. It is possible however to evaluate it numerically, together with the corresponding CHSH expression. The numerical findings, shown in Tab. 4.1, suggest that one needs the size of the RFs to scale at least quadratically with the size of entangled spins in order to observe violation of the inequality.

We can give a heuristic argument to support the numerical findings. Consider a coherent state of length j_{RF} pointing in a direction $(\vartheta, \varphi = 0)$ and a measurement of spin projection along the z-axis. The probability to obtain outcome m for the spin z component obeys a binomial distribution $p(m) = \binom{2j_{RF}}{j_{RF}+m} q^{j_{RF}+m}(1-q)^{j_{RF}-m}$, where $q = \cos^2(\frac{\vartheta}{2})$. For large j_{RF} this is approximately a Gaussian centred in $j_{RF}\cos\vartheta$ and with variance $\sigma^2 = \frac{1}{2}j_{RF}\sin(\vartheta) \sim j_{RF}$. It can be visualised as an arrow pointing toward ϑ with an angle uncertainty $\frac{1}{\sigma} \sim \frac{1}{\sqrt{2j_{RF}}}$. Using this as a RF it is impossible to distinguish between directions at angles closer than this amount. On the other hand, violation of Bell inequality requires us to measure setting directions at angles that differ at the order of $\Delta\vartheta \sim \frac{1}{j_S}$. To achieve this precision one needs $\frac{1}{\sigma} < \Delta\vartheta$, which gives the heuristic bound $j_{RF} > j_S{}^2$. Fitting our numerical results with a quadratic law we indeed find the formula $j_{RF} \simeq 6j_S^2 + 6j_S$. The quadratic curve, together with the numerical data, is plotted in Fig. 4.2. (For higher order fits we obtain coefficients close to zero for the powers higher than two).

In summary, we have shown how a bounded RF limits the ability of entangled systems to exhibit genuine quantum features, as characterised by violation of Bell's inequalities. This can be relevant in situations where, to implement quantum information tasks, only relational degrees of freedom can be exploited (for example, when the quantum channel is subject to a global noise). We focused on the restrictions derived from the lack of a directional RF, considering other restrictions would impose additional requirements on the resources needed (see, e.g., [104]). Our results suggest that a fundamental limitation on the appearance of quantum behaviour at the macroscopic level can arise from the finiteness of re-
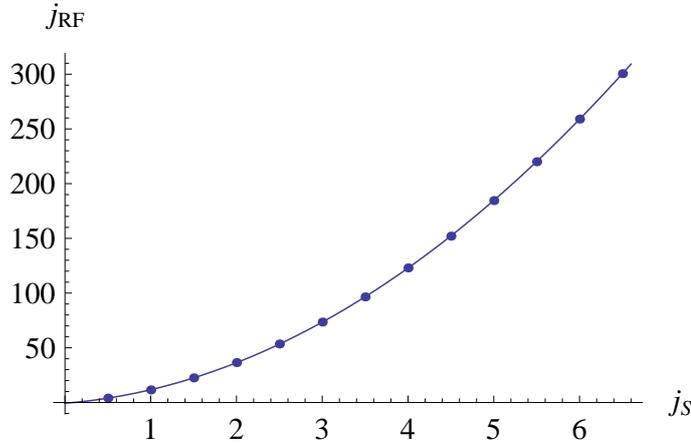
Figure 4.2: Minimal size of (spin) reference frame j_{RF} needed for violation of the Bell inequality for measurements on a pair of entangled spins of size j_S. The dots are calculated numerically, the line is the extrapolated fit $j_{RF} \simeq 6j_S^2 + 6j_S$.

sources that can be used to measure it. For example, a small iron magnet can have a magnetic field of around $100\,G$. According to our analysis, even if an entangled state of spin size $j_S \simeq \frac{\hbar 100\,G}{\mu_B} \simeq 10^{21}$ (μ_B is the Bohr magneton) were available, no violation of local realism is possible, if the RF used does not correspond to a magnetic field of the order of at least $10^4\,G$, which is much larger than what can be generally found in nature (but still not impossible to be produced).

According to the theory of decoherence [105], quantum correlations in a system are lost due to its interaction with the environment but correlations between system and environment are anyway retained. However, these correlations have no operational meaning unless a sufficiently strong RF is available. In everyday experience the size of the RFs used does not exceed that of the environment involved in the decoherence process, whereas our analysis suggests that at least a quadratic scaling would be required to demonstrate the existence of the quantum correlations.

Chapter 5

Quantum Causal Relations

Summary

The notion of causal order as an operationally-defined concept is considered. The causal order between a pair of events is defined in terms of the possibility of signalling. We pose the question whether in general operationally-defined theories, and in particular in quantum theory, events always need to be ordered in a given sequence. We consider a particular task, to be performed by two agents, that allows detecting whether the actions of the agents can be ordered according to a definite causal structure. If the actions are causally ordered, it is possible to derive a *causal inequality*, namely an upper bound on the probability of successfully performing the task. This is directly analogous to the famous violation of local realism: quantum systems allow performing a task—the violation of the Bell inequality—which is impossible if the measured quantities have pre-defined local values. The inequality considered here, unlike Bell's, concerns signalling correlations: it is based on a task that involves communication between two parties. Nevertheless, it cannot be violated if this communication takes place in a causal spacetime (independently of the physical systems used, be they classical, quantum, or even more general).

We further consider a novel framework for quantum correlations, based on the assumption that such correlations are produced by local operations that can be fully described by quantum mechanics. We do not, however, impose any constraint on the possible causal relations between the operations, not even the existence of a global spacetime on which the operations can be embedded. We derive a full characterisation of the most general correlations within the new formalism, including the special case of causally ordered ones. We further find an example of correlations that allow violating the causal inequality, showing that local quantum mechanics is consistent with the lack of a globally defined causal structure. We

also show that if locally *classical* operations are considered instead of quantum ones, it is always possible to embed the resulting correlations in a definite causal structure. We finally discuss some of the several possible implications of the results found.

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- O. Oreshkov, F. Costa, and Č. Brukner,
  "Quantum correlations with no causal order",
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5.1   An Operational Approach to Causal Relations

Recently, significant progress has been made in understanding quantum theory and the structure of quantum correlations in the context of operationalism, where primitive laboratory procedures, like measurements and preparations, are basic ingredients [106, 107, 108, 109, 110, 111, 112, 113]. Thus far, the ubiquitous approach towards understanding quantum correlations has been concerned primarily with space-like separated experiments, the main challenge being the identification of a complete set of physical principles which select the spatial quantum correlations out of the strictly larger class of no-signalling ones [114, 115, 116, 117, 118, 119, 120]. In this line of research, spacetime is typically regarded as a given, predefined "stage" in which the causal relations between events are defined. However, in a purely operational approach one should not rely on pre-existing notions of space, time, or any causal structure, but rather attempt to understand such notions in terms of primitive laboratory procedures within some general probabilistic framework.

A way to treat causal relations operationally is through the notion of *signalling*. Consider a generic bipartite experiment where to parties, *A* and *B*, perform some measurements using settings *a* and *b* and observe outcomes *x* and *y*, respectively. The statistics of the experiment is defined by the conditional probability

$$P(xy|ab). \tag{5.1}$$

We say that *A* cannot signal to *B* if the probability for observing *y* does not depend on *a*:

$$P(y|ab) := \sum_x P(xy|ab) = P(y|b),$$

If, on the other hand, correlations are found between *a* and *y*, signalling from *A* to *B* is possible (signalling from *B* to *A* is similarly defined).

If no additional assumption is made, the probabilities (5.1) are not subject to any constraint. It is however useful to delimit the physical way in which such probabilities are generated. The case often considered is the one in which the measurements *A* and *B* are performed at space-like separation and therefore, in order to comply with special relativity, the probabilities (5.1) have to be non-signalling in both directions. Here we are interested in *deducing* the causal relation between events from the observed statistics, thus less restrictive conditions should be imposed. A possible way is to imagine that each measurement is localised in an arbitrarily small region, ideally a single point, of spacetime. Given this assumption, one can deduce the causal relation between *A* and *B* (past-future, future-past, or space-like) from the direction of signalling in the probabilities (5.1) produced[1].

A different possibility, which will be exploited here, is to assume that each measurement is performed in a *closed laboratory*, which can be pictured as a finite region of spacetime bounded by two space-like surfaces, such that physical systems can enter in the laboratory only from the past surface and can exit only from the future one, while no exchange of information is possible through the time-like boundaries of the region. This implies that information can be sent from a laboratory *A* to a laboratory *B* only if the "entrance" of *B* (i.e. its past space-like boundary) is in the causal future of the "exit" of *A* (i.e. its future space-like boundary), thus the possible signalling relations between closed laboratories are the same as the possible causal relations between the spacetime points contained in the laboratories. Using the idea of closed laboratories thus allows avoiding the notion of "arbitrarily small" region and at the same allows identifying signalling relations with the underlying causal structure. In both cases it is necessary, in order to single out the class of possible probabilities (5.1) that can be produced, to specify the physical theory describing the operations that can be performed in the local region[2].

In usual situations, where the local operations can be embedded in a global spacetime (free of closed time-like curves), signalling between closed laboratories is possible at most in one direction. More generally, if the position of the local laboratories is not known with certainty, probabilistic mixtures of one-way

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[1]We assume here that measurements can be repeated an arbitrary number of times. This means that, strictly, the measurements *A* and *B* cannot be performed in the same spacetime regions for different runs of the experiment. We can however imagine that the spacetime coordinates defining these regions, operationally-defined with respect to physical clocks, rulers, etc, are reproduced in each run (e.g. by restarting the clocks at the beginning of every new experimental run).

[2]In fact, the notion of spacetime regions in which the operations are performed is not necessary, at the most general level: the class of operations that an agent can perform on a single system can be used as an abstract definition of closed laboratory.

signalling probabilities can be produced:

$$P(xy|ab) = qP^{B \nleq A}(xy|ab) + (1 - q)P^{A \nleq B}(xy|ab), \qquad 0 \leq q \leq 1, \qquad (5.2)$$

where $P^{B \nleq A}$ represents a probability distribution that does not allow signalling from B to A, i.e. $P^{B \nleq A}(x|ab) = P^{B \nleq A}(x|a)$, while $P^{A \nleq B}$ is no-signalling from A to B, $P^{A \nleq B}(y|ab) = P^{A \nleq B}(y|b)$. The main question addressed in this chapter is whether local operations must necessarily produce probabilities of this form. Alternatively, the question is whether more general causal relations are possible, once no global causal structure is assumed.

In order to appreciate the non-trivial nature of the problem, consider a deterministic model in which each party receives a classical variable, which can take the values $\lambda = 0, 1$. Let us call λ^{A_1}, λ^{A_2} the value of the variable before and after passing through the laboratory A, while λ^{B_1}, λ^{B_2} denote the variable's values before and after passing through B, respectively. Imagine now a hypothetical situation in which A and B cannot be embedded in a global causal structure, for example, consider the case where perfect correlations can be established in both directions: $\lambda^{A_2} = \lambda^{B_1}$, $\lambda^{B_2} = \lambda^{A_1}$. Signalling is possible in both directions, simply by performing operations in which the measurement outcomes are the input variables, $x = \lambda^{A_1}$, $y = \lambda^{B_1}$, and the "settings" determine the output variables, $a = \lambda^{A_2}$, $b = \lambda^{B_2}$. However, our assumption is that in each closed laboratory *all* possible operations can be performed (in this case, all possible functions $\{0, 1\} \rightarrow \{0, 1\}$). Imagine that the operation $\lambda^{A_1} \rightarrow \lambda^{A_2} = \lambda^{A_1}$ is performed in the laboratory A and the operation $\lambda^{B_1} \rightarrow \lambda^{B_2} = \lambda^{B_1} \oplus 1$ ($\oplus$ denotes the sum modulo 2) is performed in B. From the postulated perfect correlations it follows

$$\lambda^{A_1} = \lambda^{B_2} = \lambda^{B_1} \oplus 1 = \lambda^{A_2} \oplus 1 = \lambda^{A_1} \oplus 1,$$

from which one can deduce

$$\lambda^{A_1} = \lambda^{A_1} \oplus 1 \Rightarrow 0 = 1.$$

This is an example of the classical "grandfather paradox" and shows that perfect two-way signalling correlations are incompatible with local deterministic operations. As we are going to see, a stronger result holds: if the local operations are all possible classical stochastic operations, then only probabilities of the form (5.2) can be produced. Surprisingly, this is not true if locally quantum mechanics is assumed instead.

Note that, in order to interpret the correlations in (5.1) as the effects of a causal influence, a prior distinction is necessary between *freely chosen* settings, a and b, and *observed* outcomes, x and y. According to Bell [121], freely-chosen variables are, by definition, those that are only correlated with their future light cones.

Although this is a viable definition to investigate the limitations that a causal structure imposes on possible experiments, which we will consider in Sec. 5.2, it cannot be adopted in situations where no global causal structure is pre-defined. In such a situation, one can adopt the following notion: a variable *a* is "freely chosen" if it can be correlated with an arbitrary variable external to the experiment. This notion is well-defined as long as it is possible to determine which variables are relevant for the "experiment" and which ones can be considered as external, a necessary assumption in any operational framework.

5.2   Causal Inequality

The general setting that we consider involves a number of experimenters—Alice, Bob, etc.—who reside in separate laboratories. At a given run of the experiment, each of them receives a physical system (for instance, a spin-$\frac{1}{2}$ particle) and performs operations on it (e.g. measurements or rotations of the spin), after which she/he sends the system out of the laboratory. We assume that during the operations of each experimenter the respective laboratory is isolated from the rest of the world—it is only opened for the system to come in and to go out, but between these two events it is kept closed. It is easy to see that under this assumption, causal order puts a restriction on the way in which the parties can communicate during a given run. For instance, imagine that Alice can send a signal to Bob. Since Bob can only receive a signal through the system entering his laboratory, this means that Alice must act on her system before that. But this implies that Bob cannot send a signal to Alice since each party receives a system only once. Therefore, bidirectional signalling is forbidden. (More generally, probabilities of the form (5.2) can be generated if the order between the laboratories is not known with certainty.)

