An introduction to Krylov Complexity

An analytical method for calculations

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Περίληψη

Σκοπός της παρούσας εργασίας είναι να αποτελέσει εισαγωγή στην έννοια της πολυπλοκότητας Krylov. Ξεκινάμε με τη διερεύνηση της αναδρομικής μεθόδου Lanczos μέσω της οποίας, χρησιμοποιώντας τη διαδικασία Gram-Schmidt, κατασκευάζουμε την ορθοκανονική βάση Krylov και λαμβάνουμε τους λεγόμενους συντελεστές Lanczos, εργαλεία κατάλληλα για την περιγραφή της χρονικής εξέλιξης τόσο καταστάσεων όσο και τελεστών. Η προσέγγιση των τελεστών απαιτεί να προικιστεί ο χώρος των τελεστών με ένα εσωτερικό γινόμενο. Ολοκληρώνουμε το πρώτο κεφάλαιο αναφέροντας μια υπόθεση για το άνω όριο αυτών των συντελεστών. Συνεχίζουμε με τον ορισμό της πολυπλοκότητας Krylov και παρουσιάζουμε μια αναλυτική εφαρμογή στο μοντέλο SYK. Στη συνέχεια, ενισχύουμε τα θεμέλια του ορισμού μας επικαλούμενοι ένα αξίωμα ελαχιστοποίησης. Το τρίτο κεφάλαιο χρησιμεύει ως παρουσίαση του ακρογωνιαίου λίθου της αναλυτικής μας μεθόδου, των "σύμφωνων καταστάσεων". Ξεκινάμε με τις κανονικές σύμφωνες καταστάσεις, παρουσιάζοντας μια εξαγωγή και συζητώντας τις πιο σημαντικές και χρήσιμες, για τον σκοπό μας, ιδιότητες που διαθέτουν. Στη συνέχεια επιχειρούμε να ορίσουμε γενικευμένα σύνολα σύμφωνων καταστάσεων απαιτώντας συνέχεια και πληρότητα. Αυτό μας οδηγεί στην εισαγωγή των άλλων δύο πιο συνηθισμένων οικογενειών, των σπιν-σύμφωνων και των SU(1,1) σύμφωνων καταστάσεων. Μια βασική εισαγωγή στις ιδιότητες της αντίστοιχης άλγεβρας Lie παρέχεται σε κάθε περίπτωση πριν συζητήσουμε την "υπερπληρότητα", την ελάχιστη αβεβαιότητα και κάποιες σημαντικές παραμετροποιήσεις για κάθε οικογένεια. Το Κεφάλαιο 3 ολοκληρώνεται με την εισαγωγή της μετρικής Fubini-Study, η οποία μας επιτρέπει να προικίσουμε τους χώρους Hilbert με μια μετρική δομή Riemann. Στο τελευταίο κεφάλαιο, παρουσιάζουμε ένα επιχείρημα για αναλυτικές λύσεις, εφαρμόσιμο σε συγκεκριμένα συστήματα. Δείχνουμε ότι, όταν ο υπερτελεστής του Liouville μπορεί να αναλυθεί σε άθροισμα τελεστών ανύψωσης και υποβιβασμού μιας συγκεκριμένης άλγεβρας Lie, το υπολογιστικό βάρος της μεθόδου Lanczos αίρεται πλήρως. Εφαρμόζουμε τη μέθοδο αυτή σε τρία παραδείγματα. Τέλος, κατασκευάζουμε τη μετρική Fubini-Study για τις αντίστοιχες σύμφωνες καταστάσεις και επιχειρούμε να εξετάσουμε πτυχές της προσέγγισής μας χρησιμοποιώντας γεωμετρικά μεγέθη όπως ο όγκος, οι γεωδαισιακές καμπύλες και το βαθμωτό Ricci σε αυτή τη μετρική.

Abstract

The purpose of the present thesis is to introduce the concept of Krylov complexity. We start by exploring the Lanczos recursion method through which, utilizing the Gram-Schmidt process, we construct the orthonormal Krylov basis and obtain the so-called Lanczos coefficients, tools suitable for describing the time evolution of both states and operators. The operator approach requires endowing the operator space with an inner product. We finish the first chapter by mentioning a hypothesis on the upper bound of these coefficients. We continue with the definition of Krylov complexity and demonstrate an analytical application to the SYK model. Next, we strengthen the foundations of our definition by invoking a minimization axiom. The third chapter serves as a presentation of the cornerstone of our analytical method, the coherent states. We begin with the canonical coherent states, showing a derivation and discussing the most important and useful, to our cause, properties they possess. We then attempt to define generalized sets of coherent states by demanding continuity and completeness. This leads us to the introduction of the other two most common families, the spin-coherent, and the SU(1,1) coherent states. A basic introduction to the properties of the corresponding Lie Algebra is provided in each case before we discuss the overcompleteness, minimum uncertainty, and some important parametrizations for each family. Chapter 3 ends with the introduction of the Fubini-Study metric, which allows us to endow Hilbert spaces with a Riemannian metric structure. In the final chapter, we present an argument for analytical solutions, applicable to specific systems. We show that when the Liouvillian can be decomposed into the sum of raising and lowering operators of a specific Lie Algebra, the computational burden of the Lanczos method is entirely lifted. We apply this method in three examples. Finally, we construct the Fubini-Study metric for the corresponding coherent states and attempt to examine aspects of our approach using geometric quantities such as the volume, geodesic curves, and the Ricci scalar in this metric.

Acknowledgments

Krylov complexity is a very recent but quickly increasing in popularity and attention subject of theoretical physics. I am earnestly grateful to my supervisor, Professor Anastasios Petkou for recommending such an interesting, comprehensive, and currently relevant topic that I could not have discovered on my own. More than that, I would like to thank him for our numerous insightful conversations beyond the scope of this thesis thanks to which I have shaped the scientific trajectory I envision for myself and garnered a great deal of advice for its realization.

Furthermore, it goes without saying that I am indebted to my family for supporting me, but even more so, for continuously putting up with me. Their role in my endeavors has always been indispensable.

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Introduction

Quantum complexity is a rapidly blossoming field of theoretical physics that aims to provide a means for quantitative analysis of chaotic evolution and many-body dynamics in general for quantum systems. Unlike in classical dynamical systems, where extreme sensitivity to initial conditions and topological mixing of trajectories suffice to define and witness chaotic behavior, a clear definition is still pending in quantum mechanics. As such, there exists strong motivation originating from various different fields for the discovery, and creation, of probes or measures of such phenomena in the microscopic world. From quantum information theory and computing to holography and quantum gravity, condensed matter physics, or QFTs, complexity has shown great promise in providing novel insights and establishing potential connections between theories. A significant part of the discussion has been centered around the complexity and time evolution of states, or mainly, operators in the Heisenberg picture. Two very important measures are that of Nielsen, where the complexity of a unitary operator $U(t) = e^{-iHt}$ is defined as the minimal distance to the identity in the unitary group and of computational complexity defined as the minimum number of elementary quantum gates required to produce a target state $|\psi_T\rangle$ starting from a reference state $|\psi_R\rangle$. One advantage the topic of this thesis, Krylov complexity, holds over the above is that it, as we will see, does not require the inclusion of arbitrary cost functions or sets of elementary gates to be properly defined. This, along with a few other properties make it so that Kyrlov complexity is applicable in any quantum theory, turning it into a very attractive candidate for a universal complexity measure.

This thesis is not meant to be a comprehensive review of Krylov complexity by any means. In fact, a common theme throughout our analysis will be carefully picking and focusing on the appropriate depth and width of each subject at hand. Firstly, when introducing concepts from various fields of Mathematics, we avoid adopting the highest level of rigor for two main reasons. Being correct and complete in the strictest sense in every case would involve repeatedly delving into a vast amount of technical detail which, one, is beyond the scope of knowledge of the author and, two, would not positively contribute to understanding the concepts being discussed, distracting us from physical meaning. Furthermore, we follow a similar philosophy when discussing different advanced topics in Physics. In instances where a part of a specific field plays a fundamental role in our procedures, we present what we deem to be an adequate general introduction along with a brief overview of the list of properties that we require, showing calculations whenever we consider it beneficial. On the other hand, aside from the bare minimum necessary to continue, we do not concern ourselves with details of the systems and their respective parent theories to which we apply our complexity measure.

Our hope when writing this thesis was to create an introductory "manual" including an overview of the Krylov complexity formalism and a very strong method for analytical calculations presented by Caputa et. al.[1], understandable by anyone with an undergraduate level of knowledge.

Contents

Chapter 1

Time Evolution and the Krylov Basis

To properly define Krylov Complexity, we must first quantify the notion of an operator's $O(t)$, or equivalently, a state's $|\psi(t)\rangle$, spread in their associated Hilbert Spaces over their unitary evolution in time[1]. This process requires the selection of a basis to measure this spread. In this context, we will employ the Lanczos approach to many-body dynamics to construct the so-called ordered, orthonormal "Krylov basis" [2] for any particular operator (or state).

The Krylov basis $\mathcal{K}$ is highly useful as it accurately represents the part of the Hilbert space that gets explored during the time development of the initial state. While this choice seems natural for gauging the spread, given its aforementioned advantage, it's far from the only one. This degree of arbitrariness may initially appear problematic for defining complexity. We address and largely resolve this issue in a future section.

1.1 Schrödinger and Heisenberg Pictures

Quantum mechanics offers multiple equivalent mathematical frameworks for describing the dynamics of a given system. This section will focus on the Schrödinger and Heisenberg pictures. Although distinct in their approach, they yield identical physical predictions.

1.1.1 Schrödinger Picture

The Schrödinger picture presents a time-dependent state and time-independent operators. The evolution of an initial normalized state $|\psi(t_0)\rangle$ at a point in time $t = t_0$ in this framework is dictated by the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \,, \tag{1.1}$$

where $\hat{H}$ is the Hamiltonian governing the system under study. Given a Hamiltonian without explicit time-dependence, as will be all the Hamiltonians mentioned from now on, the solution to the partial differential equation (1.1) is

[1] For this thesis, we focus on unitary time evolution. Open quantum systems are an example where non-unitary time evolution is observed, i.e. the total probability of the system is not conserved.

[2] This is a bit of a misnomer, as the Krylov basis spans *a* space containing $O(t)$ (or $|\psi(t)\rangle$ respectively) for any t but does not usually span the full Hilbert Space.

$$|\psi(t)\rangle = \hat{U}_{t-t_0} |\psi(t_0)\rangle = e^{-i\hat{H}(t-t_0)} |\psi(t_0)\rangle \tag{1.2}$$

where $\hat{U}_{t-t_0}$ is the unitary time-translation/time-evolution operator. Dropping the t_0 term (setting $t_0 = 0$) for simplicity and utilizing the Taylor expansion of the exponential function of $\hat{H}$ [3] we can rewrite (1.2) as

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \hat{H}^n |\psi(0)\rangle = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} |\psi_n\rangle \tag{1.3}$$

where $|\psi_n\rangle$ represents the state which is produced by n consecutive applications of the Hamiltonian to the initial state $|\psi(0)\rangle$.