Consider, in particular, the following communication task to be performed by two parties, Alice and Bob. After a given party receives the system in her/his laboratory, she/he will have to toss a coin (or use any other means) to obtain a random bit. Denote the bits generated by Alice and Bob in this way by *a* and *b*, respectively. In addition, Bob will have to generate another random bit b', whose value, 0 or 1, will specify their goal: if $b' = 0$, Bob will have to communicate the bit *b* to Alice, while if $b' = 1$, he will have to guess the bit *a*. Without loss of generality, we will assume that the parties always produce a guess, denoted by *x* and *y* for Alice and Bob respectively, for the bit of the other (although the guess may not count depending on the value of b'). Their goal is to maximise the probability of success

$$p_{succ} := \frac{1}{2} \left[P(x = b | b' = 0) + P(y = a | b' = 1) \right]. \tag{5.3}$$
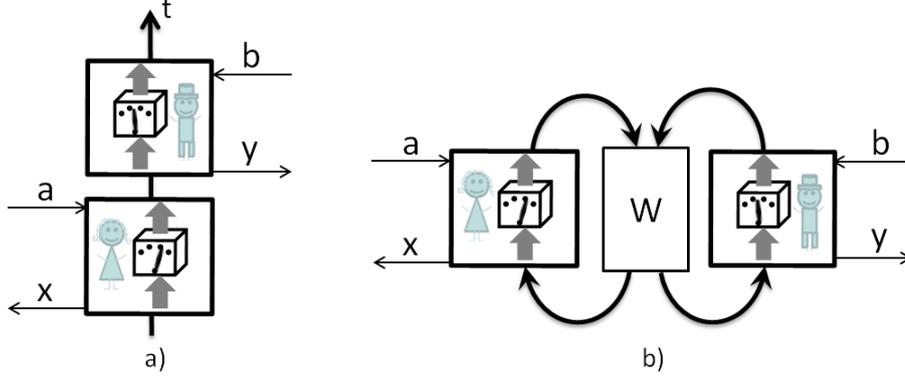
Figure 5.1: Strategy for accomplishing communication task by using processes with (a) definite and (b) indefinite causal order. (a) There exists a global background time according to which Alice's actions are strictly before Bob's. She sends her input a to Bob, who can read it out at some later time and give his estimate $y = a$. However, Bob cannot send his bit b to Alice as the system passes through her laboratory at some earlier time. Consequently, she can only make a random guess of Bob's bit. This results in a probability of success of $3/4$. (b) If the assumption of a definite order is dropped, it is possible to devise a resource (i.e. a process matrix W) and a strategy that enables a probability of success $\frac{2+\sqrt{2}}{4} > 3/4$ (see text).

If all events obey causal order, no strategy can allow Alice and Bob to exceed the bound

$$p_{succ}^{CO} \leq 3/4. \tag{5.4}$$

Indeed, as argued above, in any particular order of events, there can be at most unidirectional signalling between the parties, which means that at least one of the following must be true: Alice cannot signal to Bob, or Bob cannot signal to Alice. Consider, for example, a case where Bob cannot signal to Alice. Then, if $b' = 1$, they could in principle achieve up to $P(y = a|b' = 1) = 1$ (for instance, if Alice operates on her system before Bob, she could encode information about the bit a in the system and send it to him). However, if $b' = 0$, the best guess that Alice can make is a random one, resulting in $P(x = b|b' = 0) = 1/2$ (see Fig. 5.1). Hence, the overall probability of success in this case will satisfy $p_{succ} \leq 3/4$. The same holds if Alice cannot signal to Bob. It is easy to see that no probabilistic strategy can increase the probability of success, that is, all probabilities of the form (5.2) necessarily produce the bound (5.4).

More generally, it is possible to derive the causal inequality (5.4) from the following formal assumption:

(i) *Causal structure*—The main events in the task (a system entering a local laboratory, the parties obtaining the bits a, b, and b', and producing the guesses x and y) are localised in a causal structure. [A causal structure (such as spacetime)

is a set of event locations equipped with a partial order $\preceq$ that defines the possible directions of signalling. If $A \preceq B$, we say that A is in the *causal past* of B (or B is in the *causal future* of A). In this case, signalling from A to B is possible, but not from B to A. For more details on causal structures, see Appendix C.1.]

(ii) *Free choice*—Each of the bits a, b, and b' can only be correlated with events in its causal future (this concerns only events relevant to the task). We assume also that each of them takes values 0 or 1 with probability $1/2$.

(iii) *Closed laboratories*—x can be correlated with b only if $b \preceq A_1$, and y can be correlated with a only if $a \preceq B_1$ (this reflects the idea that each party can receive information only about events taking place in the causal past of the system entering her/his laboratory).

A formal derivation of the inequality from these assumptions is presented in Appendix C.1.

Interestingly, we will see that if the local laboratories are described by quantum mechanics, but no assumption about a global causal structure is made, it is in principle possible to violate the causal inequality in physical situations in which one would have all the reasons to believe that the bits are chosen freely and the laboratories are closed. This would imply that (i) does not hold.

5.3 Framework for Local Quantum Mechanics

The most studied, almost epitomical, quantum correlations are the non-signalling ones, such as those obtained when Alice and Bob perform measurements on two parts of an entangled state. Signalling quantum correlations exist as well, such as those arising when Alice operates on a system which is subsequently sent through a quantum channel to Bob who operates on it after that. The usual quantum formalism does not consider more general possibilities, since it does assume a global causal structure. Here we want to drop the latter assumption while retaining the validity of quantum mechanics locally. For this purpose, we consider a multipartite setting of the type outlined earlier, where each party performs an operation on a system passing once through her/his laboratory, but we make no assumption about the spatio-temporal location of these experiments, not even that there exists a spacetime or any causal structure in which they could be positioned (see Fig. 5.2). Our framework is thus based on the following central premise:

> *Local quantum mechanics*—The local operations of each party are described by quantum mechanics.
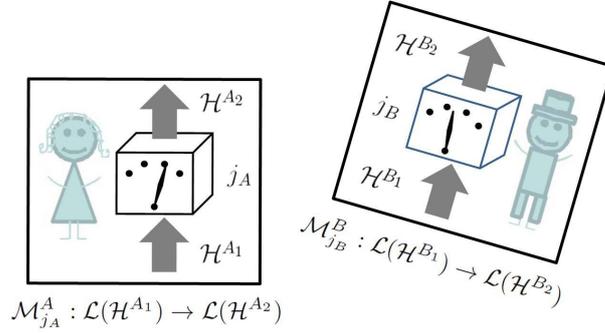
Figure 5.2: Quantum correlations with no assumption of a pre-existing causal structure, in particular of a pre-existing background time (here illustrated by the "shifted" relative orientation of the two laboratories). While the global causal order of events in the two laboratories is not fixed in advance and in general even not definite, the two agents, Alice and Bob, are each certain about the causal order of events in their respective laboratories.

5.3.1   Process Matrices

To be specific, we assume that one party, say Alice, can perform all the operations she could perform in a closed laboratory, as described in the standard spacetime formulation of quantum mechanics. These are defined as the set of *quantum instruments* [122] with an input Hilbert space $\mathcal{H}^{A_1}$ (the system coming in) and an output Hilbert space $\mathcal{H}^{A_2}$ (the system going out). (The set of allowed quantum operations can be used as a definition of "closed quantum laboratory" with no reference to a global causal structure.) A quantum instrument can most generally be realised by applying a joint unitary transformation on the input system plus an ancilla, followed by a projective measurement on part of the resulting joint system, which leaves the other part as an output. When Alice uses a given instrument, she registers one out of a set of possible outcomes, labeled by $j = 1, \ldots, n$. Each outcome induces a specific transformation from the input to the output, which corresponds to a completely positive (CP) trace-nonincreasing map [123] $\mathcal{M}_j^A : \mathcal{L}(\mathcal{H}^{A_1}) \rightarrow \mathcal{L}(\mathcal{H}^{A_2})$, where $\mathcal{L}(\mathcal{H}^X)$, $X = A_1, A_2$, is the space of matrices over a Hilbert space $\mathcal{H}^X$ of dimension d_X. The action of each $\mathcal{M}_j^A$ on any matrix $\sigma \in \mathcal{L}(\mathcal{H}^{A_1})$ can be written as [123] $\mathcal{M}_j^A(\sigma) = \sum_{k=1}^m E_{jk} \sigma E_{jk}^\dagger$, $m = d^{A1} d^{A2}$, where the matrices $E_{jk} : \mathcal{H}^{A_1} \rightarrow \mathcal{H}^{A_2}$ satisfy $\sum_{k=1}^m E_{jk}^\dagger E_{jk} \leq \mathbb{1}^{A_1}$, $\forall j$. If the operation is performed on a quantum state described by a density matrix ρ, $\mathcal{M}_j^A(\rho)$ describes the updated state after the outcome j up to normalisation, while the probability to observe this outcome is given by $P\left(\mathcal{M}_j^A\right) = \text{Tr}\left[\mathcal{M}_j^A(\rho)\right]$. The set of CP maps $\left\{\mathcal{M}_j^A\right\}_{j=1}^n$ corresponding to all the possible outcomes of a quantum instrument has the property that $\sum_{j=1}^n \mathcal{M}_j^A$ is CP and trace-preserving (CPTP), or equivalently $\sum_{j=1}^n \sum_{k=1}^m E_{jk}^\dagger E_{jk} = \mathbb{1}^{A_1}$, which reflects the fact that the probability to observe any

of the possible outcomes is unity. A CPTP map itself corresponds to an instrument with a single outcome which occurs with certainty.

In the case of more than one party, the set of local outcomes corresponds to a set of CP maps $\mathcal{M}_i^A, \mathcal{M}_j^B, \cdots$. A complete list of probabilities $P\left(\mathcal{M}_i^A, \mathcal{M}_j^B, \cdots\right)$ for all possible local outcomes will be called *process*[3]. A process can be seen as an extension of the notion of state as a list of probabilities for detection results [108] described by a positive operator-valued measure (POVM), which takes into account the transformation of the system after the measurement and can thus capture more general scenarios than just local detection. Here we will consider explicitly only the case of two parties (the generalisation to arbitrarily many parties is straightforward). We want to characterise the most general probability distributions for a pair of outcomes i, j, corresponding to CP maps $\mathcal{M}_i^A$, $\mathcal{M}_j^B$, to be observed, that is, to characterise all bipartite processes.

Linearity of Processes In quantum mechanics, operations obey a specific algebraic structure that reflects the operational relations between laboratory procedures [108]. Since we are assuming that local operations are described by quantum mechanics, we also have to assume that the algebraic structure of such operations is preserved with the usual operational interpretation. From this assumption it possible to prove that probabilities are bilinear functions of CP maps.

Consider first an instrument $\{\tilde{\mathcal{M}}_j\}_{j=1}^n$ defined as the randomisation of two different instruments $\{\mathcal{M}_j\}_{j=1}^n$ and $\{\mathcal{N}_j\}_{j=1}^n$, where the first is performed with probability p and the second with probability $(1-p)$. The probability to observe the outcome j is, by definition, $P(\tilde{\mathcal{M}}_j) = pP(\mathcal{M}_j) + (1-p)P(\mathcal{N}_j)$. In quantum mechanics randomisation is described as a convex linear combination, $\tilde{\mathcal{M}}_j = p\mathcal{M}_j + (1-p)\mathcal{N}_j$. We can then conclude that the probability must respect linear convex combinations: $P\left(p\mathcal{M}_j + (1-p)\mathcal{N}_j\right) = pP(\mathcal{M}_j) + (1-p)P(\mathcal{M}_j)$. Consider then the coarse-graining of an instrument $\{\mathcal{M}_j\}_{j=1}^n$. This is realised when two or more outcomes, for example those corresponding to the labels $j = n-1$ and $j = n$, are treated as a single one. In the resulting instrument $\{\tilde{\mathcal{M}}_j\}_{j=1}^{n-1}$ all non coarse-grained outcomes correspond to the original CP maps $\tilde{\mathcal{M}}_j = \mathcal{M}_j$ for $j = 1, \ldots n-2$, while the probability of the coarse-grained outcome is given by $P(\tilde{\mathcal{M}}_{n-1}) = P(\mathcal{M}_{n-1}) + P(\mathcal{M}_n)$. In quantum mechanics, the CP map corresponding to the coarse graining of two outcomes is represented by the sum of the respective CP maps, $\tilde{\mathcal{M}}_{n-1} = \mathcal{M}_{n-1} + \mathcal{M}_n$, from which it follows that $P(\mathcal{M}_{n-1} + \mathcal{M}_n) = P(\mathcal{M}_{n-1}) + P(\mathcal{M}_n)$. Randomisation and coarse graining together impose linearity. The argument can be repeated

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[3]It is implicitly assumed that the joint probabilities are *noncontextual*, namely that they are independent of any variable concerning the concrete implementation of the local CP maps. For example, the probability for a pair of maps $\mathcal{M}_i^A$, $\mathcal{M}_j^B$ to be realised should not depend on the particular set $\{\mathcal{M}_1^A, ..., \mathcal{M}_i^A, ..., \mathcal{M}_n^A\}$ of possible CP maps associated with Alice's operation.

for two (or more) parties, yielding the conclusion that all bipartite probabilities compatible with a local quantum mechanical description are bilinear functions, $P\left(\mathcal{M}_i^A, \mathcal{M}_j^B\right) = \omega\left(\mathcal{M}_i^A, \mathcal{M}_j^B\right) \in [0, 1]$, of the local CP and trace-nonincreasing maps $\mathcal{M}_i^A, \mathcal{M}_j^B$. Thus the study of the most general bipartite quantum correlations reduces to the study of bilinear functions of CP maps.

Process Matrices   It is convenient to represent CP maps as positive semi-definite matrices via the Choi-Jamiołkowsky (CJ) isomorphism [124, 125]. The CJ matrix $M_i^{A_1A_2} \in \mathcal{L}(\mathcal{H}^{A_1} \otimes \mathcal{H}^{A_2})$ corresponding to a linear map $\mathcal{M}_i : \mathcal{L}(\mathcal{H}^{A_1}) \rightarrow \mathcal{L}(\mathcal{H}^{A_2})$ is defined as $M_i^{A_1A_2} := [\mathcal{I} \otimes \mathcal{M}_i (|\phi^+\rangle\langle\phi^+|)]^{\mathrm{T}}$, where $|\phi^+\rangle = \sum_{j=1}^{d_{A_1}} |jj\rangle \in \mathcal{H}^{A_1} \otimes \mathcal{H}^{A_1}$ is a (not normalised) maximally entangled state, the set of states $\{|j\rangle\}_{j=1}^{d_{A_1}}$ is an orthonormal basis of $\mathcal{H}^{A_1}$, $\mathcal{I}$ is the identity map, and T denotes matrix transposition (the transposition, absent in the original definition, is introduced for later convenience).

Thanks to the CJ isomorphism, it is possible to represent bilinear functions of CP maps as bilinear functions of matrices: $\omega \leftrightarrow \tilde{\omega} : \mathcal{L}(\mathcal{H}^{A_1} \otimes \mathcal{H}^{A_2}) \times \mathcal{L}(\mathcal{H}^{B_1} \otimes \mathcal{H}^{B_2}) \rightarrow \mathbb{R}$. In general, multilinear functions on a set of vector spaces $V^1 \times V^2 \times \ldots$ are isomorphic to linear functions on $V^1 \otimes V^2 \otimes \ldots$, hence the probabilities can be written as linear functions on $\mathcal{L}(\mathcal{H}^{A_1} \otimes \mathcal{H}^{A_2} \otimes \mathcal{H}^{B_1} \otimes \mathcal{H}^{B_2})$. Using the Hilbert-Schmidt scalar product, we can identify each real linear function with an element of the same space, $\tilde{\omega} \leftrightarrow W^{A_1A_2B_1B_2} \in \mathcal{L}(\mathcal{H}^{A_1} \otimes \mathcal{H}^{A_2} \otimes \mathcal{H}^{B_1} \otimes \mathcal{H}^{B_2})$. The probability for two measurement outcomes can thus be expressed as a bilinear function of the corresponding CJ operators as follows:

$$P\left(\mathcal{M}_i^A, \mathcal{M}_j^B\right) = \mathrm{Tr}\left[W^{A_1A_2B_1B_2}\left(M_i^{A_1A_2} \otimes M_j^{B_1B_2}\right)\right], \qquad (5.5)$$

where $W^{A_1A_2B_1B_2}$ is a matrix in $\mathcal{L}(\mathcal{H}^{A_1} \otimes \mathcal{H}^{A_2} \otimes \mathcal{H}^{B_1} \otimes \mathcal{H}^{B_2})$.

The matrix W should be such that probabilities are non-negative for any pair of CP maps $\mathcal{M}_i^A, \mathcal{M}_j^B$. This imposes the restriction that W is *positive on pure tensors* (POPT) [126] with respect to the partition $A_1A_2 - B_1B_2$. By definition, these are matrices such that

$$\mathrm{Tr}\left[W^{A_1A_2B_1B_2}\left(M^{A_1A_2} \otimes M^{B_1B_2}\right)\right] \geq 0, \qquad \forall M^{A_1A_2} \geq 0, M^{B_1B_2} \geq 0. \qquad (5.6)$$

The condition has to be imposed for arbitrary positive semidefinite matrices $M^{A_1A_2}$ and $M^{B_1B_2}$ because these are the CJ matrices of CP maps. We additionally assume that the parties can share ancillary entangled states and use them in their local operations[4]. With this we mean that each party can extend the input space of

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[4]We impose this assumption because we want our formalism to be as close as possible to standard quantum mechanics, apart from the global causal structure. Without this assumption,

his/her operations to the ancillas, which we denote by A'_1 and B'_1 for Alice and Bob, respectively. The ancillas can be prepared in an arbitrary state. The extended CP maps are defined as $\mathcal{M}^A : \mathcal{L}(\mathcal{H}^{A'_1} \otimes \mathcal{H}^{A_1}) \to \mathcal{L}(\mathcal{H}^{A_2})$, $\mathcal{M}^B : \mathcal{L}(\mathcal{H}^{B'_1} \otimes \mathcal{H}^{B_1}) \to \mathcal{L}(\mathcal{H}^{B_2})$ (one can similarly extend the output systems, but this is not necessary for our argument). Given the original process matrix $W^{A_1 A_2 B_1 B_2}$, we require that its extension to the ancillary systems in a state $\psi^{A'_1 B'_1}$ has the following properties. Firstly, if only operations on the ancillas are non-trivial, namely if the CP maps have the form $\mathcal{M}^{A'} \otimes \mathcal{M}^{B'} \otimes \mathcal{I}^{AB}$, the system $A'_1 B'_1$ produces probabilities as the state $\psi^{A'_1 B'_1}$. Secondly, if only operations on the systems $A_1 B_1$ are non-trivial, with CP maps of the form $\mathcal{I}^{A'B'} \otimes \mathcal{M}^A \otimes \mathcal{M}^B$, the probabilities are given by the expression (5.5) with the original $W^{A_1 A_2 B_1 B_2}$. Since, in the current formalism, a state $\psi^{A'_1 B'_1}$ is represented by a process matrix $\psi^{A'_1 B'_1}$, these requirements imply that the extended process matrix is given by $W^{A'_1 A_1 A_2 B'_1 B_1 B_2} = \psi^{A'_1 B'_1} \otimes W^{A_1 A_2 B_1 B_2}$. If we then require that the probabilities for extended operations are non-negative, one has

$$\mathrm{Tr}\left[\psi^{A'_1 B'_1} \otimes W^{A_1 A_2 B_1 B_2} \left(M^{A'_1 A_1 A_2} \otimes M^{B'_1 B_1 B_2}\right)\right] \geq 0, \qquad (5.7)$$
$$\forall M^{A'_1 A_1 A_2}, M^{B'_1 B_1 B_2}, \psi^{A'_1 B'_1} \geq 0.$$

It was shown in Ref. [126] that condition (5.7) is satisfied if and only if $W^{A_1 A_2 B_1 B_2}$ is positive semidefinite (a class strictly smaller than POPT).

Furthermore, the probability for any pair of CPTP maps $\mathcal{M}^A$, $\mathcal{M}^B$ to be realised must be unity (they correspond to instruments with a single outcome). Since a map $\mathcal{M}^A$ is CPTP if and only if its CJ operator satisfies $M^{A_1 A_2} \geq 0$ and $\mathrm{Tr}_{A_2} M^{A_1 A_2} = \mathbb{1}^{A_1}$ (similarly for $\mathcal{M}^B$), we conclude that all bipartite probabilities compatible with local quantum mechanics are generated by matrices W that satisfy

$$W^{A_1 A_2 B_1 B_2} \geq 0 \ [\text{ non-negative probabilities}], \qquad (5.8)$$
$$\mathrm{Tr}\left[W^{A_1 A_2 B_1 B_2} \left(M^{A_1 A_2} \otimes M^{B_1 B_2}\right)\right] = 1 \qquad (5.9)$$
$$\forall M^{A_1 A_2}, M^{B_1 B_2} > 0, \ \mathrm{Tr}_{A_2} M^{A_1 A_2} = \mathbb{1}^{A_1}, \mathrm{Tr}_{B_2} M^{B_1 B_2} = \mathbb{1}^{B_1}$$
$$[\text{ sum of probabilities is one}].$$

We will refer to a matrix $W^{A_1 A_2 B_1 B_2}$ that satisfies these conditions as a *process matrix*. Conditions equivalent to Eqs. (5.8) and (5.9) were first derived as part of the definition of a "quantum comb" [127], an object that formalises quantum networks. Combs, however, are subject to additional conditions fixing a definite causal order, which are not assumed here.

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general POPT processes would be allowed, thus in particular all the processes here considered. The final result, the existence of a process that violates causal order, would thus hold in this scenario too.

5.3.2 Causally Separable Processes

A process matrix can be understood as a generalisation of a density matrix and Eq. (5.5) as a generalisation of Born's rule. In fact, when the output systems A_2, B_2 are taken to be one-dimensional (i.e. each party performs a measurement after which the system is discarded), the expression above reduces to $P\left(\mathcal{M}_i^A, \mathcal{M}_j^B\right) = \text{Tr}\left[W^{A_1B_1}\left(M_i^{A_1} \otimes M_i^{B_1}\right)\right]$, where now M_i^A, M_j^B are elements of local POVMs and Eq. (5.9) becomes $\text{Tr}\, W^{A_1B_1} = 1$, i.e. $W^{A_1B_1}$ is a quantum state. This implies that a quantum state $\rho^{A_1B_1}$ shared by Alice and Bob is generally represented by the process matrix $W^{A_1A_2B_1B_2} = \rho^{A_1B_1} \otimes \mathbb{1}^{A_2B_2}$. Signalling correlations can also be expressed in terms of process matrices. For instance, the situation where Bob is given a state ρ^{B_1} and his output is sent to Alice through a quantum channel C, which gives $P(\mathcal{M}_i^A, \mathcal{M}_j^B) = \text{Tr}\left[\mathcal{M}_i^A \circ C \circ \mathcal{M}_j^B\left(\rho^{B_1}\right)\right]$, is described by $W^{A_1A_2B_1B_2} = \mathbb{1}^{A_2} \otimes (C^{B_2A_1})^T \otimes \rho^{B_1}$, where $C^{B_2A_1}$ is the CJ matrix of the channel C from B_2 to A_1.

The most general bipartite situation typically encountered in quantum mechanics (i.e. one that can be expressed in terms of a quantum circuit) is a quantum channel with memory where, say, Bob operates on one part of an entangled state and his output plus the other part is transferred to Alice through a channel. This is described by a process matrix of the form $\mathbb{1}^{A_2} \otimes W^{A_1B_1B_2}$. Conversely, all process matrices of this form represent channels with memory [127]. This is the most general situation in which signalling from Alice to Bob is not possible, a relation that we will denote by $A \not\preceq B$ in accord with the causal notation introduced earlier. Process matrices of this kind will be denoted by $W^{A \not\preceq B}$ (note that for non-signalling processes, both $A \not\preceq B$ and $B \not\preceq A$ are true). As argued earlier, if all events are localised in a causal structure and Alice and Bob perform their experiments inside closed laboratories, at most unidirectional signalling between the laboratories is allowed. In a definite causal structure, it may still be the case that the location of each event, and thus the causal relation between events, is not known with certainty. A situation where $B \not\preceq A$ with probability $0 \leq q \leq 1$ and $A \not\preceq B$ with probability $1 - q$ is represented by a process matrix of the form

$$W^{A_1A_2B_1B_2} = qW^{B \not\preceq A} + (1-q)W^{A \not\preceq B}. \tag{5.10}$$

We will call processes of this kind *causally separable* (note that the decomposition (5.10) need not be unique since non-signalling processes can be included either in $W^{B \not\preceq A}$ or in $W^{A \not\preceq B}$). They represent the most general bipartite quantum processes for which the local experiments can be performed in closed laboratories embedded in a definite causal structure. In particular, they generate the most general quantum correlations between measurements that take place at definite (though possibly unknown) instants of time. It is clear by plugging the form (5.10) into (5.5) that causally separable processes generate probability distributions of the form (5.2)

and thus cannot be used to violate the causal inequality[5] (5.4).

5.4 A causally Nonseparable Process

The question whether all local quantum experiments can be embedded in a global causal structure corresponds to the question whether all process matrices are causally separable[6]. Mathematically, this corresponds to asking whether all matrices satisfying conditions (5.8, 5.9) can be decomposed in the form (5.10). In Appendix C.2, we provide a complete characterisation of the matrices satisfying (5.8, 5.9) via the terms allowed in their expansion in a Hilbert-Schmidt basis, which we relate to the possible directions of signalling they allow. The result is summarised in Tab. 5.1. In Tab. 5.2, the terms not appearing in a process matrix are listed, along with some possible interpretation (see also Appendix C.3).

$B \not\preceq A$	A_1, B_1, A_1B_1	A_2B_1	$A_1A_2B_1$
$A \not\preceq B$		A_1B_2	$A_1B_1B_2$
Causal order	States	Channels	Channels with memory
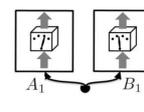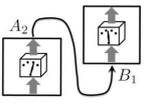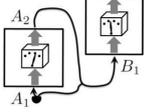
TAB. 5.1: Terms appearing in a process matrix. A matrix satisfying condition (5.8) can be expanded as $W^{A_1A_2B_1B_2} = \sum_{\mu\nu\lambda\gamma} w_{\mu\nu\lambda\gamma} \sigma_\mu^{A_1} \otimes \sigma_\nu^{A_2} \otimes \sigma_\lambda^{B_1} \otimes \sigma_\gamma^{B_2}$, $w_{\mu\nu\lambda\gamma} \in \mathbb{R}$, where the set of matrices $\{\sigma_\mu^X\}_{\mu=0}^{d_X^2-1}$, with $\sigma_0^X = \mathbb{1}^X$, $\mathrm{Tr}\sigma_\mu^X\sigma_\nu^X = d_X\delta_{\mu\nu}$, and $\mathrm{Tr}\sigma_j^X = 0$ for $j = 1, \ldots d_X^2 - 1$, provides a basis of $\mathcal{L}(\mathcal{H}^X)$. We refer to terms of the form $\sigma_i^{A_1} \otimes \mathbb{1}^{rest}$ ($i \geq 1$) as of the type A_1, terms of the form $\sigma_i^{A_1} \otimes \sigma_j^{A_2} \otimes \mathbb{1}^{rest}$ ($i, j \geq 1$) as of the type A_1A_2, and so on. In Appendix C.2 it is proven that a matrix satisfies condition (5.9) if and only if it contains the terms listed in this table. Each of the terms can allow signalling in at most one direction and can be realised in a situation in which either Bob's actions are not in the causal past of Alice's ($B \not\preceq A$) or vice versa ($A \not\preceq B$). The most general unidirectional process is a quantum channel with memory. Measurements of bipartite states that lead to non-signalling probabilities can be realised in both situations. The most general process matrix can contain terms from both rows and may not be decomposable into a mixture of quantum channels from Alice to Bob and from Bob to Alice.