1.1.2 Heisenberg Picture

Time Evolution

The Heisenberg picture offers an alternative to the above view. Here, the states are regarded as static, while the operators, the ones that are representatives of observable quantities, undertake the role of dynamic entities. This property differs from the potential explicit time dependence an observable might admit. The time evolution of a given initial operator $\hat{O}(0) = \hat{O}$ is now determined by the Heisenberg equation of motion,

$$i\hbar \frac{d}{dt}\hat{O}(t) = i\hbar \frac{\partial}{\partial t}\hat{O}(t) + [\hat{O}(t), \hat{H}] \tag{1.4}$$

where the first term on the right-hand side denotes the aforementioned explicit time dependence and will be taken equal to zero in the following analysis. The second term is the commutator of the Operator with the Hamiltonian. The solution (setting $\hbar = 1$ for simplicity) to equation (1.4) is

$$\hat{O}(t) = \hat{U}_t^{\dagger} O \hat{U}_t = e^{i\hat{H}t} \hat{O} e^{-i\hat{H}t} \tag{1.5}$$

Before continuing, it is important to demonstrate the correspondence between these two pictures and confirm their equivalence in the prediction of physical quantities. These appear as inner products in Quantum Mechanics. The subscript (superscript) H refers to the Heisenberg picture while S refers to the Schrödinger picture.

$$\begin{aligned} |\psi(t)\rangle_S &= e^{-i\hat{H}t} |\psi\rangle_H \\ \hat{O}(t)_H &= e^{i\hat{H}t} \hat{O}_S e^{-i\hat{H}t} \\ \langle\psi(t)|\hat{O}|\psi(t)\rangle_S &= \langle\psi(0)|e^{i\hat{H}t}\hat{O}_S e^{-i\hat{H}t}|\psi(0)\rangle = \langle\psi|\hat{O}(t)|\psi\rangle_H \end{aligned} \tag{1.6}$$

Baker-Haussdorff Lemma

Due to the way an operator transforms in the Heisenberg picture, executing the last step to write $\hat{O}(t)$ in the form of a "Taylor expansion" requires invoking the powerful *Baker-Haussdorf lemma*. Given any two operators $\hat{A}$,$\hat{B}$ belonging to a Lie Algebra the following equation holds[2],

[3] The exponential of $\hat{H}$ being applied to a state $|\psi(0)\rangle$ belonging to a Hilbert Space meets the requirements for the expansion to be well defined.

$$e^{\hat{B}}\hat{A}e^{-\hat{B}} = \hat{A} + [\hat{B},\hat{A}] + \frac{1}{2!}[\hat{B},[\hat{B},\hat{A}]] + \frac{1}{3!}[\hat{B},[\hat{B},[\hat{B},\hat{A}]]] + ... \tag{1.7}$$

where $[\hat{B},[\hat{B},\hat{A}]]$ for example denotes the double-nested commutator of $\hat{A}$ and $\hat{B}$, i.e.

$$[\hat{B},[\hat{B},\hat{A}]] = \hat{B}[\hat{B},\hat{A}] - [\hat{B},\hat{A}]\hat{B} = \hat{B}\hat{B}\hat{A} - \hat{B}\hat{A}\hat{B} - \hat{B}\hat{A}\hat{B} + \hat{A}\hat{B}\hat{B} = \hat{B}\hat{B}\hat{A} - 2\hat{B}\hat{A}\hat{B} + \hat{A}\hat{B}\hat{B}. \tag{1.8}$$

Given its undeniable significance in the present analysis and future sections, a proof of the lemma is provided below. Let x be a real variable and $F(x)$ a function of the form,

$$F(x) = e^{x\hat{A}}\hat{B}e^{-x\hat{A}} \tag{1.9}$$

It is easy to check that the derivatives of this function can be written recursively in the following form

$$\begin{gathered} F'(x) = \hat{A}e^{x\hat{A}}\hat{B}e^{-x\hat{A}} - e^{x\hat{A}}\hat{B}e^{-x\hat{A}}\hat{A} = [\hat{A},F(x)] \\ F''(x) = \hat{A}(\hat{A}e^{x\hat{A}}\hat{B}e^{-x\hat{A}}) - (\hat{A}e^{x\hat{A}}\hat{B}e^{-x\hat{A}})\hat{A} - \hat{A}e^{x\hat{A}}\hat{B}e^{-x\hat{A}}\hat{A} + (e^{x\hat{A}}\hat{B}e^{-x\hat{A}})\hat{A} = [\hat{A},F'(x)] \\ F^{(n)}(x) = [\hat{A},F^{(n-1)}(x)] \end{gathered} \tag{1.10}$$

Using (1.10) the derivatives of F calculated at $x = 0$ turn out to be

$$\begin{gathered} F(0) = \hat{B} \\ F'(0) = [\hat{A},\hat{B}] \\ F^{(n)}(0) = \underbrace{[\hat{A},[\hat{A},[\hat{A},[\hat{A},\ldots,}_{n-times},\hat{B}]]]\ldots] \end{gathered} \tag{1.11}$$

With these, the Taylor expansion of (1.9) around 0 and calculated at $x = 1$ is written as

$$F(1) = \sum_{n=0}^{\infty}\frac{F^{(n)}(0)}{n!}1^n = \sum_{n=0}^{\infty}\frac{F^{(n)}(0)}{n!} = \hat{B} + [\hat{A},\hat{B}] + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \ldots \tag{1.12}$$

Which finally allows us to write (1.5) as

$$\hat{O}(t) = \sum_{n=0}^{\infty}\frac{(it)^n}{n!}\tilde{O}_n \tag{1.13}$$

where $\tilde{O}_n$ are the nested commutators of $\hat{O}$ with the Hamiltonian (we have dropped the hat symbol on these terms for clarity)

$$\tilde{O}_0 = \hat{O}, \tilde{O}_1 = [\hat{H},\hat{O}], \tilde{O}_2 = [\hat{H},[\hat{H},\hat{O}]], \ldots \tag{1.14}$$

The correspondence between (1.3) and (1.13) will become clear once we properly define the Auxilliary Hilbert Space for *Operator kets* and introduce the *Liouvillian super-operator* for closed systems.

1.2 Lanczos Algorithm

Starting from the final results of the previous section, the Lanczos approach to non-equilibrium dynamics[4] works by iteratively applying the *Gram-Schmidt orthogonalization procedure* to the terms of (1.3) and (1.13). Again, we start with the simpler case of the state expansion as the $|\psi_n\rangle$ terms represent vectors belonging to a Hilbert Space. For that to hold in the case of the set $\tilde{O}_n$, the preliminary work is significantly more involved.

1.2.1 Gram-Schmidt orthogonalization procedure

Although the Gram-Schmidt process was originally defined on finite-dimensional inner product spaces[5], in the case of an infinite-dimensional, yet separable Hilbert space – that is, a space with a countable basis – we can still employ it to derive an orthonormal basis [4]. The process goes as follows.

Given an initial set of linearly independent vectors, $\{v_i\}$, the orthonormal basis is sequentially crafted. The first basis vector u_1 is just a normalized version of v_1,

$$u_1 = \frac{v_1}{\langle v_1|v_1\rangle^{\frac{1}{2}}} \tag{1.15}$$

where $\langle v_1|v_1\rangle$ denotes the inner product of v_1 with itself in Dirac notation.

Then, to construct a vector orthogonal to u_1, the projection of v_2 onto u_1 is removed from v_2. Finally, the new vector is normalized.

$$z_2 = v_2 - \langle v_2|u_1\rangle\, u_1, \tag{1.16a}$$

$$u_2 = \frac{z_2}{\langle z_2|z_2\rangle}. \tag{1.16b}$$

Likewise, removing the projections of v_3 onto u_1 and u_2 from itself and normalizing, produces u_3.(Note that these projections are always of the form seen in (1.16a) and independent of each other due to the orthogonality of $\{u_i\}$). The general iterative formula thus is

$$z_n = v_n - \sum_{i=0}^{n-1} \langle v_n|u_i\rangle\, u_i,$$

$$u_n = \frac{z_n}{\langle z_n|z_n\rangle}. \tag{1.17}$$

1.2.2 Krylov state basis

We start by applying the above algorithm to the set of vectors$\{\hat{H}^n\,|\psi(0)\rangle\}$, generated by the Hamiltonian in (1.3). Throughout the following analysis, the hermiticity of $\hat{H}$ is assumed which allows for its "moving" from the ket to the bra position and vice versa. This is in fact what will

[4]The terms "many-body" and "non-equilibrium" refer to distinct types of systems with significant overlap between them. They will be used interchangeably throughout this thesis.

[5]These are, of course, not limited to the vector spaces used below, see [3]

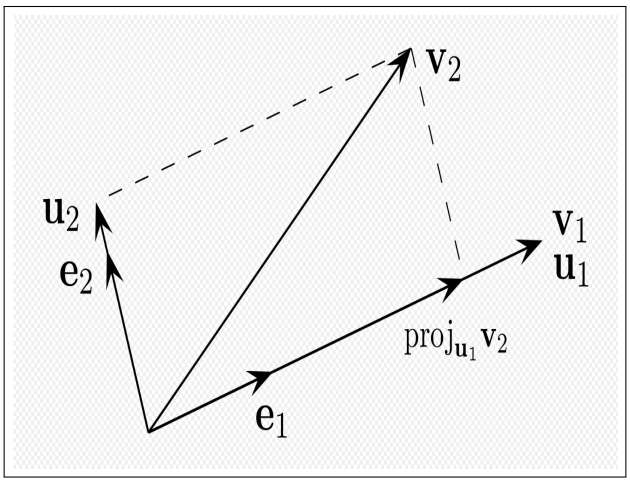

Figure 1.1: Schematic representation of the Gram-Schmidt orthogonalization procedure.

significantly simplify this procedure. We picked $|\psi(0)\rangle$ to be normalized so the first term of the Krylov State Basis is $|K_0\rangle = |\psi(0)\rangle = |\psi_0\rangle$. $|K_1\rangle$ is, according to (1.17),

$$\begin{aligned} |z_1\rangle &= \hat{H}\,|K_0\rangle - a_0\,|K_0\rangle\,, \\ |K_1\rangle &= \frac{|z_1\rangle}{\langle z_1|z_1\rangle}. \end{aligned} \tag{1.18}$$

where,

$$a_0 = \langle K_0|\hat{H}|K_0\rangle \tag{1.19}$$

Normally, we would proceed with K_2 by subtracting the previous two vectors, K_3 by subtracting the previous 3 vectors, and so forth. However, here lies the strength of the Lanczos algorithm. Following [5], the iterative formula for $|K_n\rangle$ can inductively be proven to be

$$\begin{aligned} |z_{n+1}\rangle &= (\hat{H} - a_n)\,|K_n\rangle - b_n\,|K_{n-1}\rangle\,, \\ |K_n\rangle &= b_n^{-1}\,|z_n\rangle\,. \end{aligned} \tag{1.20}$$

$$\langle K_n|K_m\rangle = \delta_{nm} \tag{1.21}$$

a_n, b_n represent the, by default real, *Lanczos coefficients* with units of energy defined by

$$a_n = \langle K_n|\hat{H}|K_n\rangle\,, \tag{1.22}$$

$$\begin{aligned} b_n &= \langle z_n|z_n\rangle^{\frac{1}{2}} \\ b_0 &\equiv 0 \end{aligned} \tag{1.23}$$

To prove by induction that the Lanczos algorithm (1.20) produces an orthonormal set of vectors, we first remind that $|K_0\rangle = |\psi_0\rangle$ (which is normalized) and $b_0 = 0$. Already, we can see how (1.18)

does follow the algorithm. That is the first step. Now, to complete the proof, we need to show that a state $|z_n\rangle$ produced by (1.20) is orthogonal to any $|K_m\rangle$ such that $m < n$. We proceed as follows,

$$\begin{aligned}\langle z_n|K_m\rangle &= \langle(\hat{H} - a_{n-1})K_{n-1}|K_m\rangle - \langle b_{n-1}K_{n-2}|K_m\rangle\,,\\ &= \langle K_{n-1}|\hat{H}|K_m\rangle - a^*_{n-1}\langle K_{n-1}|K_m\rangle - b^*_{n-1}\langle K_{n-2}|K_m\rangle\,,\\ &= \langle K_{n-1}|\hat{H}|K_m\rangle - a_{n-1}\delta^m_{n-1} - b_{n-1}\delta^m_{n-2}. \end{aligned} \tag{1.24}$$

We continue by applying the Hamiltonian above to $\langle K_{n-1}|$ and using (1.26). We get

$$\begin{aligned}\langle z_n|K_m\rangle &= \langle a_{n-1}K_{n-1}|K_m\rangle + \langle b_nK_n|K_m\rangle + \langle b_{n-1}K_{n-2}|K_m\rangle - a_{n-1}\delta^m_{n-1} - b_{n-1}\delta^m_{n-2},\\ &= a_{n-1}\delta^m_{n-1} + b_n\delta^m_n + b_{n-1}\delta^m_{n-2} - a_{n-1}\delta^m_{n-1} - b_{n-1}\delta^m_{n-2} = 0. \end{aligned} \tag{1.25}$$

This concludes the proof by induction. The normalization of $|z_n\rangle$ was not relevant to the proof and thus was not included.

The essence of (1.20) is that we do not need to explicitly subtract the projections along the previous vectors in each step but the orthogonality is, in a way, ensured by just the two terms containing the Lanczos coefficients (Which correspond to the last two constructed orthonormal vectors). This greatly reduces the number of calculations needed to, analytically and numerically, construct this orthonormal basis. This effect becomes more apparent by rearranging (1.20) in the following way,

$$\hat{H}\,|K_n\rangle = a_n\,|K_n\rangle + b_{n+1}\,|K_{n+1}\rangle + b_n\,|K_{n-1}\rangle \tag{1.26}$$

This equation demonstrates that the matrix representation of the Hamiltonian operator becomes tridiagonal[6] in the Krylov Basis $\mathcal{K}$. It is straightforward to see that the diagonal elements are given by a_n, whereas the elements above and below are given by b_n as shown below.

$$H_{nm} := \langle K_n|\hat{H}|K_m\rangle = \begin{pmatrix} a_1 & b_1 & 0 & 0 & \cdots\\ b_1 & a_2 & b_2 & 0 & \cdots\\ 0 & b_2 & a_3 & b_3 & \cdots\\ 0 & 0 & b_3 & a_4 & \ddots\\ \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix} \tag{1.27}$$

We can make an important observation about the application of the Gram-Schmidt orthogonalization procedure to the $\{\hat{H}^n\,|\psi_0\rangle\}$ set of vectors. It is not obvious that they are *linearly independent*. In fact, it may very well be the case that they are not. If so, the iterative process stops after a finite number of steps, say L. The Krylov Basis $\mathcal{K}$ then spans an L-Dimensional subspace of the Hilbert Space in which the initial state belongs. Keeping (1.3) in mind, it is now evident why $\mathcal{K}$ is said to represent the part of the Hilbert space that is explored during time evolution.

Already, it can be seen how the spread of the state will be measured using this Basis. Large dimensionality of the Krylov Subspace indicates that the initial state requires a greater part of the Hilbert Space to be properly described, and can thus be thought of as "more complex". This statement will become specific when we define Krylov Complexity.

[6] This is one of the original purposes of the Lanczos recursion method, see [6]

Putting the above results to use, the time evolved state $|\psi(t)\rangle$ can be written as,

$$|\psi(t)\rangle = \sum_{n=0}^{L-1} \phi_n(t) \, |K_n\rangle \tag{1.28}$$

where the sum is over $\{K_n\}$ and $\phi_n(t)$ are the probability amplitudes for each vector. Probability conservation requires that

$$\sum_{n=0}^{L-1} |\phi_n(t)|^2 \equiv \sum_n p_n(t) = 1 \tag{1.29}$$

Knowledge of all ϕ_n is required to completely determine the dynamics of the system. Inserting (1.28) into the Schrödinger equation (setting $\hbar = 1$)(1.1) yields[7],

$$\sum_n i \frac{\partial \phi_n(t)}{\partial t} \, |K_n\rangle = \sum_n \phi_n(t) \hat{H} \, |K_n\rangle \tag{1.30}$$

Combining (1.30) with the action of the Hamiltonian on the Krylov Basis vectors (1.26) gives

$$\sum_n i \frac{\partial \phi_n(t)}{\partial t} \, |K_n\rangle = \sum_n \phi_n(t)(a_n \, |K_n\rangle + b_{n+1} \, |K_{n+1}\rangle + b_n \, |K_{n-1}\rangle) \tag{1.31}$$

Remembering that, by convention, $b_0 = \phi_{-1} = 0$ and $b_L = 0$ (if it exists) and changing the summation variables accordingly to rearrange the terms, we reach an equation with sums left and right over $\{K_n\}$ that can be split, due to orthogonality, into differential equations for each $\phi_n(t)$,

$$i \frac{\partial \phi_n(t)}{\partial t} = a_n \phi_n(t) + b_{n+1} \phi_{n+1}(t) + b_n \phi_{n-1}(t), \tag{1.32}$$

with the expected initial conditions, $\phi_n(0) = \delta_{n0}$. As is obvious from (1.32), knowing the Lanczos coefficients amounts to knowing the dynamics of the system as they provide an algebraic procedure for calculating all ϕ_n. Starting from b_0 and $\phi_0(t)$, which, thanks to (1.28), is connected to the so-called *auto-correlation function*, or *survival amplitute* by

$$C(t) = \langle \psi(t) | \psi(0) \rangle = \langle \psi(t) | K_0 \rangle = \phi_0(t)^* \tag{1.33}$$

we can solve for $\phi_1(t)$ and likewise continue with the rest.

1.3 Krylov operator basis

In the context of time evolution within the Heisenberg Picture, applying the Lanczos Algorithm directly to the terms of (1.13) presents a problem: these terms are not vectors, but operators—specifically, nested commutators of operators. To address this, we must associate each nested commutator with a vector within a Hilbert Space of operators. For this, we need to define an inner product. The rationale behind this requirement is to endow the operator algebra with the

[7]Given the potential infinite dimensionality of the Krylov Space, the summation terms appearing below don't explicitly denote the range of the sum

structure of a Hilbert Space. As this process involves several complex steps and requires a considerable level of technical knowledge, we dedicate this entire section to it. We follow the *GNS (Gel'fand-Naimark-Segal) construction* outlined in [7].

In the subsequent discourse, we will lay out definitions and coin terms with the aim of capturing the essential characteristics of the concepts under study. Although these constructs could be generalized and defined with a higher degree of mathematical rigor, doing so would delve into technicalities that are beyond the scope of this thesis. Instead, the definitions provided here will be specifically tailored to meet our immediate requirements.

We will shed light on concepts such as algebras, von Neumann algebras, linear functionals, the dual space, the GNS construction, and the Thermofield Double State (TFD). A foundational understanding of terms like vector space, inner product space and Hilbert Space is assumed. A refresher on these terms is provided in (A.1).

In crafting our auxiliary Hilbert space and redefining our operators as states, we will need to employ thermal expectation values. This requires the use of density matrix formalism. However, as this formalism does not hold a pivotal conceptual role in this segment, we include a brief introduction for completeness purposes in (A.2).

1.3.1 Construction of the auxiliary Hilbert Space

We start by providing a brief glossary of mathematical terms that will be subsequently used.

Definition 1 *A subset $\mathcal{S}$ of all the bounded, linear operators $\mathcal{B}(\mathcal{H})$ acting on a Hilbert Space $\mathcal{H}$ is called an algebra*[8] *if*

(i) it is closed under linear combination over the complex numbers, i.e. for any $A,B \in \mathcal{S}$ and $\alpha, \beta \in \mathbb{C}$, $\alpha A + \beta B \in \mathcal{S}$ as well (the structure of a vector space),

(ii) it is closed under a binary operation, which in the case of operators is their consecutive application on a state of $\mathcal{H}$. That means that for $A,B \in \mathcal{S}$, $AB \in \mathcal{S}$ as well (this, along with the existence of an identity and inverse elements, endow the subset with the structure of a group).

An algebra according to Def. 1 is called an *-algebra if furthermore for any $A, \in \mathcal{S}$ its adjoint $A^\dagger$ also belongs to $\mathcal{S}$. We will not delve into the addition of topological closure arguments here, even though they are crucial for analysis, as they are not directly relevant to our objectives (see [8] for more information on the subject). They allow us to define *C*-algebras* and, finally, a subset of theirs which contain the Identity Operator[9], the *von Neumann* algebras.

This series of sequential definitions paints a picture of the most important properties of these constructs and was vital for our analysis as most if not all operators encountered in Quantum Mechanics form C*-algebras or von Neumann algebras.

The GNS construction generates a Hilbert space $\mathcal{H}_\omega$ from an abstract C* -algebra $\mathcal{A}$ and a linear functional (state) ω from $\mathcal{A}$ to $\mathbb{C}$, together with a pair of (equivalent) *representations of the algebra* $\pi(\mathcal{A}), \bar{\pi}(\mathcal{A})$ acting on it.

[8] The notion of an algebra extends beyond sets of operators acting on Hilbert Spaces.

[9] The requirement that the unit operator shall be contained in them is not always considered as part of the definition of a von Neumann ring.

Definition 2 *A representation of a (group) algebra[9] $\tilde{\mathcal{G}}$ is a mapping from $\tilde{\mathcal{G}}$ to a set of linear operators $\{U\}$ on a vector space $\mathcal{V}$ which preserve the group algebra structure: if $q,r \in \tilde{\mathcal{G}}$ and $U(q), U(r)$ are their images, then $U(\alpha q + \beta r) = \alpha U(q) + \beta U(r)$, and $U(qr) = U(q)U(r)$.*

Definition 3 *States ω are positive and normalized linear functionals from $\mathcal{A}$ to $\mathbb{C}$, i.e. for any $\alpha,\beta \in \mathbb{C}$ and $A,B \in \mathcal{A}$ they satisfy*

(i)
$$\omega(\alpha A + \beta B) = \alpha\omega(A) + \beta\omega(B),$$

(ii)
$$\omega(A^* A) \geq 0, \tag{1.34}$$

(iii)
$$\omega(\mathbb{I}) = 1.$$

Now, let $\mathcal{A}$ be von Neumann Operator Algebra. Considering the above, $\mathcal{A}$ is already a vector space over $\mathbb{C}$. What remains for the construction of a proper Hilbert Space $\mathcal{H}_\omega$ is the addition of an inner product following the restrictions set by Definition 9. This role is played by ω in the following way. Let's consider any two operators A and B in $\mathcal{A}$. Their inner product, defined using Dirac notation, is expressed as

$$\langle A|B\rangle = \omega(A^\dagger B) \tag{1.35}$$

This inner product satisfies all the requirements (A.7) except for the existence of non-zero operators W satisfying $\omega(W^\dagger W) = 0$. Resolving this issue is a technical procedure that requires further algebra theory knowledge and will not be demonstrated here. Curious readers are encouraged to refer to the sources cited before.