---

[5]The classical "tosses" a, b can be encoded in the choice of the local operations, while the "guesses" x, y can be decoded from the outcome. Thus a probability (5.1) is generally reproduced by plugging into (5.5) matrices of the form $M_x^{A_1A_2}(a)$ and $M_y^{B_1B_2}(b)$

[6]Note that this is not a question about entanglement: all possible entangled states, and more generally all quantum circuits, correspond to matrices of the form $W^{B\not\preceq A}$ or $W^{A\not\preceq B}$, while the nonseparable processes we are looking for cannot be written as quantum circuits or even as probabilistic mixtures of different circuits.

$A_2, B_2, A_2 B_2$	$A_1 A_2, B_1 B_2$	$A_1 A_2 B_2, A_2 B_1 B_2$	$A_1 A_2 B_1 B_2$
Postselection	Local Loops	Local Loops & Postselection	Global Loops

TAB. 5.2: Terms not appearing in a process matrix. These terms are not compatible with local quantum mechanics because they yield non-unit probabilities for some completely positive trace-preserving maps. A possible interpretation of these terms within the present framework is that they correspond to statistical sub-ensembles of possible processes. For example, terms of the type A_2 can be understood as postselection. One specific case is when a system enters a laboratory in a maximally mixed state, is subject to the map $\mathcal{M}$ and, after going out of the laboratory, is measured to be in some state $|\psi\rangle$. The corresponding probability is given by $\mathrm{Tr}|\psi\rangle\langle\psi|\mathcal{M}(\frac{1\!\!1}{d})$, generated in the present formalism by $W^{A_1 A_2} = \frac{1\!\!1}{d}^{A_1} \otimes |\psi\rangle\langle\psi|^{A_2}$. Notably, correlations of the type $A_1 A_2$ have been exploited in models for describing closed time-like curves [128, 129], as is discussed in Appendix C.3. The pictures are only suggestive of the possible interpretations.

Using such a characterisation, it is simple to see that the following is a valid process matrix:

$$W^{A_1 A_2 B_1 B_2} = \frac{1}{4}\left[1\!\!1^{A_1 A_2 B_1 B_2} + \frac{1}{\sqrt{2}}\left(\sigma_z^{A_2}\sigma_z^{B_1} + \sigma_z^{A_1}\sigma_x^{B_1}\sigma_z^{B_2} \right) \right], \qquad (5.11)$$

where A_1, A_2, B_1, and B_2 are two-level systems (e.g. the spin degrees of freedom of a spin-$\frac{1}{2}$ particle) and σ_x and σ_z are the Pauli spin matrices.

As we are about to see, having such a resource Alice and Bob can play the game described in Sec. 5.2 and exceed the bound on the probability of success (5.4) imposed by causal order. Before delving into the proof, notice that if Bob measures in the z basis and detects one of the states $|z_\pm\rangle$, the corresponding CJ operator contains the factor $|z_\pm\rangle\langle z_\pm|^{B_1}$. Inserting this, together with Eq. (5.11), into the expression (5.5) for the probabilities, the term containing $\sigma_x^{B_1}$ in the process matrix is annihilated and what remains corresponds to a noisy channel from Alice to Bob. If Alice encodes her bit in the z basis with the CJ operator $|z_\pm\rangle\langle z_\pm|^{A_2}$, this channel allows Bob to guess Alice's bit with probability $P(y = a) = \frac{2+\sqrt{2}}{4}$. If, on the other hand, Bob measures in the x basis, Eq. (5.11) is reduced to a similar noisy channel from Bob to Alice. Bob is thus able to activate a channel in the desired direction by choosing the measurement basis (we refer to the Appendix for a detailed calculation and analysis of the protocol). In this way they can achieve

$$p_{succ} = \frac{2 + \sqrt{2}}{4} > \frac{3}{4} \qquad (5.12)$$

for the success probability (5.3), which proves that (5.11) is not causally separable.

Protocol for Violating the Causal Inequality   The process described by the matrix (5.11) can be exploited for the task described in Sec. 5.2 in the following way. Alice always measures the incoming qubit in the z basis, assigning the value $x = 0$ to the outcome $|z_+\rangle$ and $x = 1$ to $|z_-\rangle$. She then reprepares the qubit, encoding a in the same basis, and sends it away. Using the the inverse direction of the CJ isomorphism,

$$\mathcal{M}(\rho^{A_1}) := \left(\mathrm{Tr}_{A_1} \left[\rho^{A_1} M^{A_1 A_2} \right] \right)^{\mathrm{T}}, \tag{5.13}$$

it is easy to see that the CP map corresponding to the detection of a state $|\psi\rangle$ and repreparation of another state $|\phi\rangle$ has CJ matrix $|\psi\rangle\langle\psi|^{A_1} \otimes |\phi\rangle\langle\phi|^{A_2}$. Accordingly, the possible operations performed by Alice can be represented compactly by the CJ matrix

$$\xi^{A_1 A_2}(x, a) = \frac{1}{4} \left[\mathbb{1} + (-1)^x \sigma_z \right]^{A_1} \otimes \left[\mathbb{1} + (-1)^a \sigma_z \right]^{A_2}. \tag{5.14}$$

Bob adopts the following protocol. If he wants to read Alice's bit ($b' = 1$), he measures the incoming qubit in the z basis and assigns $y = 0$, $y = 1$ to the outcomes $|z_+\rangle$, $|z_-\rangle$, respectively (the repreparation is unimportant in this case). If he wants to send the bit ($b' = 0$), he measures in the x basis and, if the outcome is $|x_+\rangle$, he encodes b in the z basis of the outgoing qubit as $0 \rightarrow |z_+\rangle$, $1 \rightarrow |z_-\rangle$, while, if the outcome is $|x_-\rangle$, he encodes it as $0 \rightarrow |z_-\rangle$, $1 \rightarrow |z_+\rangle$. The CJ matrix representing Bob's CP maps is

$$\eta^{B_1 B_2}(y, b, b') = b' \eta_1^{B_1 B_2}(y, b) + (b' \oplus 1) \eta_2^{B_1 B_2}(y, b), \tag{5.15}$$

$$\eta_1^{B_1 B_2}(y, b) = \frac{1}{2} \left[\mathbb{1} + (-1)^y \sigma_z \right]^{B_1} \otimes \rho^{B_2}, \tag{5.16}$$

$$\eta_2^{B_1 B_2}(y, b) = \frac{1}{4} \left[\mathbb{1} + (-1)^y \sigma_x \right]^{B_1} \otimes \left[\mathbb{1} + (-1)^{b+y} \sigma_z \right]^{B_2}, \tag{5.17}$$

where ρ^{B_2} is the arbitrary state prepared when $b' = 1$ (with $\mathrm{Tr}\rho^{B_2} = 1$) and $\oplus$ denotes the sum modulo 2. Note that, in Eq. (5.17), Bob's assignment $|x_+\rangle \rightarrow y = 0$, $|x_-\rangle \rightarrow y = 1$ for the outcomes of his measurement is arbitrary, since, for $b' = 0$ he is not trying to correlate y with a.

The probabilities for different possible outcomes, when the described protocol is applied to the process (5.11), are given, according to (5.5), by

$$P(xy|abb') = \mathrm{Tr} \left[W^{A_1 A_2 B_1 B_2} \left(\xi^{A_1 A_2}(x, a) \eta^{B_1 B_2}(y, b, b') \right) \right].$$

In order to calculate the probability of success (5.3), we need as intermediate steps the marginals $P(y|ab, b' = 1) = \sum_x P(xy|ab, b' = 1)$ and $P(x|ab, b' = 0) = \sum_y P(xy|ab, b' = 0)$. Notice that when the outcome of one party is ignored, it is

always possible to identify a specific state in which the other party receives the qubit. For example, to average out Alice's outcomes one has to calculate

$$
\sum_x \mathrm{Tr}\left[W^{A_1A_2B_1B_2}\left(\xi^{A_1A_2}(x,a)\eta^{B_1B_2}(y,b,b')\right)\right]
$$

$$
= \mathrm{Tr}_{B_1B_2}\left\{\eta^{B_1B_2}(y,b,b')\mathrm{Tr}_{A_1A_2}\left[W^{A_1A_2B_1B_2}\left(\sum_x \xi^{A_1A_2}(x,a)\right)\right]\right\}.
$$

The process observed by Bob is therefore described by the reduced matrix

$$
\overline{W}^{B_1B_2}(a) := \mathrm{Tr}_{A_1A_2}\left[W^{A_1A_2B_1B_2}\left(\sum_x \xi^{A_1A_2}(x,a)\right)\right]. \tag{5.18}
$$

The matrix $\sum_x \xi^{A_1A_2}(x,a)$ represents the CPTP map performed by Alice when the outcomes of her measurement are ignored (the explicit dependence on a accounts for the possibility of signalling). Using (5.14) we find $\sum_x \xi^{A_1A_2}(x,a) = \frac{1}{2}\mathbb{1}^{A_1} \otimes [\mathbb{1} + (-1)^a\sigma_z]^{A_2}$ which, plugged into Eq. (5.18) together with Eq. (5.11), gives

$$
\overline{W}^{B_1B_2}(a) = \frac{1}{2}\left[\mathbb{1} + (-1)^a\frac{1}{\sqrt{2}}\sigma_z\right]^{B_1} \otimes \mathbb{1}^{B_2}. \tag{5.19}
$$

When this is measured with the map (5.16), we find

$$
P(y|ab,b'=1) = \mathrm{Tr}\left[\eta_1^{B_1B_2}(y,b)\overline{W}^{B_1B_2}(a)\right] = \frac{1}{2}\left[1 + \frac{(-1)^{y+a}}{\sqrt{2}}\right], \tag{5.20}
$$

from which we get $P(y=a|b'=1) = \frac{2+\sqrt{2}}{4}$.

Consider now the case when $b' = 0$. When Bob's outcomes are ignored, he performs the CPTP map described by $\sum_y \eta^{B_1B_2}(y,b) = \frac{1}{2}\left[\mathbb{1} + (-1)^b\sigma_x^{B_1}\sigma_z^{B_2}\right]$. From this we can calculate, as in the previous case, the effective state received by Alice, which is

$$
\overline{W}^{A_1A_2}(b,b'=0) = \frac{1}{2}\left[\mathbb{1} + (-1)^b\frac{1}{\sqrt{2}}\sigma_z\right]^{A_1} \otimes \mathbb{1}^{A_2}, \tag{5.21}
$$

from which we find $P(x=b|b'=0) = \frac{2+\sqrt{2}}{4}$. By averaging the two probabilities of signalling in the probability of success (5.3), we find

$$
p_{succ} = \frac{1}{2}\left(\frac{2+\sqrt{2}}{4} + \frac{2+\sqrt{2}}{4}\right) = \frac{2+\sqrt{2}}{4} > \frac{3}{4}.
$$

We see that, depending on his choice, Bob can effectively end up "before" or "after" Alice, each possibility with a probability $\sqrt{2}/2$. This is remarkable,

since if Alice and Bob perform their experiments inside laboratories that they believe are isolated from the outside world for the duration of their operations (e.g. by walls made of impenetrable material), and if they believe that they are able to freely choose the bits a, b, and b' (e.g. by tossing a coin), they will have to conclude that the events in their experiment do not take place in a causal sequence. Indeed, the framework only assumes that the local operations from the input to the output system of each party are correctly described by quantum mechanics, and it is compatible with any physical situation in which one would have all the reasons to believe that each party's operations are freely chosen in a closed laboratory.

Interestingly, both the classical bound (5.4) and the quantum violation (5.12) match the corresponding numbers in the CHSH-Bell inequality [102], which resembles closely inequality (5.4). However, the physical situations to which these inequalities correspond is very different: Bell inequalities can be violated in space-like separated laboratories, while (5.12) cannot be achieved neither with space-like nor with time-like separated laboratories. It is an open question whether (5.12) is the maximal possible violation allowed by quantum mechanics.

5.5 Classical Processes Are Causally Separable

It is possible to see that if the operations of the local parties are classical, they can always be understood as taking place in a global causal structure. This is a generalisation of the argument given in Sec. 5.1: every combination of classical operations that does not satisfy a causal order generates some "grandfather paradox" and is therefore excluded if one assumes that each party must be free to perform an arbitrary operation. The intuition behind this result is that classical processes are stochastic mixtures of deterministic processes. Thus, in each individual run of a classical experiment, there is a classical variable with a well-defined value associated with the entrance and the exit of each laboratory. On the other hand, each signalling correlation between the two laboratories can also be seen as a classical mixture of deterministic functions, connecting the variable at the exit of a laboratory with the one at the entrance of the other laboratory. This means that, if a process allows non-separable, bi-directional signalling correlation, for some run of the experiment the variables must be deterministically correlated. Thus, for those particular experimental runs, the argument leading to the grandfather paradox can be applied.

The actual proof of this fact is a little more lengthy and goes through the quantum formalism. Classical operations can be described by transition matrices $M_j^{(\lambda_2 \lambda_1)} = P(\lambda_2, j | \lambda_1)$, where $P(\lambda_2, j | \lambda_1)$ is the conditional probability that the measurement outcome j is observed and the classical output state λ_2 is prepared given that the input state is λ_1. They can be expressed in the quantum formalism as

CP maps diagonal in a fixed ("pointer") basis, and the corresponding CJ operators are $M_j = \sum_{\lambda_1 \lambda_2} M_j^{(\lambda_2 \lambda_1)} |\lambda_1\rangle\langle\lambda_1|^{A_1} \otimes |\lambda_2\rangle\langle\lambda_2|^{A_2}$. Thus, in order to express arbitrary bipartite probabilities of classical maps, it is sufficient to consider process matrices which are diagonal in the pointer basis. In Appendix C.4 we provide a detailed proof that all such processes are causally separable.

5.6   Possible Implications

We have seen that, by relaxing the assumption of global causal order and requiring that the standard quantum formalism holds only locally, we obtain the possibility for global causal relations that are not included in the usual formulation of quantum mechanics. The latter is reminiscent of the situation in general relativity, where by requiring that locally the geometry is that of flat Minkowski spacetime, one obtains the possibility of having more general, curved spacetimes.