The two representations induced by the GNS Construct act on $\mathcal{H}_\omega$ in the following way,

$$\begin{aligned} \pi(A)\,|B\rangle &= |AB\rangle\,, \\ \bar{\pi}(A)\,|B\rangle &= |BA^\dagger\rangle \end{aligned} \tag{1.36}$$

Additionally, the two representations allow for the unitary transformations of the operators, such as time evolution, to be transferred to the corresponding states. With these, the construction of the Auxiliary Hilbert Space is complete. A ket can be attributed to each operator and its evolution can be seen as a conventional state evolution. Of course, (1.34) shows that we can choose an unlimited amount of different, but potentially related, inner products which will uniquely affect our definition of complexity.

This ambiguity, or freedom, of this approach, needs to be addressed in the same manner as arbitrarily picking the Krylov Basis for measuring the spread as we mentioned in this chapter's introduction.

1.3.2 Choice of Inner Product

For now, we proceed with the discussion of a particular family of inner products given by the following form,

$$(A|B)^g_\beta = \int_0^\beta g(\lambda)\, \langle e^{\lambda H} A^\dagger e^{-\lambda H} B \rangle_\beta \, d\lambda \tag{1.37}$$

In this formula, the braket $\langle \rangle_\beta$ denotes the thermal expectation value in the density matrix formalism at temperature $T = \frac{1}{k_B \beta} = \frac{1}{\beta}$,

$$\begin{aligned} \langle A \rangle_\beta &= \frac{1}{Z} \mathrm{Tr}(e^{-\beta H} A), \\ Z &= \mathrm{Tr}(e^{-\beta H}). \end{aligned} \tag{1.38}$$

where k_B refers to the Boltzmann constant. Also, for this definition to be a proper inner product (9), the weight function $g(\lambda)$ has to satisfy the following conditions,

$$\begin{aligned} g(\lambda) &\geq 0, \\ g(\beta - \lambda) &= g(\lambda), \\ \frac{1}{\beta} \int_0^\beta g(\lambda)\, d\lambda &= 1. \end{aligned} \tag{1.39}$$

Examples of different weight functions that can be used are[10]

$$\begin{aligned} g(\lambda) &= 1, \\ g(\lambda) &= \frac{1}{2}\beta(\delta(\lambda) + \delta(\beta - \lambda)), \\ g(\lambda) &= \delta(\lambda - \frac{\beta}{2}), \end{aligned} \tag{1.40}$$

The last example in (1.40) is called the Wightmann Inner Product, most commonly used in quantum field theory, and it will be our main focus. It is a physical choice that amounts to taking the expectation value of the operators in the *thermofield double state (TFD)*, with operators A and B inserted in the two different copies [1]. In this case, (1.37) becomes

$$(A|B)_\beta = \langle e^{H\frac{\beta}{2}} A^\dagger e^{-H\frac{\beta}{2}} B \rangle_\beta \tag{1.41}$$

To enhance comprehension of the previously mentioned content, we'll proceed with a succinct review of some fundamental aspects of quantum statistical mechanics and an introduction to the concept of the Thermofield Double State.

1.3.3 Quantum Statistical Mechanics and TFD

According to the postulates of Statistical Mechanics [10], the state of a system in equilibrium may be regarded as an *incoherent* superposition of eigenstates (see A.2). We can think of a system as one member of an infinite collection of systems, each of which is in an eigenstate of the Hamiltonian describing it. Equivalently, it is possible to form a mental picture of each system prepared one at a time. This mental picture generalizes the Gibbsian Ensemble in the context of quantum mechanics. As such, it becomes clear that the density matrix formulation is suitable for describing the systems of quantum statistical mechanics.

[10]The first weight function corresponds to the Kubo Inner Product.

For the purposes of this thesis, we describe the canonical ensemble in statistical mechanics. The canonical ensemble or NVT ensemble (representing constant number of particles, volume, and temperature) is a statistical ensemble representing the possible states of a system in thermal equilibrium with a heat reservoir. As we will see, utilizing the density matrix, the results are easily recognizable by their classical counterparts.

The matrix elements of the density operator for the canonical ensemble of systems governed by a Hamiltonian $\hat{H}$ are given by

$$\rho_{mn} = \delta_{mn} e^{-\beta E_n} \tag{1.42}$$

where $\{E_n\}$ denotes the energy spectrum of the Hamiltonian,

$$\hat{H} \left|\Psi_n\right\rangle = E_n \left|\Psi_n\right\rangle, \tag{1.43}$$

and the exponential part as a whole is the usual relative probability, the Boltzmann factor. Consequently, the partition function of a canonical ensemble in quantum mechanics is

$$Z = \sum_n e^{-\beta E_n} = \mathrm{Tr}(\rho) \tag{1.44}$$

where the sum is over all states to account for degeneracies. Taking into account the completeness of the set of energy eigenstates $\{\Psi_n\}$ and starting from the decomposition of ρ, it can be rewritten into,

$$\rho = \sum_n e^{-\beta E_n} \left|\Psi_n\right\rangle \left\langle\Psi_n\right| = e^{-\beta \hat{H}} \sum_n \left|\Psi_n\right\rangle \left\langle\Psi_n\right| = e^{-\beta \hat{H}} \tag{1.45}$$

Finally, the thermal average, or ensemble average, in the canonical ensemble for any observable represented by an operator O, following (A.16) is given by

$$\left\langle O\right\rangle_\beta = \frac{\mathrm{Tr}(\rho O)}{\mathrm{Tr}(\rho)} = \frac{1}{Z}\mathrm{Tr}(e^{-\beta \hat{H}} O) \tag{1.46}$$

Thermofield Double State

The Thermofield approach is a formalism originally created to incorporate thermal effects in Quantum Field Theories (see [11] for a detailed introduction). The difference with the density operator formalism briefly presented above, is that it describes systems at finite temperatures by means of a structure of a Hilbert Space. This of course is achieved by following the procedures of the GNS construction showcased in (1.3.1).

In this case, it is proven by contradiction that the degrees of freedom describing the system need to be doubled. We construct the Hilbert Space $\mathcal{H}_\omega$ as the direct product of the original $\mathcal{H}$ with itself, also known as a double copy. To be more precise, the direct product is taken with its "tilde conjugate", also referred to as dual. The two spaces are equivalent in structure, but they differ when it comes to the applications of Operators. Different sets of operators act on each copy of the Hilbert Space and the application on one copy does not affect the other.

Enlarging the Hilbert Space in this way results in the purification of the system, i.e. we can describe it by means of pure states instead of the mixed states used in normal quantum statistical mechanics. Physically, this procedure corresponds to taking two copies of the system and describing them together.

The aim is to associate each density matrix ρ_β used to calculate a thermal average in (1.46) with a state $|0(\beta)\rangle$ called a thermofield vacuum[11]

$$\langle O \rangle_\beta = \langle 0(\beta)|O|0(\beta)\rangle \,. \tag{1.47}$$

After proving that the original Hilbert Space of the Energy Eigenstates, called Fock states in this context, $\{|n\rangle\}$ cannot produce the desired result, we set $|0(\beta)\rangle \in \mathcal{H} \otimes \tilde{\mathcal{H}}$ where $\tilde{\mathcal{H}}$ is the aforementioned copy. We write our new state as a linear combination of the combined Fock States $|n\rangle \otimes |\tilde{n}\rangle = |n, \tilde{n}\rangle$

$$|0(\beta)\rangle = \sum_n g_n(\beta)\, |n, \tilde{n}\rangle \,, \tag{1.48}$$

where the probability amplitudes $g_n(\beta)$ need to be determined. Demanding that (1.47) holds for all O, we expectedly get more than one possible results. The definition is finally given by,

$$|0(\beta)\rangle = \frac{1}{\sqrt{Z}} \sum_n e^{-\beta \frac{E_n}{2}} |n, \tilde{n}\rangle = \frac{1}{\sqrt{Z}} \sum_n e^{-\beta \frac{\hat{H}}{2}} |n, \tilde{n}\rangle \,. \tag{1.49}$$

With this definition, we can understand the physical meaning of (1.41) as the expectation value of two operators A and B being inserted in the two different copies.

1.3.4 Applying the Lanczos Algorithm

After fulfilling the prerequisite groundwork, we can finally apply the Lanczos Algorithm to the set of Operators, now considered states in the space of Operators, in (1.13). For clarity purposes, we adopt a better-suited formalism and define the Liouvillian super-operator[12] $\mathcal{L}$,

$$\mathcal{L} = [\hat{H}, \cdot]. \tag{1.50}$$

With this definition, equation (1.13) can be rewritten as,

$$\hat{O}(t) = \sum_{n=0} \frac{(it)^n}{n!} \tilde{O}_n = \sum_{n=0} \frac{(it)^n}{n!} \mathcal{L}^n O = e^{i\mathcal{L}t} O. \tag{1.51}$$

where $\mathcal{L}^n$ refers to acting with the Liouvillian on $\hat{O}$ n times, i.e. taking the n nested commutators with the Hamiltonian We have reformulated our expansion in such a way that the correspondence with the Krylov State Basis now becomes clear thanks to the comparisons of (1.51) with equations (1.2) and (1.3). Additionally, it has become apparent that the Lanczos Algorithm will be applied to the set of operator-states $\{\mathcal{L}^n|O)\}$.

Before proceeding with the recursive formula for constructing the Krylov Operator Basis $|\mathcal{O})$, we will make a few simple observations to greatly simplify our analysis. Firstly, keeping in mind the Hermiticity of $\hat{H}$ and any other operator O corresponding to a physical observable as well as the properties of the Trace of operators, it becomes obvious that $(\tilde{O}_0|\tilde{O}_1) = 0$ with respect to

[11] The terminology generally used originates from quantities encountered in QFT.

[12] The Liouvillian, and all operators acting on operators, are called super-operators to distinguish them from the usual operators which act on states. In our particular instance, we might have opted against adopting this terminology, given our decision to associate nested commutators with specific states.

the Wightmann inner product we have chosen. (This expression is equal to zero for all the inner products belonging to the family (1.37)). This means that we can write the first two steps of our algorithm as,

$$\begin{aligned} |\mathcal{O}_0) \equiv |\tilde{O}_0) = |O_0) = |O), \\ |z_1\rangle = \mathcal{L}|O), \\ |\mathcal{O}_1) = \frac{\mathcal{L}|O)}{(O\mathcal{L}|\mathcal{L}O)^{\frac{1}{2}}} = b_1^{-1}\mathcal{L}|O). \end{aligned} \tag{1.52}$$

Essentially, we have again set $b_0 = 0$ just as in 1.2.2, only this time a_0 also happens to be zero. In fact, it can be proven that

$$(A|\mathcal{L}A) = 0, \tag{1.53}$$

holds for any arbitrary operator A[13]. This important statement sets all the emerging a_n Lanczos coefficients to zero. This simplifies the iterative orthogonalization considerably and leads to the following set of relations for $|\mathcal{O}_n\rangle$,

$$\begin{aligned} |z_n\rangle = \mathcal{L}|\mathcal{O}_{n-1}) - b_{n-1}|\mathcal{O}_{n-2}), \\ |\mathcal{O}_n) = b_n^{-1}\,|z_n\rangle\,, \\ b_n = \langle z_n|z_n\rangle^{\frac{1}{2}}\,. \end{aligned} \tag{1.54}$$

Verifying the validity of this formula is the exact same process as the one demonstrated in the previous subsection. We have again successfully constructed an orthonormal basis suitable for describing the time evolution of an observable in this context. The matrix representation of the Liouvillian, which in the case of operator dynamics plays the role of the Hamiltonian we showed in (1.27), is again made clear after we rearrange (1.54) to get,

$$\mathcal{L}|\mathcal{O}_n) = b_{n+1}|\mathcal{O}_{n+1}) + b_n|\mathcal{O}_{n-1}), \tag{1.55}$$

which leads to,

$$\mathcal{L}_{nm} := (O_n|\mathcal{L}|O_m) = \begin{pmatrix} 0 & b_1 & 0 & 0 & \cdots \\ b_1 & 0 & b_2 & 0 & \cdots \\ 0 & b_2 & 0 & b_3 & \cdots \\ 0 & 0 & b_3 & 0 & \ddots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}. \tag{1.56}$$

All the previously discussed aspects of this analysis regarding the dimensionality of the Krylov subspace hold in this case as well. We now expand our time-evolved operator in a slightly different manner than we did in (1.28),

$$|O(t)) = \sum_n i^n \phi_n(t)|\mathcal{O}_n), \tag{1.57}$$

where the probability amplitudes $\phi_n(t)$ turn out to be real and of course conserve probability identically to (1.29). The discrete set of "Schrödinger" equations governing these amplitudes is derived in the same way which gives,

$$\frac{\partial \phi_n(t)}{\partial t} = b_n\phi_{n-1}(t) - b_{n+1}\phi_{n+1}(t). \tag{1.58}$$

[13]Equivalently, it can be proven that $i^n\mathcal{O}_n$ is always hermitian.

Starting from the same initial conditions $\phi_n(0) = \delta_{n0}$ (and $b_0 = \phi_{-1} = 0$) and with knowledge of the Lanczos coefficients, we can solve for these amplitudes and completely determine the dynamics of our system.

Before we conclude with the final part of this chapter, a proposal on a universal upper bound for the growth of the $\{b_n\}$ Lanczos coefficients, we draw some comparisons between the state and operator approaches. When referring to the same system's time evolution, the Lanczos coefficients yielded are in general different between the two approaches. Even more apparent is the fact that in the context of operator dynamics, our setup was such that the Liouvillian always had zero expectation value, i.e. zero diagonal elements, in our basis. Though we could have followed the more general path of including $\{a_n\}$, the main argument we present in this thesis, following [1], remains relatively unchanged, in the qualitative sense at least, with this simplification. We will comment on the physical meaning of these coefficients as well as the potentially critical quantitative effect their inclusion has in the following chapter. It is easy to argue that the "State" approach is more comprehensive as it necessitates -and subsequently provides- an increased amount of important parameters of the system and thus can potentially give more fine-grained information about the quantum dynamics.

1.3.5 A universal Operator Growth Hypothesis

In this chapter's final subsection, we present one last interesting idea proposed in [12] which can be correctly expressed without the need to explicitly define Krylov Complexity. As we previously discussed, the more terms the expansions (1.28) and (1.51) have, the more nested commutators appear and the more difficult it becomes to describe the system's evolution, increasing its complexity. From the set of equations (1.58), we can surmise that the rate at which each new term in the expansion becomes more relevant is determined by $\{b_n\}$. Borrowing the vocabulary from condensed matter physics, these coefficients can be seen as the hopping amplitudes from each "site" ϕ_n of a one-dimensional chain to the next.

This concept is the foundation of Krylov Complexity and will be studied in a more detailed and precise sense in the following chapter. For now, we simply state the following hypothesis, "Suppose that H describes an infinite, non-integrable, many-body system in dimension $d \geq 1$ and O is a local operator having zero overlap with any conserved quantity (in particular, $(O|H) = 0$). Then the Lanczos coefficients are asymptotically linear:

$$b_n = \alpha n + \gamma + o(1)" \tag{1.59}$$

where α and γ are system-dependent constants. α denotes the growth rate for the coefficients and must be positive.

A noteworthy weight of evidence in the form of analytical and numerical examples has been amassed in favor of this hypothesis which in a way states that the maximal growth of these coefficients, which we expect to observe in chaotic systems, turns out to be linear. Given the relative ambiguity in the definition of chaotic quantum systems, integrability in this context refers to the existence of an extensive number of quasi-local conserved quantities. After we introduce Krylov Complexity, the growth rate α will offer another definition for quantum chaos in the form of a *Lyapunov exponent*. In classical dynamical systems, these are defined as follows,

Definition 4 *Consider a dynamical system governed by the differential equation $\dot{x} = f(x)$, where $x \in \mathbb{R}^n$, and let $\phi_t(x)$ denote the flow of the system, i.e., the trajectory of a point x in phase space after time t.The derivative of the flow at point x after time t is denoted by $D\phi_t(x)$, which represents the Jacobian matrix of partial derivatives of the flow after time t. Now, consider two initially close points in phase space, $x(0)$ and $x(0) + \delta x(0)$. The trajectories of these points as time evolves are $x(t)$ and $x(t) + \delta x(t)$ respectively. The Lyapunov exponent $\lambda(x, v)$, for an initial perturbation v, quantifies the exponential rate of separation of these two trajectories and is defined by:*

$$\lambda(x, v) = \lim_{t\to\infty} \frac{1}{t} \log |D\phi_t(x)v| \tag{1.60}$$

Under the assumption of small initial separations and provided that the limit exists, this can be approximated by observing the exponential separation of trajectories:

$$|\delta x(t)| \approx e^{\lambda t} |\delta x(0)| \tag{1.61}$$

Here, λ is the Lyapunov exponent, $\delta x(t)$ is the separation between the two trajectories at time t, and $\delta x(0)$ is the initial separation at $t = 0$.

Positive Lyapunov exponents indicate chaotic behavior, as two arbitrarily close trajectories diverge from each other at an exponential rate (see [13] for a more rigorous treatment).

Lastly, it is interesting to note that the Lanczos recursion method can be also applied to classical systems in almost the exact same manner. A somewhat weaker bound on the growth of the Lanczos coefficients can in fact be proven to hold for classical chaotic systems.

Chapter 2

Krylov Complexity

Having acquired our most important ingredient in describing the time evolution of a state, or alternatively an operator, an ordered orthonormal basis, we can now define the complexity of a system. From the beginning, our purpose has been to find a way to quantify the spread inside a Hilbert Space during time evolution. We achieve this by essentially following a fundamental idea often encountered in similar definitions of quantum, computational, or otherwise complexity. "*The complexity of an object, or class of objects, should be understood as the number of simple components required to assemble it.*"[14]. In our case, these components are of course none other than the Krylov basis states $\{|K_n\rangle\}$ or $\{|\mathcal{O}_n)\}$.

After presenting the physical quantity we dub *Krylov Complexity*, we will attempt to build an intuition for what it represents, and show the results from a well-known example of a chaotic quantum system that is also analytically solvable. The technical difficulties which arise when one tries to calculate all the involved quantities we have thus far mentioned offer a good motive for the most important part of this thesis, an alternative geometric perspective on the Lanczos approach first proposed in [1]. The description of this geometric argument which attempts to both correlate Krylov Complexity with a certain geometric quantity and simplify the required calculations is, however, left for a subsequent chapter.

Before that, we strengthen the foundations of this formalism by addressing the ambiguities we encounter in the previous sections regarding the choices of basis and, in the case of operator growth, inner product. We resolve this issue by borrowing another axiom from information theory pertaining to the definition of complexity. This axiom generally stipulates that the complexity of an object, when defined using a set of tools, is the minimum value we can assign to it using that specific set.

2.1 Definition

In subsequent sections, we fluidly interchange between the state and operator Krylov bases. Although initially coined for the operator basis, the term "Krylov complexity" has been expansively applied to the state basis as well. As we mentioned before, Krylov Operator complexity can be perceived as a less encompassing version of State Krylov complexity within an auxiliary Hilbert space. It's noteworthy that this State complexity, upon its debut in [14], was referred to as "spread complexity".

Given the fact that we expect more complex time evolution will spread $|\psi(t)\rangle$ more widely over the Hilbert space relative to the initial state $|\psi\rangle$ and thus require more terms in (1.28), our complexity must be a cost function relative to $\mathcal{K}$,

$$K_\psi = \sum_n c_n |\langle \psi(t)|K_n\rangle|^2 = \sum_n c_n |\phi_n(t)|^2 = \sum_n c_n p_n(t), \tag{2.1}$$

where c_n must obviously be a positive, increasing sequence of real numbers and the rest of the terms are the ones encountered in (1.28). We opt for the sequence $c_n = n$, which gives us the following equations,

$$\begin{aligned} K_\psi &= \sum_n n|\phi_n(t)|^2, \\ K_\mathcal{O} &= \sum_n n|\phi_n(t)|^2. \end{aligned} \tag{2.2}$$

To build proper intuition for this choice we observe that the dynamics in equations (1.58) and (1.32) can be interpreted as those of a quantum particle moving on a one-dimensional chain, called the *Krylov chain*. The term "quantum" refers to the fact that the particle is in a coherent superposition of all sites on the chain, with probability amplitudes $\{\phi_n\}$. Of course, the sites on this chain are the Krylov basis states $\{|K_n\rangle\}$ or $\{|\mathcal{O}_n)\}$ and the hopping/transition amplitudes are given by $\{b_n\}$. In this context, (2.2) represent the average position of the particle on this chain as time progresses, i.e.

$$K_\mathcal{O} = \langle \hat{n}(t)\rangle\,, \tag{2.3}$$

where $\hat{n}(t)$ is the number, or position operator on the one-dimensional chain. This way, Krylov complexity can be more formally written as the expectation value in the evolving state $|\mathcal{O}(t))$ of the "Krylov complexity operator" (or number operator) whose spectral decomposition is,

$$\hat{K}_\mathcal{O} = \sum_n n|\mathcal{O}_n)(\mathcal{O}_n|, \tag{2.4}$$

such that Krylov complexity reads

$$K_\mathcal{O} = (\mathcal{O}(t)|\hat{K}_\mathcal{O}|\mathcal{O}(t)). \tag{2.5}$$