The natural question is whether "non-causal" quantum correlations of the kind described by our formalism can be found in nature. One can speculate that they may arise in situations in which both quantum mechanics and general relativity are relevant. Given that the conformal spacetime metric is a description of the causal relation between spacetime points [130, 131], it is natural to expect that extending general relativity to the quantum domain would involve some kind of "superpositions of causal orders". The fact that the most general process matrices contain terms corresponding to well-defined causal orders (Tab. 5.1), yet are not classical mixtures of these, suggests that our formalism could describe such superpositions. Furthermore, our result that classical theories can always be understood in terms of a global causal structure suggests the possibility that the observed causal order of spacetime might not be a fundamental property of nature but rather emerge from a more fundamental theory [132, 133, 63] in a quantum-to-classical transition due to, for example, decoherence [134] or coarse-grained measurements [18]. Indeed, once a causal structure is present, it is possible to derive relativistic spacetime from a causally ordered set of elements under appropriate conditions [135, 136].

It is also worth noting that exotic causal structures already appear in the classical theory of general relativity. For example, there exist solutions to the Einstein equation containing closed time-like curves (CTCs) [137]. In this context, it should be noted that any process matrix W in our framework can be interpreted as a CPTP map from the outputs, A_2, B_2, of the parties, to their inputs, A_1, B_1. In other words, any process can be thought of as having the form of a CTC, where information is sent back in time through a noisy channel (see also Fig. 5.1 b). The existence of processes that do not describe definite causal order is therefore not incompatible with general relativity in principle. It is sometimes argued that CTCs should not exist since they generate logical paradoxes, such as an agent going back

in time and killing his grandfather. The possible solutions that have been proposed [138, 128, 129, 139, 140, 141], in which quantum mechanics and CTCs might co-exist, involve non-linear extensions of quantum theory that deviate from quantum mechanics already at the level of local experiments. Our framework, on the other hand, is by construction linear and in agreement with local quantum mechanics, and yet paradoxes are avoided, in accordance with the Novikov principle [142], due to the noise in the evolution "backward in time".

We should point out that instances of indefinite causal order may also emerge in situations closer to possible laboratory implementations. As already noted, our formalism describes more general correlations than those that can be realised with a quantum circuit, that is, as a sequence of quantum gates. Recently, a new model of quantum computation which goes beyond the causal paradigm of quantum circuits by using superpositions of the "wires" connecting different gates was proposed [143]. This possibility may allow breaking the assumption that events are localised in a causal structure. Since the instant when a system enters a device depends on how the device is wired with the rest of the computer's architecture, superpositions of wires may allow creating situations in which events are not localised in time (similarly to the way in which a quantum particle may not be localised in space). While it is an open question whether violating the causal inequality (5.4) can be achieved by similar means, the findings presented suggest that new quantum resources for information processing might be available—beyond entanglement, quantum memories, and even "superpositions of wires"—and the formalism introduced provides a natural framework for exploring them.

Finally, the present framework can be extended beyond quantum mechanics to generalised probabilistic theories, where operations are described as elements of more general convex spaces [108, 144, 145, 146]. It is an interesting research program to find physical principles which single out quantum correlations, with and without definite causal structure, out of the more general correlations predicted by such theories. In this respect, it would be helpful to understand if the probability for successfully accomplishing our task, $p_{succ} = \frac{2+\sqrt{2}}{4}$, is the largest allowed by quantum mechanics, i.e. if it represents a "Tsirelson bound [147] for non-causallly ordered correlations".

Conclusions and Outlook

The topics addressed in this thesis involve the notions of space, time and causal structures in quantum mechanics. The results presented bring new insights into the notions of locality and causality within the quantum formalism.

In regimes of sufficiently low energies, one typically assumes the existence of a classical spacetime background on which quantum degrees of freedom are defined. As discussed in the first chapters, even in such regimes (in fact, even for flat spacetime) the definition of familiar notions such as particles and regions of space within the quantum formalism gives rise to several conceptual problems. It is usually assumed in quantum field theory that the observables associated to a point of space $\vec{x}$ are the covariant fields $\phi(\vec{x})$, $\pi(\vec{x})$. The results of the first chapters of the present work, however, suggest that such an identification might not necessarily correspond to the degrees of freedom actually measured by "localised" devices. As seen in Chapter 1, the particle content of a relativistic quantum field can be defined operationally in terms of a particle detector model. If the natural assumption is made that ground and excited states of the detector correspond to the eigenstates of an interacting theory, the effective degrees of freedom seen by the detector are not localised in the standard sense.

The standard identification between regions of space and quantum observables produces unusual divergences in the calculation of thermodynamic quantities. As seen in Chapter 2, these can be cured if, instead of the covariant fields, the Newton-Wigner position operators are used to identify the region of space. This result does not answer the question of which degrees of freedom should be associated with regions of space "at a fundamental level". The Newton-Wigner localisation is problematic in this respect, since the corresponding field operators are not covariant and would yield superluminal signalling. The results of Chapter 3 suggest that a solution to this problem might be that different localisations should be adopted for regimes of different measurement accuracies. The results show that, given a minimal space resolution, the Hilbert space $\mathcal{H}$ of a field decomposes into a tensor product $\mathcal{H} = \mathcal{H}_{coll} \otimes \mathcal{H}_{fine}$, where $\mathcal{H}_{coll}$ contains the degrees of freedom measurable with the given resolution (via measurement of collective operators), while the fine-structure degrees of freedom in $\mathcal{H}_{fine}$ cannot

be accessed. Therefore, given a decomposition of space in two regions R_1, R_2, one should not consider a corresponding decomposition in subsystems of $\mathcal{H}$, but rather of $\mathcal{H}_{coll} = \mathcal{H}_{R_1} \otimes \mathcal{H}_{R_2}$. If only a resolution worse than typical correlation lengths in the field is available, the vacuum turns out to be a product state in the resulting tensor decomposition, just as in the Newton-Wigner localisation[7]. One can imagine, by arbitrarily increasing the resolution, to access regimes where the vacuum entanglement becomes more and more accessible, although the divergent entropy associated with it will always be confined in the $\mathcal{H}_{fine}$ subsystem. In this picture, the standard localisation associated with the covariant fields does not have any direct operational meaning, since it could only be approximated in the limit of infinite precision but never reached exactly.

Thermodynamic considerations in relativistic quantum field theory (addressed in Chapters 2 and 3) are based on non-covariant notions: a thermal state is defined in some given inertial reference frame and the related thermodynamic quantities are calculated in the corresponding space-like plane. Notions such as regions of space, entanglement, coarse-graining, and collective operators all depend on the assigned space-like surface on which they are defined. In applications to special and general relativity, it would be natural to seek generalisations of such notions to covariant spacetime properties. A starting point for constructing such notions could be the general framework of information theory, which has already been shown to provide solid foundations to thermodynamics and statistical mechanics [150]. However, quantum information too, although formulated with no direct reference to a physical space, does assume a sharp division between "space-like" objects (such as quantum states) and "time-like" ones (such as unitary operators). The framework outlined in Chapter 5 goes beyond such a division and can be a starting point for the construction of a "covariant" quantum information, which could in turn provide the basis for relativistic thermodynamics. In the formalism developed, quantum states and evolutions are special instances of more general objects, which we called *processes*. A process describes a general situation where a number of local operations are performed, with no prior assumption about how such operations are embedded in a global spacetime. The local operations correspond to the most general quantum operations that can be performed in a localised spacetime volume, thus one can think of them as *defining* a small region of space time (in the limit, a point). A process describes all the possible measurement outcomes of the local operations and can then be seen as an abstract description

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[7]Note that, as in the NW localisation, the decomposition $\mathcal{H}_{coll} = \mathcal{H}_{R_1} \otimes \mathcal{H}_{R_2}$ is not covariant (in fact, covariance is already broken in the definition of coarse-graining, i.e. in the decomposition $\mathcal{H} = \mathcal{H}_{coll} \otimes \mathcal{H}_{fine}$). However, such a lack of covariance does not lead to possible non-local effects (such as signalling between space-like separated regions), because the effective localisation is only a consequence of the lack of precision in determining the position of local operations which, at a fundamental level, are still defined according to the covariant fields $\phi(x)$, $\pi(x)$.

of the geometry in which such regions are embedded. In Chapter 5 the causal relations between regions defined by processes have been studied, the structure and properties of processes are however still largely unexplored; it is still to be understood what the sensible notions are that generalise information-theoretical concepts such as entanglement, entropy, channel capacity, etc. It is natural to expect that "covariant" properties of processes would provide a better insight into the foundational issues regarding relativistic quantum systems considered in the first chapters.

The analysis of causal relations in quantum theory opens several possible research directions. An important aspect is understanding when and how situations with no causal order, such as the abstract example given in Chapter 5, can arise in nature. A viable approach is to consider gedankenexperiments that could lead to superpositions of spacetime metrics in the light of the new formalism developed. It is important to stress that the treatment of such experiments should not rely on detailed calculations in some quantum-gravity formalism. Rather, similarly to the EPR and Bell examples, only minimal assumptions about the underlying theory should be used. It is however also interesting to understand whether different approaches to quantum gravity lead to different possible operationally-defined causal relations.

A theme underlying large part of the work is the correspondence principle. If fundamental theories have counterintuitive features, one should also find a reason why such features are not observable at the level of everyday experience. More generally, it is important to assess the range of validity of specific theories and under which conditions they reduce to less fundamental, effective theories. The coarse-graining approach has proved surprisingly versatile in providing a general guiding line for understanding emergent properties. It has been shown in Chapter 3 that all quantum measurements in phase space can be described in terms of classical probability distributions as long as the measurement precision is small enough. This suggest a general criterion for the emergence of classicality: the classical limit can be understood as the $\frac{\hbar}{\sigma^2} \to 0$ limit, where σ^2 quantifies the minimal precision available in the measurement of phase space observables. It is noteworthy that the classical limit seems to provide "for free" a limit of causal order. As seen in Chapter 5, the assumption of local classical operations implies the existence of a global causal structure. There are however regimes, nowadays largely accessible in the laboratory, where quantum phenomena can be observed (thus far from the classical limit), but for which a global causal structure seems to be well-defined. A possible explanation is that the observed causal structure in quantum experiments relies on the fact that the spacetime location of quantum operations and measurements is determined by instruments well into the classical limit, which therefore define "classical reference frames" for spacetime. In the presence of large superpositions of mass-energy one could expect such reference

frames not to be available. An interesting possibility is to consider such situations in terms of relative degrees of freedom between quantum systems and quantum reference frames, applying the methods used in Chapter 4. A possible development is a reconsideration of the equivalence principle to include reference frames in quantum superpositions, which could provide a new approach to the study of the interplay between general relativity and quantum mechanics.

Appendix A

A.1 Convergence of High-Energy Loops

Let us consider the integral

$$J = \int_{R_0} dx_0 \cdots \int_{R_{n+1}} dx_{n+1} \frac{m_0 m_1 \cdots m_{n+1}}{[m_0^2 + (x_0 - x_1)^2] \cdots [m_{n+1}^2 + (x_{n+1} - x_0)^2]} \quad \text{(A.1)}$$

where the ranges R_i can be the interval $I_L = [-L/\beta, L/\beta]$ or the set $E_L = (-\infty, -L/\beta] \cup [L/\beta, \infty)$, and $n \geq 1$ (the case $n = 0$ can be verified by a direct computation). Without loss of generality, we can assume $R_{n+1} = E_L$. We can perform the integration in dx_{n+1} by means of the formula

$$\int dx \frac{ab}{[a^2 + (x - y)^2][b^2 + (z - x)^2]} =$$
$$= \frac{b[b^2 - a^2 + (z - y)^2] \arctan \frac{x-y}{a} + a[a^2 - b^2 + (z - y)^2] \arctan \frac{x-z}{b}}{[(y - z)^2 + (a + b)^2][(y - z)^2 + (a - b)^2]}$$
$$- \frac{ab(y - z) \log \frac{a^2 + (x-y)^2}{b^2 + (x-z)^2}}{[(y - z)^2 + (a + b)^2][(y - z)^2 + (a - b)^2]}, \quad \text{(A.2)}$$

so that

$$W(m_n, m_{n+1}; x_n, x_0; \beta) = \int_{E_L} dx_{n+1} \frac{m_n m_{n+1}}{[m_n^2 + (x_n - x_{n+1})^2][m_{n+1}^2 + (x_{n+1} - x_0)^2]} =$$
$$= - \frac{m_{n+1}[m_{n+1}^2 - m_n^2 + (x_0 - x_n)^2] \arctan \frac{\frac{L}{\beta} - x_n}{m_n}}{[(x_n - x_0)^2 + (m_n + m_{n+1})^2][(x_n - x_0)^2 + (m_n - m_{n+1})^2]}$$
$$- \frac{m_n[m_n^2 - m_{n+1}^2 + (x_0 - x_n)^2] \arctan \frac{\frac{L}{\beta} - x_0}{m_{n+1}}}{[(x_n - x_0)^2 + (m_n + m_{n+1})^2][(x_n - x_0)^2 + (m_n - m_{n+1})^2]}$$
$$+ \frac{m_n m_{n+1}(x_n - x_0) \log \frac{m_n^2 + (\frac{L}{\beta} - x_n)^2}{m_{n+1}^2 + (\frac{L}{\beta} - x_0)^2}}{[(x_n - x_0)^2 + (m_n + m_{n+1})^2][(x_n - x_0)^2 + (m_n - m_{n+1})^2]}$$

$$-(\beta \to -\beta) + \frac{\pi(m_{n+1} + m_n)[(m_{n+1} - m_n)^2 + (x_0 - x_n)^2]}{[(x_n - x_0)^2 + (m_n + m_{n+1})^2][(x_n - x_0)^2 + (m_n - m_{n+1})^2]} \quad (A.3)$$

Next, a very careful analysis is needed, distinguishing the cases if R_0, R_n are of type I_L and/or E_L. Note that it is an odd function of β, apart from a term which does not contain β. Indeed such term imply $W(m_n, m_{n+1}; x_n, x_0; \beta) \to 0$ if $\beta \to 0^+$. It is possible to see that one can find a set of positive constants K_{ab} such that

$$W(a, b; x_n, x_0; \beta) \leq \frac{K_{ab}}{(x_n - x_0)^2 + (a + b)^2} \frac{\beta}{L}. \quad (A.4)$$

After substitution in (A.1), we see that in the worst case[1] J takes the form (2.29) so that the limit $\beta \to 0^+$ exists.

---

[1]that is, when all the remaining insertions are the black ones

Appendix B

B.1 Estimation of Gaussian Convolution

Consider the integral

$$I := \int d^d y \, G_{\frac{1}{4\epsilon^2}}(\vec{a} - \vec{y})\varphi(\|\vec{y}\|), \tag{B.1}$$

where φ is a positive bounded function, $0 \leq \varphi(y) \leq \varphi_0 \, \forall y \geq 0$, with $\varphi(y') \leq \varphi(y)$ $\forall y' \geq y$, $y > r$, for some $r > 0$. In order to find an upper bound for I we write, for some $\alpha > r$,

$$I = \left(\int_{\|\vec{y}\| \leq \alpha} + \int_{\|\vec{y}\| > \alpha} \right) d^d y \, G_{\frac{1}{4\epsilon^2}}(\vec{y})\varphi(\|\vec{y} + \vec{a}\|)$$

$$\leq \varphi(|a - \alpha|) \int_{\|\vec{y}\| \leq \alpha} d^d y \, G_{\frac{1}{4\epsilon^2}}(\vec{y}) + \varphi_0 \int_{\|\vec{y}\| > \alpha} d^d y \, G_{\frac{1}{4\epsilon^2}}(\vec{y})$$

$$\leq \varphi(|a - \alpha|) + \varphi_0 \int_{\|\vec{y}\| > \alpha} d^d y \, G_{\frac{1}{4\epsilon^2}}(\vec{y}),$$

where $a = \|\vec{a}\|$ and we used $\int d^d y \, G_{\frac{1}{4\epsilon^2}}(\vec{y}) = 1$. By integrating the angular degrees of freedom, one obtains

$$\int_{\|\vec{y}\| > \alpha} d^d y \, G_{\frac{1}{4\epsilon^2}}(\vec{y}) = \frac{1}{(8\pi\epsilon^2)^{d/2}}\gamma_d \int_\alpha^\infty dr \, r^{d-1} e^{-\frac{r^2}{4\epsilon^2}} = \frac{2}{\Gamma(\frac{d}{2})} \int_{\frac{\alpha}{2\epsilon}}^\infty dr \, r^{d-1} e^{-r^2},$$

where $\gamma_d = \frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})}$ is the surface of the d-sphere and Γ is the Euler gamma function. For $\alpha \gg \epsilon$, one has

$$I \leq \varphi(|a - \alpha|) + \frac{2\varphi_0}{\Gamma(\frac{d}{2})} e^{-\frac{\alpha^2}{4\epsilon^2}} \left[\left(\frac{\alpha}{2\epsilon} \right)^{d-2} + O\left(\frac{\alpha}{2\epsilon} \right)^{d-4} \right].$$

By choosing $\alpha = sa$ for some $s \in (0, 1)$, we obtain the upper bound

$$I \leq \varphi((1 - s)a) + \frac{2\varphi_0}{\Gamma(\frac{d}{2})} e^{-\frac{s^2 a^2}{16\epsilon^2}} \left[\left(\frac{sa}{4\epsilon} \right)^{d-2} + O\left(\frac{sa}{4\epsilon} \right)^{d-4} \right], \tag{B.2}$$

from which we derive

$$\int d^d y \, G_{\frac{1}{4\epsilon^2}}(\vec{a} - \vec{y})\varphi(\|\vec{y}\|) \to \varphi(a)$$

for $\frac{a}{\epsilon} \gg 1$. (It is enough to take $s \to 0$ in (B.2), e.g. by setting $s = \sqrt{\frac{\epsilon}{a}}$.)

B.2 Discretisation of the Klein-Gordon Field

We review the relation between a massive, scalar, bosonic field and a lattice of harmonic oscillators in d space dimension. The same correspondence holds both for quantum and classical systems; here we only present it in the quantum formalism. A field of mass M confined in a d-dimensional box of size L is described by the Hamiltonian

$$\hat{H} = \frac{1}{2} \int_{[0,L]^d} d^d x \left\{ M^2 \hat{\phi}^2(\vec{x}) + \hat{\pi}^2(\vec{x}) + \sum_{s=1}^{d} \left[\frac{\partial}{\partial x_s} \hat{\phi}(\vec{x}) \right]^2 \right\}, \qquad \text{(B.3)}$$

where the conjugate field operators satisfy the continuous canonical commutation relation

$$[\hat{\phi}(\vec{x}), \hat{\pi}(\vec{y})] = i \, \delta(\vec{x} - \vec{y}). \qquad \text{(B.4)}$$

We assume periodic boundary conditions, such that, for $s = 1, \ldots, d$, $\hat{\phi}(\vec{x} + \vec{u}_s L) = \phi(\vec{x})$, $\hat{\pi}(\vec{x} + \vec{u}_s L) = \pi(\vec{x})$, where $\vec{u}_s$ are the d-dimensional unit vectors $\vec{u}_1 = (1, 0, \ldots, 0), \ldots, \vec{u}_d = (0, \ldots, 0, 1)$.

The integral (B.3) is the $N \to \infty$ limit of the expression

$$\hat{H}_{\text{dis}} = \frac{\epsilon^d}{2} \sum_{j_1 \ldots j_d = 1}^{N} \left\{ M^2 \hat{\phi}^2(\vec{j}\epsilon) + \hat{\pi}^2(\vec{j}\epsilon) + \sum_{s=1}^{d} \left[\frac{\hat{\phi}((\vec{j} + \vec{u}_s)\epsilon) - \hat{\phi}(\vec{j}\epsilon)}{\epsilon} \right]^2 \right\}, \qquad \text{(B.5)}$$

where $\epsilon = \frac{L}{N}$ and $\frac{\phi((\vec{j} + \vec{u}_s)\epsilon) - \phi(\vec{j}\epsilon)}{\epsilon}$ is the discretised partial derivative along the s-th coordinate. The fields evaluated at discrete points have commutation relations $[\hat{\phi}(\vec{j}\epsilon), \hat{\pi}(\vec{l}\epsilon)] = i \, \delta\left((\vec{j} - \vec{l})\epsilon\right) = \frac{1}{\epsilon^d} \delta_{\vec{j}\vec{l}}$. A convenient choice of dimensionless, discrete degrees of freedom with canonical commutation relations is

$$\hat{q}_{\vec{j}} := \sqrt{E}\epsilon^{d/2}\hat{\phi}(\vec{j}\epsilon), \qquad\qquad \hat{p}_{\vec{j}} := \frac{\epsilon^{d/2}}{\sqrt{E}}\hat{\pi}(\vec{j}\epsilon),$$

with $E := \frac{1}{\epsilon}\sqrt{M^2\epsilon^2 + 2d}$. Substituting these into (B.5) we can write the discretised Hamiltonian has

$$\hat{H}_{\text{dis}} = \frac{E}{2} \sum_{j_1, \ldots, j_d = 1}^{N} \left[\hat{q}_{\vec{j}}^2 + \hat{p}_{\vec{j}}^2 - \alpha \sum_{s=1}^{d} \hat{q}_{\vec{j}}\hat{q}_{\vec{j} + \vec{u}_s} \right], \qquad \text{(B.6)}$$

where $\alpha := \frac{2}{E^2 \epsilon^2} = \frac{1}{d + \frac{1}{2}\epsilon^2 M^2}$.

The Hamiltonian (B.6) can be diagonalised introducing the operators

$$
\begin{aligned}
\hat{a}_{\vec{k}} &:= \frac{1}{\sqrt{2N^d}} \sum_{j_1,\dots,j_d=1}^{N} e^{i\frac{2\pi}{N}\vec{j}\cdot\vec{k}} \left(\sqrt{\nu_{\vec{k}}}\hat{q}_{\vec{j}} + \frac{i}{\sqrt{\nu_{\vec{k}}}}\hat{p}_{\vec{j}} \right), \\
\hat{a}_{\vec{k}}^{\dagger} &:= \frac{1}{\sqrt{2N^d}} \sum_{j_1,\dots,j_d=1}^{N} e^{-i\frac{2\pi}{N}\vec{j}\cdot\vec{k}} \left(\sqrt{\nu_{\vec{k}}}\hat{q}_{\vec{j}} - \frac{i}{\sqrt{\nu_{\vec{k}}}}\hat{p}_{\vec{j}} \right),
\end{aligned}
\tag{B.7}
$$

where $\nu_{\vec{k}} := \sqrt{E\left(1 - \alpha \sum_{s=1}^{d} \cos\frac{2\pi}{N}k_s\right)}$. The inverse relation reads

$$
\begin{aligned}
\hat{q}_{\vec{j}} &= \frac{1}{\sqrt{2N^d}} \sum_{k_1,\dots,k_d=1}^{N} \frac{1}{\sqrt{\nu_{\vec{k}}}} \left(e^{-i\frac{2\pi}{N}\vec{j}\cdot\vec{k}}\hat{a}_{\vec{k}} + e^{i\frac{2\pi}{N}\vec{j}\cdot\vec{k}}\hat{a}_{\vec{k}}^{\dagger} \right), \\
\hat{p}_{\vec{j}} &= -\frac{i}{\sqrt{2N^d}} \sum_{k_1,\dots,k_d=1}^{N} \sqrt{\nu_{\vec{k}}} \left(e^{-i\frac{2\pi}{N}\vec{j}\cdot\vec{k}}\hat{a}_{\vec{k}} - e^{i\frac{2\pi}{N}\vec{j}\cdot\vec{k}}\hat{a}_{\vec{k}}^{\dagger} \right),
\end{aligned}
$$

which, plugged into Eq. (B.6), gives the diagonalised Hamiltonian

$$
\hat{H}_{\text{dis}} = \sum_{k_1,\dots,k_d=1}^{N} \nu_{\vec{k}} \left(\hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{k}} + \frac{1}{2} \right).
\tag{B.8}
$$

Appendix C

C.1 Formal Derivation of the Causal Inequality

A causal structure (for instance, spacetime) is a set of event locations equipped with a partial ordering relation $\preceq$ that defines the possible causal relations between events at these locations. If A and B are two such locations, $A \preceq B$ reads "A is in the *causal past* of B", or equivalently, "B is in the *causal future* of A" (e.g. if A and B are spacetime points, $A \preceq B$ corresponds to A being in the past light cone of B). Operationally, if $A \preceq B$, an agent at A can *signal* to an agent at B by encoding information in events at A that get correlated with events at B which the other agent can observe. The fact that the relation $\preceq$ is a partial order means that it satisfies the following conditions: 1) $A \preceq A$ (reflexivity); 2) if $A \preceq B$ and $B \preceq C$, then $A \preceq C$ (transitivity); and 3) if $A \preceq B$ and $B \preceq A$, then $A = B$ (antisymmetry). The last condition says that if A and B are two different locations, there can either be signalling from A to B, or vice versa, but no signalling in both directions is possible (i.e. there are no causal loops). If A is *not* in the causal past of B, we will write $A \npreceq B$. Note that in a causal structure both $A \npreceq B$ and $B \npreceq A$ may hold (as in the case when A and B are space-like separated), and at least one of the two *must* hold for $A \neq B$. We will denote the situation where both $A \npreceq B$ and $B \npreceq A$ hold by $A \npreceq\npreceq B$.

Since every event specifies an event location, we will use the same notation directly for events. For instance, if X and Y are two events such that the location of X is in the causal past of the location of Y, we will write $X \preceq Y$ (similarly for $\npreceq$ and $\npreceq\npreceq$).

The main events in our communication task are the systems entering Alice's and Bob's laboratories, which we will denote by A_1 and B_1, respectively, and the parties producing the bits a, b, b', x, and y, which we will denote by the same letters as the corresponding bits. The fact that Alice generates the bit a and produces her guess x *after* the system enters her laboratory means that $A_1 \preceq a, y$. Similarly, we have $B_1 \preceq b', b, y$.

The assumptions behind the causal inequality are:

(i) *Causal structure*—The events A_1, B_1, a, b, b', x, y are localised in a causal structure.

(ii) *Free choice*—Each of the bits a, b, and b' can only be correlated with events in its causal future (this concerns only events relevant to the task). We assume also that each of them takes values 0 or 1 with probability $1/2$.

(iii) *Closed laboratories*—x can be correlated with b only if $b \preceq A_1$, and y can be correlated with a only if $a \preceq B_1$.

We want to show that these assumptions imply

$$p_{succ} = \frac{1}{2} p(x = b|b' = 0) + \frac{1}{2} p(y = a|b' = 1) \leq \frac{3}{4} \tag{C.1}$$

for the success probability that Alice and Bob can achieve in their task.

First, notice that assumption (ii) implies that the bits a, b, and b' are independent of each other. Indeed, there are two general ways in which the three bits could be correlated—two of them are correlated with each other while the third one is independent, or each of them is correlated with the other two. In the first case, the free-choice assumption implies that the two correlated bits would have to be in each other's causal pasts, which is impossible. In the second case, each of the bits would have to be in the causal past of the other two, which is again impossible. Hence, the bits are uncorrelated.