Now, we can make use of the proposed bound on the Lanczos coefficients we outlined in 1.3.5. Asymptotically linear growth of the Lanczos coefficients translates to the expectation value of the position in the chain, i.e. the Krylov Complexity increasing at most exponentially. For non-chaotic systems or chaotic systems at late times, the complexity can expectedly grow much slower, as we will demonstrate in subsequent chapters. In any case, a bound for the behavior of $K_\mathcal{O}$ is given by,

$$K_\mathcal{O} \sim e^{2\alpha t}, \tag{2.6}$$

where α is the system-dependent constant in (1.59). The behavior in (2.6) was originally proposed as a definition for quantum chaotic systems in [15]. It becomes clear why this constant was named the growth rate and that its relation to the Lyapunov exponent is

$$\lambda = 2\alpha. \tag{2.7}$$

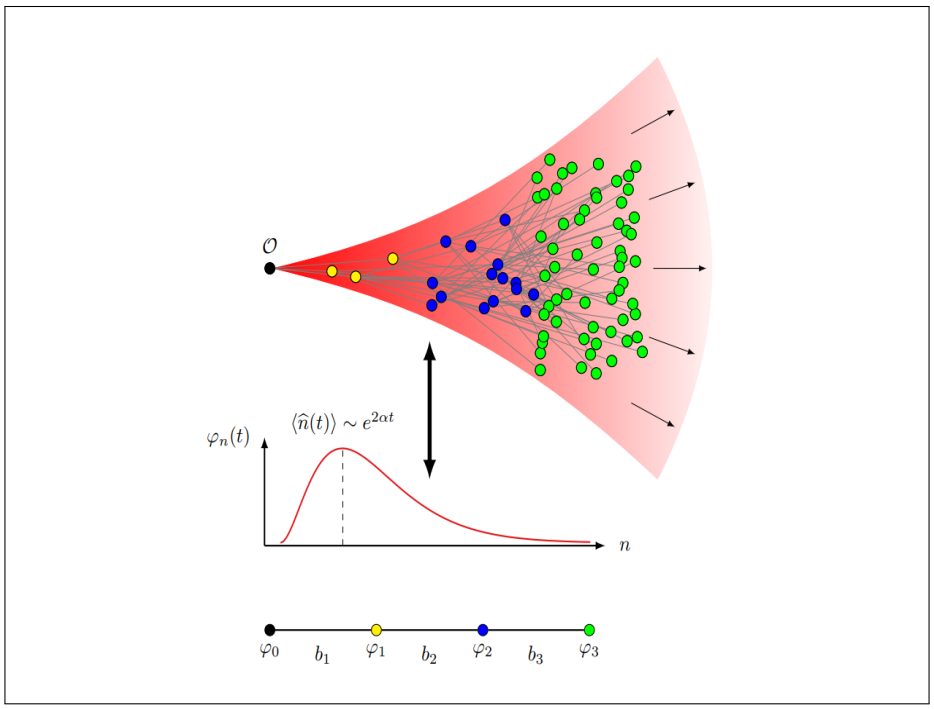

Figure 2.1: Schematic representation of the space of operators and its relation to the 1d chain defined by the Lanczos algorithm starting from a simple operator $\mathcal{O}$. The region of more and more complex operators corresponds to larger n, or moving to the right. (starting from the black dot, and reaching the green, which corresponds to a larger sum of operators needed to describe the state). The middle graph shows the probability amplitudes for each site.

Another success of this result is that at, finite temperatures, the calculated growth rate bounds the Lyapunov exponent in a way that coincides with another prediction on a universal bound on chaos proposed in [16] based on out-of-time-order correlation functions, such as the one in (1.33). The growth rate in those examples becomes $\alpha = \frac{\pi}{\beta}$.

Even though we stated that in the process of defining Krylov complexity, we interchange between the state and operator approaches, it is important to note that in general, they have different uses. Krylov operator complexity allows us to read out the Lyapunov exponents, as we will see, and the *scrambling time*[1] which characterize the exponential growth of the operator size. Krylov state complexity is more suitable for describing late-time chaos in systems due to its connection to the *Spectral Form Factor*. The Spectral Form Factor (SFF) is a measure used to study the statistical properties of energy spectra in quantum systems, particularly in the context of quantum chaos. It characterizes the correlations between energy levels and provides insights into the level-spacing distribution. It can help identify whether a system exhibits quantum chaotic or integrable behavior.

Besides the differences in application, the inclusion of the a_n Lanczos coefficients in Krylov state complexity can drastically change the evolution of the complexity, both quantitatively and qualitatively. After completing our explicit calculations using the geometric approach in the operator context, we will briefly compare them with the results, in the exact same system, when taking $\{a_n\}$ into consideration.

[1]Scrambling time refers to the duration a quantum system takes to disperse information irretrievably.

2.2 Application to the SYK Model

This section will serve as the first and only example of using exclusively the tools we have constructed thus far to study a system. The choice of the SYK Model, which we will superficially present (see [17] for an in-depth analysis), is a deliberate one. For starters, it is a well-known and thoroughly researched system introduced to study various aspects of quantum gravity, holography, and black hole physics. Additionally, it exhibits maximally chaotic dynamics as a many-body system and is exactly solvable at large N (or q in our case, to be more precise). This special combination of properties makes it ideal as a first representative of the potential of our formalism as well as the expected behavior (2.6).

The SYK model consists of N Majorana fermions, i.e. fermions that are their own anti-particles and can annihilate with themselves, with all-to-all random interactions (as opposed to nearest-neighbor interactions) involving an even number of q of them at a time. This many-body non-local character of the system gives it its chaotic behavior. The Hamiltonian for this setup is,

$$H = (i)^{\frac{q}{2}} \sum_{1\leq i_1\leq i_2<\cdots<i_q\leq N} J_{i_1 i_2\cdots i_q}\psi_{i_1}\psi_{i_2}\cdots\psi_{i_q}, \tag{2.8}$$

where $\{\psi_{i_q}\}$ with $1 \leq i \leq N$ are the Majorana fermions and $\{J_{i_1 i_2\cdots i_q}\}$ represent the coupling constants. These are chosen randomly from a Gaussian distribution and have a mean value of 0 and variance,

$$\langle J^2_{i_1 i_2\cdots i_q}\rangle = \frac{\mathbf{J}^2(q-1)!}{N^{q-1}} = \frac{2^{q-1}}{q}\frac{\mathcal{J}^2(q-1)!}{N^{q-1}}, \tag{2.9}$$

where $\mathbf{J}$, or $\mathcal{J}$ is a dimension-one parameter.

Though there are numerous nuanced physics principles and technical details not included in our analysis, they fall outside the scope of our thesis and beyond the expertise of the author. As such, we can proceed with presenting the calculated relative quantities (taken from [12] and [1]). The operator $\mathcal{O}$ to whom we apply the Lanczos algorithm corresponds to one Majorana fermion, i.e. $\mathcal{O} = \sqrt{2}\psi_1$.

The first step to solving the dynamics of the system is in, as we have mentioned, calculating the auto-correlation function which, at low temperatures, turns out to be,

$$C(t) = \cosh^{-\eta}\left(\frac{\pi t}{\beta}\right), \tag{2.10}$$

where $\eta = \frac{2\gamma}{\alpha} + 1$. In this case, the Lanczos coefficients can be obtained analytically and are given by,

$$b_n = \frac{\pi}{\beta}\sqrt{n(n-1+\eta)}. \tag{2.11}$$

Following the methodology we outlined in order to solve (1.58), we get the amplitudes,

$$\phi_n(t) = \sqrt{\frac{\Gamma(\eta+n)}{n!\,\Gamma(\eta)}}\frac{\tanh^n(\alpha t)}{\cosh^{\eta}(\alpha t)}. \tag{2.12}$$

Confirming the proposed bound, the operator Krylov complexity with amplitudes grows exponentially with $\lambda = \frac{2\pi}{\beta}$,

$$K_{\mathcal{O}} = \eta\sinh^2(\alpha t) \sim \frac{\eta}{4}e^{2\alpha t}. \tag{2.13}$$

We again remark that these results refer to the system at very large N. We will briefly comment upon the behavior for smaller systems, which is a more general pattern of behavior for Krylov State complexity. As we will see, the Lanczos coefficients do not asymptotically grow.

We refrain from showing analytical calculations on the quantities until we introduce the geometric argument. The reason is that the required work to obtain the Lanczos coefficients in this system, even more so in others, is significantly demanding. In fact, they are calculated in a roundabout way. It is important that we mention the existence of other very useful quantities frequently encountered in the recursion method such as the *Green function* $G(z)$, the *spectral function* $\Phi(\omega)$ and the so-called *moments* μ_{2n}. These will not be used in our thesis but they can be utilized to produce our results in a multitude of cases. An insightful overview is provided in Appendix A of [12].

Our last important comment regarding the SYK model is its relation to conformal symmetry, which is described by the SL(2,R) Lie algebra. The Majorana fermions behave as primaries[2] transforming in specific representations of the SL(2,R) algebra. In other words, we may be able to consider the SYK system to be governed by the SL(2,R) symmetry group given some scaling adjustments.

2.3 Minimization Principle

As we have pointed out, picking the Krylov basis $\mathcal{K}$ as the basis upon which we measure the *spread* of a state in its Hilbert space during time evolution, is a natural choice, given its construction method. However, it remains arbitrary and thus creates concerns about the validity of the use of the term "complexity". This happens because many original definitions, mainly stemming from information science, include a sense of minimization in complexity.

For example, Kolmogorov's crucial proposal for the complexity of a sequence was that of the length of the *shortest* Turing machine program producing it[18]. Another instance is Rissanen's definition of the complexity of an ensemble of messages as their *minimal* codelength, averaged over the ensemble. Even in the domain of complexity in quantum mechanics, Nielsen's definition of the complexity of the time evolution operator $U(t) = e^{-i\hat{H}t}$ is the minimal distance in the unitary group between the identity and $U(t)$.

This reasoning of ensuring minimization in order to properly define complexity, though axiomatic, is most certainly based on common sense. We give a very simple example to illustrate this point.

Consider the task of moving from point A to point B in Figure 2.2 using only vertical and horizontal steps. We can conjure infinitely many arbitrarily long routes, but the shortest, and simplest, is one which consists only of one horizontal and one vertical step. Given a specific task or object, our measure of its complexity using a specific set of tools should be the minimal value we can assign to it.

In our case, the object under study is the spread of the state/operator during time evolution and our tool set is all the possible, appropriate bases of the Hilbert Space. In the case of State complexity, we only have to consider the possible choices of basis. Operator complexity on the other

[2]In the context of conformal field theories, primary operators (or fields) are the basic building blocks of the theory, from which all other fields can be derived

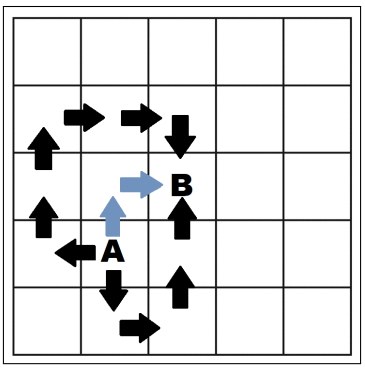

Figure 2.2: Cartoon of the minimization principle in defining complexity. It is reasonable to assume that the path with grey arrows is less complex than the two longer paths made up of black arrows.

hand involves another level of ambiguity regarding the inner product. We start from the former and only comment on the findings in relation to the latter.

2.3.1 Minimizing over the choice of basis

Attempting to quantify the spread of our initial state in its Hilbert space during time evolution forces us to pick a base upon which to measure. It is our duty to ensure that we choose the base which minimizes the value we attribute to the spread of *any* state. We follow the proof in [14].

Start by defining the previously mentioned cost function only this time relative to any complete, ordered, orthonormal basis $\mathcal{B} = \{|B_n\rangle : n = 0, 1, 2, \cdots\}$,

$$\mathcal{C}_{\mathcal{B}}(t) = \sum_n c_n |\langle \psi(t) | B_n \rangle|^2 \equiv \sum_n c_n p_{\mathcal{B}}(n, t), \tag{2.14}$$

where c_n is again an increasing positive sequence of real numbers and the completeness of $\mathcal{B}$ along with conservation of probability imply

$$\sum_n p_{\mathcal{B}}(n, t) = 1 \tag{2.15}$$

As a first attempt, we could try to define our complexity as,

$$\mathcal{C}(t) = \min_{\mathcal{B}} \mathcal{C}_{\mathcal{B}}(t) \tag{2.16}$$

which minimizes our cost function over all bases for each moment in time. This definition however does not provide any useful information as for any time t_0, any basis with $|B_0\rangle = |\psi(t_0)\rangle$ will minimize (2.16), achieving $\mathcal{C}(t_0) = c_0$.

As such, we need to minimize over a finite *amount* of time. This means that in our procedure we seek a "functional minimization" for $\mathcal{C}_{\mathcal{B}}(t)$.