Next, consider the following three possibilities that can be realised in a causal structure: $A_1 \preceq B_1$, $B_1 \preceq A_1$, $A_1 \npreceq\npreceq B_1$. Since these possibilities are mutually exclusive and exhaustive, their probabilities satisfy $p(A_1 \preceq B_1) + p(B_1 \preceq A_1) + p(A_1 \npreceq\npreceq B_1) = 1$. From assumption (ii) it follows that the bits a, b, and b' are independent of which of these possibilities is realised. To see this, consider for instance b'. Since $B_1 \preceq b'$, we have that b' must be independent of whether A_1 takes place in the causal past of B_1 or not, i.e. $p(A_1 \preceq B_1|b') = p(A_1 \preceq B_1)$. Similarly, b' must be independent of whether A_1 takes place in the larger region which is a complement of the causal future of B_1, which implies $p(B_1 \npreceq A_1|b') = p(B_1 \npreceq A_1)$. But $p(B_1 \npreceq A_1|b') = p(A_1 \preceq B_1|b') + p(A_1 \npreceq\npreceq B_1|b') = p(A_1 \preceq B_1) + p(A_1 \npreceq\npreceq B_1|b')$, while $p(B_1 \npreceq A_1) = p(A_1 \preceq B_1) + p(A_1 \npreceq\npreceq B_1)$, which implies $p(A_1 \npreceq\npreceq B_1|b') = p(A_1 \npreceq\npreceq B_1)$. Finally, since $p(A_1 \preceq B_1|b') + p(A_1 \npreceq\npreceq B_1|b') + p(B_1 \preceq A_1|b') = p(A_1 \preceq B_1) + p(A_1 \npreceq\npreceq B_1) + p(B_1 \preceq A_1|b') = 1 = p(A_1 \preceq B_1) + p(A_1 \npreceq\npreceq B_1) + p(B_1 \preceq A_1)$, we have $p(B_1 \preceq A_1|b') = p(B_1 \preceq A_1)$. An analogous argument shows that a and b are also independent of the causal relation between A_1 and B_1.

Using the above, the success probability can be written

$$
p_{succ} = \frac{1}{2}p(x = b|b' = 0) + \frac{1}{2}p(y = a|b' = 1)
$$

$$
= \frac{1}{2}p(x = b|b' = 0; A_1 \preceq B_1)p(A_1 \preceq B_1)
$$

$$
+ \frac{1}{2}p(x = b|b' = 0; B_1 \preceq A_1)p(B_1 \preceq A_1)
$$

$$
+ \frac{1}{2}p(x = b|b' = 0; A_1 \npreceq\nsucceq B_1)p(A_1 \npreceq\nsucceq B_1)
$$

$$
+ \frac{1}{2}p(y = a|b' = 1; A_1 \preceq B_1)p(A_1 \preceq B_1)
$$

$$
+ \frac{1}{2}p(y = a|b' = 1; B_1 \preceq A_1)p(B_1 \preceq A_1)
$$

$$
+ \frac{1}{2}p(y = a|b' = 1; A_1 \npreceq\nsucceq B_1)p(A_1 \npreceq\nsucceq B_1)
$$

$$
= \left(\frac{1}{2}p(x = b|b' = 0; A_1 \preceq B_1) + \frac{1}{2}p(y = a|b' = 1; A_1 \preceq B_1)\right)
$$

$$
\times p(A_1 \preceq B_1)
$$

$$
+ \left(\frac{1}{2}p(x = b|b' = 0; B_1 \preceq A_1) + \frac{1}{2}p(y = a|b' = 1; B_1 \preceq A_1)\right)
$$

$$
\times p(B_1 \preceq A_1)
$$

$$
+ \left(\frac{1}{2}p(x = b|b' = 0; A_1 \npreceq\nsucceq B_1) + \frac{1}{2}p(y = a|b' = 1; A_1 \npreceq\nsucceq B_1)\right)
$$

$$
\times p(A_1 \npreceq\nsucceq B_1). \tag{C.2}
$$

If $A_1 \preceq B_1$ (which implies $B_1 \npreceq A_1$), from the transitivity of partial order it follows that $A_1 \preceq b$ (and thus $b \npreceq A_1$). From assumption (iii), x can only be correlated with b if b is in the causal past of A_1, thus $p(b|x; A_1 \preceq B_1) = p(b|A_1 \preceq B_1) = \frac{1}{2}$ [the last equality follows from the independence of b from the causal relations between A_1 and B_1, together with assumption (ii)]. Using also that b and b' are independent, we thus obtain $p(x = b|b' = 0; A_1 \preceq B_1) = p(b = 0; x = 0|b' = 0; A_1 \preceq B_1) + p(b = 1, x = 1|b' = 0; A_1 \preceq B_1) = p(b = 0|x = 0; b' = 0; A_1 \preceq B_1)p(x = 0|b' = 0; A_1 \preceq B_1) + p(b = 1|x = 1; b' = 0; A_1 \preceq B_1)p(x = 1|b' = 0; A_1 \preceq B_1) = \frac{1}{2}p(x = 0|b' = 0; A_1 \preceq B_1) + \frac{1}{2}p(x = 1|b' = 0; A_1 \preceq B_1) = \frac{1}{2}$.

If $B_1 \preceq A_1$ (which implies $A_1 \npreceq B_1$), by an analogous argument we obtain $p(y = a|b' = 1; B_1 \preceq A_1) = \frac{1}{2}$. Finally, if $A_1 \npreceq\nsucceq B_1$, we have both $p(y = a|b' = 1; A_1 \npreceq\nsucceq B_1) = \frac{1}{2}$ and $p(x = b|b' = 0; A_1 \npreceq\nsucceq B_1) = \frac{1}{2}$. Substituting this in Eq. (C.2), we obtain

$$p_{succ} = \left(\frac{1}{4} + \frac{1}{2}p(y = a|b' = 1; A_1 \preceq B_1)\right)p(A_1 \preceq B_1)$$

$$+ \left(\frac{1}{2}p(x = b|b' = 0; B_1 \preceq A_1) + \frac{1}{4}\right)p(B_1 \preceq A_1)$$

$$+ \left(\frac{1}{4} + \frac{1}{4}\right)p(A_1 \npreceq\nsucceq B_1)$$

$$\leq \frac{3}{4}p(A_1 \preceq B_1) + \frac{3}{4}p(B_1 \preceq A_1) + \frac{3}{4}p(A_1 \npreceq\nsucceq B_1) = \frac{3}{4}. \qquad \text{(C.3)}$$

This completes the proof.

C.2   Characterisation of Process Matrices

We derive necessary and sufficient conditions for a matrix to satisfy Eqs. (5.8) and (5.9) in terms of an expansion of the matrix in a Hilbert-Schmidt basis. A Hilbert-Schmidt basis of $\mathcal{L}(\mathcal{H}^X)$ is given by a set of matrices $\{\sigma_\mu^X\}_{\mu=0}^{d_X^2-1}$, with $\sigma_0^X = \mathbb{1}^X$, $\text{Tr}\sigma_\mu^X\sigma_\nu^X = d_X\delta_{\mu\nu}$, and $\text{Tr}\sigma_j^X = 0$ for $j = 1,\dots d_X^2 - 1$. A general element of $\mathcal{L}(\mathcal{H}^{A_1} \otimes \mathcal{H}^{A_2} \otimes \mathcal{H}^{B_1} \otimes \mathcal{H}^{B_2})$ can be expressed as

$$W^{A_1A_2B_1B_2} = \sum_{\mu\nu\lambda\gamma} w_{\mu\nu\lambda\gamma}\sigma_\mu^{A_1}\sigma_\nu^{A_2}\sigma_\lambda^{B_1}\sigma_\gamma^{B_2}, \quad w_{\mu\nu\lambda\gamma} \in \mathbb{C} \qquad \text{(C.4)}$$

(we omit tensor products and identity matrices whenever there is no risk of confusion). Since a process matrix has to be Hermitian, we consider only the cases

$$w_{\mu\nu\lambda\gamma} \in \mathbb{R}. \qquad \text{(C.5)}$$

We will refer to terms of the form $\sigma_i^{A_1} \otimes \mathbb{1}^{rest}$ ($i \geq 1$) as of the type A_1, terms such as $\sigma_i^{A_1} \otimes \sigma_j^{A_2} \otimes \mathbb{1}^{rest}$ ($i, j \geq 1$) as of the type A_1A_2, and so on. The properties of a process matrix can be analysed with respect to the terms it contains. For example, terms of the type A_1B_1 produce non-signalling correlations between the measurements, terms such as A_2B_1 correlate Alice's outputs with Bob's inputs, yielding signalling from Alice to Bob, etc., as illustrated in Tab. 5.1. Note that not all terms are compatible with the condition (5.9). We will prove that a matrix W satisfies condition (5.9) if and only if it only contains the terms listed in Tab. 5.1.

The CJ (Choi-Jamiołkowsky) matrix of a local operation can be similarly written $M^{X_1X_2} = \sum_{\mu\nu} r_{\mu\nu}\sigma_\mu^{X_1}\sigma_\nu^{X_2}$, $r_{\mu\nu} \in \mathbb{R}$. The condition $\text{Tr}_{X_2}M^{X_1X_2} = \mathbb{1}^{X_1}$ is equivalent to the requirement $r_{00} = \frac{1}{d_{X_2}}$, $r_{i0} = 0$ for $i > 0$. Thus CJ matrices corresponding to

CPTP maps have the form

$$M^{X_1 X_2} = \frac{1}{d_{X_2}} \left(\mathbb{1}^{X_1 X_2} + \sum_{i>0} a_i \sigma_i^{X_2} + \sum_{ij>0} t_{ij} \sigma_i^{X_1} \sigma_j^{X_2} \right), \tag{C.6}$$

$$a_i, t_{ij} \in \mathbb{R}.$$

Let us consider first the case of a single party, say, Alice. Since the set of matrices $M^{A_1 A_2} \geq 0$ is a substantial set, condition (5.9) can be equivalently imposed on arbitrary matrices of the form (C.6) and, for a single party, it can be rewritten as

$$\frac{1}{d_{A_2}} \mathrm{Tr} \left[W^{A_1 A_2} \left(\mathbb{1}^{A_1 A_2} + \sum_{i>0} a_i \sigma_i^{A_2} + \sum_{ij>0} t_{ij} \sigma_i^{A_1} \sigma_j^{A_2} \right) \right] = 1,$$

$$\forall \ a_i, t_{ij} \in \mathbb{R}.$$

Using an expansion of the process matrix in the same basis in a similar way, $W^{A_1 A_2} = \sum_{\mu\nu} w_{\mu\nu} \sigma_\mu^{A_1} \sigma_\nu^{A_2}$, $w_{\mu\nu} \in \mathbb{R}$, the above condition becomes

$$d_{A_1} \left(w_{00} + \sum_{i>0} w_{0i} a_i + \sum_{ij>0} w_{ij} t_{ij} \right) = 1,$$

$$\forall \ a_i, t_{ij} \in \mathbb{R},$$

and one obtains $w_{00} = \frac{1}{d_{A_1}}$, $w_{0i} = w_{ij} = 0$ for $i, j > 0$. Thus the most general process matrix observed by a single party has the form

$$W^{A_1 A_2} = \frac{1}{d_{A_1}} \left(\mathbb{1}^{A_1 A_2} + \sum_{i>0} v_i \sigma_i^{A_1} \right), \tag{C.7}$$

$$v_i \in \mathbb{R}, \quad W^{A_1 A_2} \geq 0,$$

which can be recognised as a state. This result—that all probabilities a single agent can observe are described by quantum states—is an extension of Gleason's theorem from POVMs [148, 149] to CP maps (note that here the linear structure of quantum operations is assumed, while in Gleason's theorem for POVMs it is derived from different hypotheses. However, by a similar argument one could derive linearity for CP maps too).

Let us now consider a bipartite process matrix, $W^{A_1 A_2 B_1 B_2} = \sum_{\mu\nu\lambda\gamma} w_{\mu\nu\lambda\gamma} \sigma_\mu^{A_1} \sigma_\nu^{A_2} \sigma_\lambda^{B_1} \sigma_\gamma^{B_2}$, $w_{\mu\nu\lambda\gamma} \in \mathbb{R}$. We have to impose (5.9) for arbitrary matrices $M^{A_1 A_2}$, $M^{B_1 B_2}$ of the form (C.6). First, if we fix $M^{B_1 B_2} = \frac{\mathbb{1}^{B_1 B_2}}{d_{B_2}}$, we obtain

$$d_{A_1} d_{B_1} \left(w_{0000} + \sum_{i>0} w_{0i00} a_i + \sum_{ij>0} w_{ij00} t_{ij} \right) = 1$$

$$\forall \ a_i, t_{ij} \in \mathbb{R},$$

which imposes $w_{0000} = \frac{1}{d_{A_1} d_{B_1}}$ and $w_{0i00} = w_{ij00} = 0$ for $i, j > 0$. Similarly, by fixing $M^{A_1 A_2} = \frac{\mathbb{1}^{A_1 A_2}}{d_{A_2}}$, we can derive $w_{000i} = w_{00ij} = 0$ for $i, j > 0$. Finally, imposing (5.9) for arbitrary

$$M^{A_1 A_2} = \frac{1}{d_{A_2}} \left(\mathbb{1}^{A_1 A_2} + \sum_{i>0} a_i \sigma_i^{A_2} + \sum_{ij>0} t_{ij} \sigma_i^{A_1} \sigma_j^{A_2} \right),$$

$$M^{B_1 B_2} = \frac{1}{d_{B_2}} \left(\mathbb{1}^{B_1 B_2} + \sum_{k>0} b_k \sigma_k^{B_2} + \sum_{kl>0} s_{kl} \sigma_k^{B_1} \sigma_l^{B_2} \right),$$

we obtain

$$\sum_{ik>0} w_{0i0k} a_i b_k + \sum_{ikl>0} w_{0ikl} a_i s_{kl}$$
$$+ \sum_{ijk>0} w_{ij0k} t_{ij} b_k + \sum_{ijkl>0} w_{ijkl} t_{ij} s_{kl} = 0,$$
$$\forall\ a_i, t_{ij}, b_k, s_{kl} \in \mathbb{R},$$

from which we conclude that the most general matrix that satisfies (5.9) has the form

$$W^{A_1 A_2 B_1 B_2} = \frac{1}{d_{A_1} d_{B_1}} \left(\mathbb{1} + \sigma^{B \preceq A} + \sigma^{A \preceq B} + \sigma^{A \npreceq \nsucceq B} \right),$$

$$\sigma^{B \preceq A} := \sum_{ij>0} c_{ij} \sigma_i^{A_1} \sigma_j^{B_2} + \sum_{ijk>0} d_{ijk} \sigma_i^{A_1} \sigma_j^{B_1} \sigma_k^{B_2},$$

$$\sigma^{A \preceq B} := \sum_{ij>0} e_{ij} \sigma_i^{A_2} \sigma_j^{B_1} + \sum_{ijk>0} f_{ijk} \sigma_i^{A_1} \sigma_j^{A_2} \sigma_k^{B_1},$$

$$\sigma^{A \npreceq \nsucceq B} := \sum_{i>0} v_i \sigma_i^{A_1} + \sum_{i>0} x_i \sigma_i^{B_1} + \sum_{ij>0} g_{ij} \sigma_i^{A_1} \sigma_j^{B_1},$$

where $c_{ij}, d_{ijk}, e_{ij}, f_{ijk}, g_{ij}, v_i, x_i \in \mathbb{R}$.

This form, together with the condition $W^{A_1 A_2 B_1 B_2} \geq 0$, completely characterises the most general bipartite process matrix.

C.3 Terms not Appearing in Process Matrices

The terms not-allowed in a process matrix (i.e. those incompatible with the normalisation condition (5.9)) are listed in Tab. 5.2, along with possible interpretations. Particularly interesting are the cases involving terms of the type $A_1 A_2$.

These would correlate Alice's output with her input and not give unit probabilities for some CPTP maps that she can choose to perform. This kind of correlations resemble a "backward in time" transmission of information: one can imagine that they can be generated by a quantum channel "in the inverse order", from the output A_2 to the input A_1. It is worth noting that a recently proposed model of closed time-like curves [128, 129] can be expressed precisely in this way. Using our terminology, such a model considers an agent receiving two quantum systems in her laboratory: a chronology-respecting system A and a second system A' which, after leaving the laboratory, is sent back in time to the laboratory's entrance, see Fig. C.1. This can be described by the process matrix $W^{A_1 A_1' A_2 A_2'} = \sigma^{A_1} \otimes \mathbb{1}^{A_2} \otimes \left(U \otimes \mathbb{1} | \phi^+ \rangle \langle \phi^+ |^{A_1' A_2'} U^\dagger \otimes \mathbb{1} \right)$, where σ^{A_1} is the state of the chronology-respecting system when it enters the laboratory and $\left(U \otimes \mathbb{1} | \phi^+ \rangle \langle \phi^+ |^{A_1' A_2'} U^\dagger \otimes \mathbb{1} \right)$ is a process matrix corresponding to a unitary U from A_2' to A_1', describing the evolution back in time of the chronology-violating system. (The labels A_1, A_1' represent the two systems entering the laboratory, while A_2, A_2' represent the systems going out. Note that, here, the two systems A and A' pass through the same laboratory and thus they can undergo any joint operation.) In this model, probabilities have to be renormalised in order to sum up to one: if the agent performs a quantum instrument described by the set of CJ matrices $\{M_j^{A_1 A_1' A_2 A_2'}\}$, the probability of observing the outcome j is given by

$$P(M_j^{A_1 A_1' A_2 A_2'}) = \frac{\text{Tr}\left[M_j^{A_1 A_1' A_2 A_2'} W^{A_1 A_1' A_2 A_2'} \right]}{\text{Tr}\left[\sum_j M_j^{A_1 A_1' A_2 A_2'} W^{A_1 A_1' A_2 A_2'} \right]}.$$

This makes the probabilities non-linear functions of the local operations $M_j^{A_1 A_1' A_2 A_2'}$, therefore the model violates our original assumptions (in particular, as opposed to quantum mechanics, probabilities are contextual in this model, since it is necessary to specify the events that do not occur in order to perform the renormalisation step). A similar conclusion can be drawn for Deutsch's model of closed time-like curves [138], which is also non-linear (although it uses a different mechanism to obtain well-defined probabilities) and thus violates our premise that ordinary quantum mechanics holds locally in each laboratory.

C.4 Casual Order in the Classical Limit

Let us now show that in the classical limit all correlations are causally ordered. Classical operations can be described by transition matrices $M_j^{(ki)} = P(k, j|i)$, where $P(k, j|i)$ is the conditional probability that the measurement outcome j is observed and the classical output state k is prepared given that the input state is i.
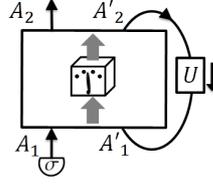
Figure C.1: Nonlinear model of closed time-like curve. In the model of closed time-like curves considered in Refs. [128, 129], a chronology-respecting system A, initially in a state σ, interacts with a second system, A', which travels back in time according to a unitary U. This model can be represented in our formalism by an "unphysical" process matrix, i.e. one for which probabilities do not sum up to one.

They can be expressed in the quantum formalism as CP maps diagonal in a fixed ("pointer") basis, and the corresponding CJ matrices are $M_j = \sum_{ki} M_j^{(ki)} |i\rangle\langle i|^{A_1} \otimes |k\rangle\langle k|^{A_2}$. In order to express arbitrary bipartite probabilities of classical operations, it is sufficient to consider process matrices of the standard form

$$W^{A_1A_2B_1B_2} = \frac{1}{d_{A_1}d_{B_1}}\left(\mathbb{1} + \sigma^{B \nleq A} + \sigma^{A \nleq B}\right),\tag{C.8}$$

where $\sigma^{B \nleq A}$ and $\sigma^{A \nleq B}$ are diagonal in the pointer basis. Probabilities are still given by Eq. (5.5).

We will show that any such diagonal process matrix can be written in the form

$$W^{A_1A_2B_1B_2} = \frac{1}{d_{A_1}d_{B_1}}\left(\rho^{A_1A_2B_1} \otimes \mathbb{1}^{B_2} + \rho^{A_1B_1B_2} \otimes \mathbb{1}^{A_2}\right),\tag{C.9}$$

where $\rho^{A_1A_2B_1}$ and $\rho^{A_1B_1B_2}$ are positive semidefinite matrices. This is sufficient to conclude that $W^{A_1A_2B_1B_2}$ is causally separable. Indeed, if $W^{A_1A_2B_1B_2}$ can be written in the form (C.9), we know that $\rho^{A_1A_2B_1}$ does not contain Hilbert-Schmidt terms of the types A_1A_2 or A_2 (which are not allowed in a process matrix), since by assumption these terms are not part of $W^{A_1A_2B_1B_2}$. Therefore, the matrix

$$W^{B \nleq A} \equiv \frac{\rho^{A_1A_2B_1}}{\mathrm{Tr}\rho^{A_1A_2B_1}} d_{A_2}d_{B_2},\tag{C.10}$$

which is positive semidefinite, has trace $d_{A_2}d_{B_2}$, and contains only terms of the allowed types, is a valid process matrix with no signalling from B to A. Similarly,

$$W^{A \nleq B} \equiv \frac{\rho^{A_1B_1B_2}}{\mathrm{Tr}\rho^{A_1B_1B_2}} d_{A_2}d_{B_2}\tag{C.11}$$

is a valid process matrix with no signalling from A to B. The whole process matrix can then be written in the causally separable form

$$W^{A_1A_2B_1B_2} = qW^{B \nleq A} + (1-q)W^{A \nleq B},\tag{C.12}$$

where

$$q \equiv \frac{\mathrm{Tr}\rho^{A_1 A_2 B_1}}{d_{A_1} d_{A_2} d_{B_1} d_{B_2}}. \tag{C.13}$$

Note that $0 \le q \le 1$ since $\rho^{A_1 A_2 B_1}$ and $\rho^{A_1 B_1 B_2}$ in Eq. (C.9) are positive semidefinite and $\mathrm{Tr} W^{A_1 A_2 B_1 B_2} = d_{A_2} d_{B_2}$.

To prove Eq. (C.9), we will construct $\rho^{A_1 A_2 B_1}$ and $\rho^{A_1 B_1 B_2}$ from the general form in Eq. (C.8). Let the minimum eigenvalue of $\sigma^{B \not\preceq A} + \sigma^{A \not\preceq B}$ be m. Since $W^{A_1 A_2 B_1 B_2}$ is positive semidefinite and $\sigma^{B \not\preceq A} + \sigma^{A \not\preceq B}$ is traceless, we have $m \in [-1, 0]$. Define the matrices

$$\kappa^{A_1 A_2 B_1} = -m\mathbb{1} + \sigma^{B \not\preceq A}, \tag{C.14}$$

$$\kappa^{A_1 B_1 B_2} = \sigma^{A \not\preceq B}. \tag{C.15}$$

The full process matrix can then be written

$$W^{A_1 A_2 B_1 B_2} = \frac{1}{d_{A_1} d_{B_1}} \left((1+m)\mathbb{1} + \kappa^{A_1 A_2 B_1} + \kappa^{A_1 B_1 B_2} \right), \tag{C.16}$$

where $\kappa^{A_1 A_2 B_1} + \kappa^{A_1 B_1 B_2}$ is positive semidefinite.

We are now going to modify $\kappa^{A_1 A_2 B_1}$ and $\kappa^{A_1 B_1 B_2}$ by adding matrices of the form $\kappa^{A_1 B_1}$ to $\kappa^{A_1 A_2 B_1}$ and subtracting them from $\kappa^{A_1 B_1 B_2}$ (therefore leaving $\kappa^{A_1 A_2 B_1} + \kappa^{A_1 B_1 B_2}$ unchanged), until we transform both $\kappa^{A_1 A_2 B_1}$ and $\kappa^{A_1 B_1 B_2}$ in Eq. (C.16) into positive semidefinite matrices.

Denote the pointer basis of system X by $|i\rangle^X$, $i = 1, ..., d_X$, $X = A_1, A_2, B_1, B_2$. All matrices we consider are diagonal in the basis $\{|i\rangle^{A_1}|j\rangle^{A_2}|k\rangle^{B_1}|l\rangle^{B_2}\}$. Let $m_1(i, j, k, l)$ denote the eigenvalues of $\kappa^{A_1 A_2 B_1}$ corresponding to the eigenvectors $|i\rangle^{A_1}|j\rangle^{A_2}|k\rangle^{B_1}|l\rangle^{B_2}$, and let $m_2(i, j, k, l)$ be the eigenvalues of $\kappa^{A_1 B_1 B_2}$ corresponding to the same vectors. For every i and k, we do the following. Define

$$\tilde{m}_1(i, k) = \min_{j,l} m_1(i, j, k, l), \tag{C.17}$$

$$\tilde{m}_2(i, k) = \min_{j,l} m_2(i, j, k, l). \tag{C.18}$$

Note that $m_1(i, j, k, l)$ do not depend on l since $\kappa^{A_1 A_2 B_1}$ acts trivially on B_2, and similarly $m_2(i, j, k, l)$ do not depend on j. This means that for given i and k, the minimum of the eigenvalues of $\kappa^{A_1 A_2 B_1} + \kappa^{A_1 B_1 B_2}$ for all eigenvectors of the type $|i\rangle^{A_1}|j\rangle^{A_2}|k\rangle^{B_1}|l\rangle^{B_2}$ is equal to $\tilde{m}_1(i, k) + \tilde{m}_2(i, k)$. But by construction $\kappa^{A_1 A_2 B_1} + \kappa^{A_1 B_1 B_2}$ is positive semidefinite, so we have

$$\tilde{m}_1(i, k) + \tilde{m}_2(i, k) \ge 0. \tag{C.19}$$

Now, if both $\tilde{m}_1(i, k)$ and $\tilde{m}_2(i, k)$} are non-negative, we will not modify $\kappa^{A_1 A_2 B_1}$ and $\kappa^{A_1 B_1 B_2}$. However, if one of these numbers is negative, say $\tilde{m}_1(i, k) < 0$ (both cannot be negative due to (C.19)), we will add the term $-\tilde{m}_1(i, k)|i\rangle\langle i|^{A_1} \otimes \mathbb{1}^{A_2} \otimes |k\rangle\langle k|^{B_1} \otimes \mathbb{1}^{B_2}$ to $\kappa^{A_1 A_2 B_1}$ and subtract the same term from $\kappa^{A_1 B_1 B_2}$. After this step, the modified $\kappa^{A_1 A_2 B_1}$ is such that the eigenvalues $m_1(i, j, k, l)$ have been changed to $m_1(i, j, k, l) - \tilde{m}_1(i, k) \geq \tilde{m}_1(i, k) - \tilde{m}_1(i, k) = 0$, i.e. $\kappa^{A_1 A_2 B_1}$ does not have any more negative eigenvalues $m_1(i, j, k, l)$ for the given i and k. The same holds for $\kappa^{A_1 B_1 B_2}$ since the eigenvalues $m_2(i, j, k, l)$ change to $m_2(i, j, k, l) + \tilde{m}_1(i, k) \geq \tilde{m}_2(i, k) + \tilde{m}_1(i, k) \geq 0$. In other words, the eigenvalues of the modified $\kappa^{A_1 A_2 B_1}$ and $\kappa^{A_1 B_1 B_2}$ satisfy

$$m_1(i, j, k, l), \ m_2(i, j, k, l) \geq 0, \quad \forall j, l. \tag{C.20}$$

By performing this procedure for all i and k, we eventually transform $\kappa^{A_1 A_2 B_1}$ and $\kappa^{A_1 B_1 B_2}$ into matrices all of whose eigenvalues are non-negative. Denote the resultant positive semidefinite matrices by $\tilde{\kappa}^{A_1 A_2 B_1}$ and $\tilde{\kappa}^{A_1 B_1 B_2}$. We can now add the term $(1 + m)\mathbb{1}$ in Eq. (C.16) for instance to $\tilde{\kappa}^{A_1 A_2 B_1}$ (recall that $m \in [-1, 0]$), defining the positive semidefinite matrices

$$\rho^{A_1 A_2 B_1} \equiv (1 + m)\mathbb{1} + \tilde{\kappa}^{A_1 A_2 B_1}, \tag{C.21}$$

$$\rho^{A_1 B_1 B_2} \equiv \tilde{\kappa}^{A_1 B_1 B_2}. \tag{C.22}$$

We thus arrive at the desired form (C.9) which implies (C.12) as argued above.

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Curriculum Vitae

Professional history

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