Consider two bases $\mathcal{B}_1, \mathcal{B}_2$ whose cost functions $\mathcal{C}_{\mathcal{B}_1}(t)$ and $\mathcal{C}_{\mathcal{B}_2}(t)$ have convergent Taylor expansions over a time interval T ($0 \leq t \leq T$),

$$\begin{aligned}\mathcal{C}_{\mathcal{B}_1}(t) &= \sum_m^\infty \frac{\mathcal{C}_{\mathcal{B}_1}^{(m)}}{m!} t^m, \mathcal{C}_{\mathcal{B}_1}^{(m)} \equiv {}^{d^m \mathcal{C}_{\mathcal{B}_1}(t)}/_{dt^m}|_{t=0} \\ \mathcal{C}_{\mathcal{B}_2}(t) &= \sum_m^\infty \frac{\mathcal{C}_{\mathcal{B}_2}^{(m)}}{m!} t^m, \mathcal{C}_{\mathcal{B}_2}^{(m)} \equiv {}^{d^m \mathcal{C}_{\mathcal{B}_2}(t)}/_{dt^m}|_{t=0}.\end{aligned} \tag{2.17}$$

Suppose also that there exists a natural number k such that $\mathcal{C}_{\mathcal{B}_1}^{(m)} = \mathcal{C}_{\mathcal{B}_2}^{(m)}$ for $m < k$ and $\mathcal{C}_{\mathcal{B}_1}^{(m)} < \mathcal{C}_{\mathcal{B}_2}^{(m)}$ for $m = k$. We can say with certainty that $\mathcal{C}_{\mathcal{B}_1}(t) < \mathcal{C}_{\mathcal{B}_2}(t)$ for an interval $0 \leq t \leq \tau$ with $\tau < T$. Our aim is to minimize the cost function in this sense in the vicinity of $t = 0$. We only need the sequences of derivatives from each Taylor expansion so, when the above condition holds we write $\mathcal{S}_{\mathcal{B}_1} < \mathcal{S}_{\mathcal{B}_2}$ where,

$$\mathcal{S}_{\mathcal{B}} = \left(\mathcal{C}_{\mathcal{B}}^{(0)}, \mathcal{C}_{\mathcal{B}}^{(1)}, \mathcal{C}_{\mathcal{B}}^{(2)}, \cdots\right). \tag{2.18}$$

As we have mentioned in previous sections, the Krylov Basis $\mathcal{K}$ may not span the full Hilbert Space, but rather a K-dimensional subspace of it. Thus, there may exist orthonormal ordered bases of the Hilbert space whose K first vectors coincide with the Krylov Basis (in the correct order). We will prove that for any such basis, which we say belongs to the class of *complete Krylov bases* $\mathcal{K}_C$, the derivative sequence $\mathcal{S}$, and thus the cost function, is minimized in the vicinity of $t = 0$.

We proceed by inductively showing that any $\mathcal{B}$ whose first N elements coincide with the Krylov basis satisfies $\mathcal{S}_{\mathcal{B}} < \mathcal{S}_{\mathcal{B}'}$ for all bases $\mathcal{B}'$ whose first N elements do not coincide with $\mathcal{K}$. The first part involves showing that this holds for just 1 coinciding element against none, i.e. $|B_0\rangle = |K_0\rangle = |\psi(0)\rangle$ (see 1.2.2). In this case, considering that $\langle \mathcal{B}_{i>0} | \psi(0)\rangle = 0$ by definition,

$$\begin{aligned}\mathcal{C}_{\mathcal{B}}^{(0)} &= \mathcal{C}_{\mathcal{B}}(0) = \sum_n c_n |\langle \psi(0)|B_n\rangle|^2 = c_0, \\ \mathcal{C}_{\mathcal{B}'}^{(0)} &= \mathcal{C}_{\mathcal{B}'}(0) = \sum_n c_n p_{\mathcal{B}'}(n,0) \geq c_0,\end{aligned} \tag{2.19}$$

which immediately allows us to write $\mathcal{S}_{\mathcal{B}} < \mathcal{S}_{\mathcal{B}'}$, if we remember (2.15). The inductive step is somewhat more involved. We start by explicitly calculating the derivatives $\mathcal{C}_{\mathcal{B}}^{(m)}$ using equations (1.1) and (2.14). Starting from[3]

$$\begin{aligned}&\partial_t p_{\mathcal{B}}(n,t) = \partial_t |\langle \psi(t)|B_n\rangle|^2 = \partial_t(\langle \psi(t)|B_n\rangle \langle B_n|\psi(t)\rangle) = \\ &= \partial_t(\langle \psi(t)|)\,|B_n\rangle \langle B_n|\psi(t)\rangle + \langle B_n|\,\partial_t(|\psi(t)\rangle)\,\langle \psi(t)|B_n\rangle = \\ &= i\,\langle \psi(t)|\hat{H}|B_n\rangle \langle B_n|\psi(t)\rangle - i\,\langle \psi(t)|B_n\rangle \langle B_n|\hat{H}|\psi(t)\rangle\,,\end{aligned} \tag{2.20}$$

and keeping in mind that $\hat{H}$ has no explicit time dependence, we observe that each consecutive derivative is given, as per the General Leibniz rule and (1.1), by a "binomial expansion",

$$\frac{d^m p_{\mathcal{B}}(n,t)}{dt^m} = p_{\mathcal{B}}^{(m)}(n,t) = i^m \sum_{k=0}^m (-1)^k \binom{m}{k} \langle \psi(t)|\hat{H}^{m-k}|B_n\rangle \langle B_n|\hat{H}^k|\psi(t)\rangle\,. \tag{2.21}$$

[3]We use the notation $\partial_t \equiv \frac{\partial}{\partial t}$ for clarity whenever deemed necessary.

We can then write,

$$\mathcal{C}_{\mathcal{B}}^{(m)} = \sum_n c_n p_{\mathcal{B}}^{(m)}(n,0). \tag{2.22}$$

Our first important observation is that for any coinciding elements in two bases, all the derivatives of their respective probability functions also coincide, i.e. for $|\mathcal{B}_i\rangle = |\mathcal{B}'_i\rangle$,

$$p_{\mathcal{B}}^{(m)}(i,t) = p_{\mathcal{B}'}^{(m)}(i,t), \tag{2.23}$$

for *all* m. The same cannot be said for the derivatives of the cost functions, as each of them is a sum of derivatives of probabilities over the whole basis. To surpass this issue, we must notice that thanks to the structure of equation (2.22), the derivatives of the probability functions for any basis $\mathcal{B}$ whose first N elements coincide with those of K, up to an irrelevant phase factor, have the following property,

$$p_{\mathcal{B}}^{(m)}(n,0) = 0 \text{ for } n \geq N, m < 2N. \tag{2.24}$$

We start by observing that for any $k < N$, $\hat{H}^k |\psi(0)\rangle$ is, by definition, a linear combination of $|B_0\rangle, \cdots, |B_{N-1}\rangle$ (as they are the first N elements of the Krylov basis). So, due to orthogonality of $\{|B_n\rangle\}$, for any $n \geq N$ we can write,

$$\begin{aligned} \langle \hat{H}^k \psi(0) | B_n \rangle = \langle B_n | \hat{H}^k \psi(0) \rangle = \\ = \langle \psi(0) | \hat{H}^k | B_n \rangle = \langle B_n | \hat{H}^k | \psi(0) \rangle = 0. \end{aligned} \tag{2.25}$$

To ensure that any of the two inner products in equation (2.21) is zero for $n \geq N$, i.e. that either $k < N$ or $m - k < N$ we must impose the second constraint, $m \leq 2N - 1$. At this point, it is crucial to notice that this relation holds for the Krylov basis itself. The arguments about orthogonality hold for $\mathcal{K}$ as well. $\hat{H}^k |\psi(0)\rangle$ is orthogonal to $|K_n\rangle$ for $k < N$ and $n > N - 1$. As a result, we again have,

$$p_{\mathcal{K}}^{(m)}(n,0) = 0 \text{ for } n \geq N, m < 2N. \tag{2.26}$$

We remind that in order to prove that $\mathcal{S}_{\mathcal{B}_1} < \mathcal{S}_{\mathcal{B}_2}$ in the vicinity of $t = 0$, we need to find and integer M such that $\mathcal{C}_{\mathcal{B}_1}^{(M)} < \mathcal{C}_{\mathcal{B}_2}^{(M)}$ (with the previous terms of the sequence coinciding). Given the emerging restriction, our aim is to show that $\mathcal{C}_{\mathcal{K}}^{(2N)} \leq \mathcal{C}_{\mathcal{B}}^{(2N)}$ for any $\mathcal{B}$ with N coinciding vectors with $\mathcal{K}$, completing the inductive step. The equality will hold when $\mathcal{K}$ itself consists only of those N basis vectors (and $\mathcal{B}$ is actually a complete Krylov basis $\mathcal{K}_C$) or when $|B_n\rangle = |K_n\rangle$ holds as well. Taking into consideration (2.23), (2.24) and (2.26) we see that for our $\mathcal{B}$, $\mathcal{S}_{\mathcal{B}}$ and $\mathcal{S}_{\mathcal{K}}$ are identical up to the term $\mathcal{C}_{\mathcal{K}}^{(2N-1)}$.

We start by considering all the $p_{\mathcal{B}}^{(2N)}(n,0)$ terms with $n \geq N$. Based on the previous arguments, it is easy to see that they *all* consist of only one non-zero term, namely

$$\begin{aligned} p_{\mathcal{B}}^{(2N)}(n,0) = i^{2N}(-1)^N \binom{2N}{N} \langle \psi(0) | \hat{H}^N | B_n \rangle \langle B_n | \hat{H}^N | \psi(0) \rangle = \\ = \binom{2N}{N} \langle \hat{H}^N \psi(0) | B_n \rangle \langle B_n | \hat{H}^N \psi(0) \rangle . \end{aligned} \tag{2.27}$$

To get a better understanding of this term, we can write the vector $\hat{H}^N |\psi(0)\rangle$ as,

$$\hat{H}^N |\psi(0)\rangle = \xi_\perp |K_n\rangle + \xi_{||} |K_{||}\rangle , \tag{2.28}$$

where we have decomposed the original vector into the part ($K_{||}$) that is a linear combination of the previous Krylov basis vectors $\{|K_n\rangle : n = 0, 1, \cdots, N-1\}$ and the orthogonal part which is, by construction, proportional to K_n. With this decomposition, we can rewrite expression (2.27) as,

$$p_{\mathcal{B}}^{(2N)}(n,0) = |\xi_\perp|^2 \binom{2N}{N} \langle K_N|B_n\rangle \langle B_n|K_N\rangle , \tag{2.29}$$

where we have taken into account the orthogonality of $\mathcal{B}$. Finally, the $2N$th derivative of our cost function can be written in the following way,

$$\begin{aligned} \mathcal{C}_{\mathcal{B}}^{(2N)} &= \sum_n c_n p_{\mathcal{B}}^{(2N)}(n,0) = \\ &= \sum_{n=0}^{N-1} c_n p_{\mathcal{B}}^{(2N)}(n,0) + |\xi_\perp|^2 \binom{2N}{N} \sum_{n=N}^{D} c_n \langle K_N|B_n\rangle \langle B_n|K_N\rangle . \end{aligned} \tag{2.30}$$

where D is the dimension of the full Hibert space, which can be infinite. Here, we can distinguish two different scenarios. One, $\mathcal{K}$ only consists of these N vectors and $\mathcal{B} = \mathcal{K}_C$. It then becomes obvious that $\xi_\perp = 0$ and thus

$$\begin{aligned} \mathcal{C}_{\mathcal{B}}^{(2N)} &= \sum_{n=0}^{N-1} c_n p_{\mathcal{B}}^{(2N)}(n,0) \\ &= \sum_{n=0}^{N-1} c_n p_{\mathcal{K}}^{(2N)}(n,0) = \mathcal{C}_{\mathcal{K}}^{(2N)}, \end{aligned} \tag{2.31}$$

thanks to (2.23). This last equality gives $\mathcal{S}_{\mathcal{B}} = \mathcal{S}_{\mathcal{C}}$. The second case implies that $\xi_\perp \neq 0$. Remembering the completeness condition we assumed for our bases and that c_n is a positive increasing sequence, we can write,

$$\begin{aligned} \sum_n |B_n\rangle \langle B_n| &= \hat{I}, \\ \sum_n \langle K_N|B_n\rangle \langle B_n|K_N\rangle &= \langle K_N|K_N\rangle = 1, \\ \sum_{n=N}^{D} c_n \langle K_N|B_n\rangle \langle B_n|K_N\rangle &\leq c_N. \end{aligned} \tag{2.32}$$

that in turn allows us to write the inequality,

$$\mathcal{C}_{\mathcal{B}}^{(2N)} \geq \sum_{n=0}^{N-1} c_n p_{\mathcal{B}}^{(2N)}(n,0) + |\xi_\perp|^2 \binom{2N}{N} c_N = \mathcal{C}_{\mathcal{K}}^{(2N)}. \tag{2.33}$$

The last equality holds thanks to arguments similar to (2.26). With this, we can finally write $\mathcal{S}_{\mathcal{K}} < \mathcal{S}_{\mathcal{B}}$. We have successfully proven that our measure of complexity in terms of the spread of an initial state in an ordered orthonormal basis during time evolution is minimized by any complete Krylov Basis $\mathcal{K}_C$ for a finite amount of time after $t = 0$. With this process, we have managed to strengthen the foundations of our definition by endowing it with a strong axiom present in many other influential definitions.

2.3.2 Choice of inner product

As we previously discussed, the GNS construct requires the choice of an inner product between any two operator states. In the context of the recursion method we have been using, all choices belong to the family of inner products (1.37). Even though we provided the "physical" explanation of the Wightmann inner product we decided upon in 1.3.2, we have picked arbitrarily from a myriad of available weight functions $g(\lambda)$ for which the process remains valid (see 1.3.4).

Thankfully, it has been shown in Appendix A of [7] that out of all possible inner products, the weight function $g(\lambda) = \delta(\lambda - \frac{\beta}{2})$ actually produces the slowest growth of complexity. This type of "minimization" qualitatively differs from the one we pursued in the previous subsection, but is still acceptable, desirable even. Essentially, it produces the slowest growth of the Lanczos coefficients and, as we outlined in 1.3.5, sets the correct Lyapunov exponents.

The proof, starting from the survival amplitude, consists of a series of mathematical manipulations such as the Fourier transform, an analytic continuation in imaginary time, complex integrations, etc. We have opted against including the procedure in our thesis.

Chapter 3

Coherent States

The geometric approach to Krylov complexity relies heavily on the concept of *coherent states* in quantum mechanics. By making the identification between the Krylov basis and the basis vectors associated with the representation of the symmetry group governing our system, we will make the connection between the time evolution of our operator and the corresponding coherent states. As such, a firm grasp on a variety of their inner workings and unique properties is critical, if we want to present the procedure properly. Given the significant bulk of knowledge around this topic, we dedicate this chapter solely to an overview of the coherent states.

In the context of classical mechanics, we describe the states of dynamical systems as points belonging to a phase space (or via density distributions more generally) and their evolution in time, such as a trajectory of a mass in real space, as *flows* in that phase space. However, this treatment doesn't directly translate to quantum mechanics, where systems are described by vectors in a Hilbert space or, alternatively, via density operators. What's more, Heisenberg's *uncertainty principle* precludes the point-representation of variables in any phase space.

An attempt to bridge this gap, i.e. find a way to enable a seamless transition between the classical and quantum description of systems, the harmonic oscillator in particular, was what originally lead Schrödinger to discover the so-called canonical or standard coherent states. The terminology, however, is owed to Glauber who, along with Klauder and Sudarshan rediscovered these states (a different representation of them to be exact) decades later in the context of quantum optics.

Today, a plethora of families of coherent states have been constructed for different kinds of systems and the concept has found use in numerous fields of physics, quantum or otherwise. Following [19], we will go through the procedure of producing the standard coherent states in their "Fock representation" used by Glauber (For Schrödinger's states, an overview is given in ([20],[21]), from which we take most of what we present in this chapter).

After presenting some of the most important properties of these states, such as the fact that they *minimize uncertainty*, they form an *overcomplete basis* etc., we elaborate on the parts which lead us to a more general, widely acknowledged but not unique definition for what constitutes a set of coherent states. Another very important aspect we study is their evolution in time. We also comment on the relation to aspects of *group theory* by pointing out that coherent states are generated by the unitary action of a group on the ground state of the system (by means of a displacement operator), from where we can construct the second family of use to us, the *spin coherent states*. Our final set is the *generalized coherent states* of the SL(2,R) group which we can generate following Perelomov's work [22]. We finish by introducing the crucial *Fubini-Study metric*,

which allows us to connect any set of coherent states with a metric tensor, opening up the potential for the Geometrization of a Hilbert Space.

It is important to remember that our presentation omits several aspects of these families of states and does not delve into their physical interpretations. We simply provide and in some cases derive a select few important results which will come into play in the next chapter.

3.1 Canonical Coherent States

We study the, most widely used, canonical coherent states in the context of the quantum harmonic oscillator. A brief reminder on the basics of the oscillator is given and we start by deriving the states in a relatively contrived way which, however, is intuitive, before introducing a more general approach. The one-dimensional quantum harmonic oscillator is a system governed by the Hamiltonian

$$\hat{H} = \frac{\hat{p_x}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2, \tag{3.1}$$

where m is the particle's mass and ω its angular frequency. The wavefunction solutions to the time-independent version of equation (1.1) are the energy eigenstates of the system and form an orthonormal basis,

$$\psi_n(x) = \frac{\mathcal{N}e^{-\frac{x^2}{2}}}{2^{\frac{n}{2}}\sqrt{n!}}H_n(x), \tag{3.2}$$

where $\mathcal{N}$ is a normalization constant and $H_n(x)$ is the n-th physicist's Hermite polynomial. We will refer to these states as Fock states and write them as $\{|n\rangle\}$. For our purposes, it is useful to introduce the *annihilation* (lowering) and *creation* (raising) operators, namely,

$$\hat{a} = \sqrt{\frac{m}{2\hbar\omega}}(\omega\hat{x} + i\hat{\dot{x}}), \tag{3.3}$$

$$\hat{a}^\dagger = \sqrt{\frac{m}{2\hbar\omega}}(\omega\hat{x} - i\hat{\dot{x}}). \tag{3.4}$$

These operators obey the following important relations,

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle\,,\ \hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,, \tag{3.5}$$

and,

$$[\hat{a}, \hat{a}^\dagger] = \hat{I}. \tag{3.6}$$

The Fock states $\{|n\rangle\}$ can be generated by consecutive applications of $\hat{a}^\dagger$ on the ground state $|0\rangle$ (hence the name),

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\,|0\rangle\,, \tag{3.7}$$

or, in adjoint form,

$$\langle n+1| = \langle 0|\,\frac{\hat{a}^{n+1}}{\sqrt{(n+1)!}}. \tag{3.8}$$

Also, we can rewrite (3.1) using these operators,

$$\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2}), \tag{3.9}$$

where $\hat{N} = \hat{a}^\dagger\hat{a}$ is appropriately called the *number operator*, acting on the Fock states as,

$$\hat{N}\,|n\rangle = n\,|n\rangle \tag{3.10}$$

and giving the commutation relations,

$$[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger,\ [\hat{N}, \hat{a}] = -\hat{a} \tag{3.11}$$

3.1.1 Initial Derivation

A first intuitive step towards constructing a set of quantum states which will resemble their classical counterparts is to demand that they have minimum uncertainty. It is well known that the ground state of the harmonic oscillator is a "minimum uncertainty" state in the sense that the product $\Delta\hat{x}\Delta\hat{p}$ saturates the limit given by Heisenberg's uncertainty principle. The ground state $|0\rangle$ is also an eigenvector of $\hat{a}$ with,

$$\hat{a}\,|0\rangle = 0\,|0\rangle\,. \tag{3.12}$$

The position-momentum uncertainty relation is only one instance of the generalized uncertainty relation[23],

$$\Delta\hat{A}\Delta\hat{B} \geq \frac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle\,|. \tag{3.13}$$

Another equally valid, and more useful to us, way to write it is through the creation and annihilation operators. Using their properties from above, it is straightforward to show that their uncertainty relation reads,

$$\langle\hat{a}^\dagger\hat{a}\rangle \geq \langle\hat{a}^\dagger\rangle\,\langle\hat{a}\rangle\,. \tag{3.14}$$

Thanks to (3.12), it becomes apparent that $|0\rangle$ is a minimum-uncertainty state. In fact, (3.14) shows that any arbitrary state $|z\rangle$ which happens to be an eigenstate of $\hat{a}$, i.e.

$$\hat{a}\,|z\rangle = z\,|z\rangle\,, \tag{3.15}$$

is also a minimum uncertainty state, considering that,

$$\begin{aligned}\langle z|\hat{a}|z\rangle &= z,\\ \langle z|\hat{a}^\dagger|z\rangle &= z^*,\\ \langle z|\hat{a}^\dagger\hat{a}|z\rangle &= |z|^2,\end{aligned} \tag{3.16}$$

if we observe that (3.15) implies

$$\langle z|\,z^* = \langle z|\,\hat{a}^\dagger. \tag{3.17}$$

This set $\{|z\rangle\}$ of states are thus the coherent states we are searching for. We must now find an explicit expression for them. We start by exploiting the completeness of the Fock states,

$$|z\rangle = \sum_n |n\rangle\,\langle n|z\rangle \tag{3.18}$$

Our aim is to calculate the amplitudes $\langle n|z\rangle$, which we achieve using equations (3.8),(3.15),(3.17) to get,

$$\langle n|z\rangle = \frac{\langle n|\hat{a}|z\rangle}{z} = \frac{\sqrt{n+1}}{z}\langle n+1|z\rangle = \frac{\hat{a}^n}{\sqrt{n!}}\langle 0|z\rangle\,. \tag{3.19}$$

The states become,

$$|z\rangle = \langle 0|z\rangle \sum_n \frac{z^n}{\sqrt{n!}}|n\rangle\,. \tag{3.20}$$

The final step is normalization, taking into account the orthonormality of the set $|n\rangle$,

$$\begin{aligned}\langle z|z\rangle = |\langle 0|z\rangle|^2 \sum_n \sum_m \frac{z^n (z^*)^m}{\sqrt{n!\,m!}}\langle m|n\rangle = |\langle 0|z\rangle|^2 \sum_n \frac{(|z|^2)^n}{n!} = \\ = |\langle 0|z\rangle|^2 e^{|z|^2} = 1,\end{aligned} \tag{3.21}$$

given our freedom to define states in Hilbert spaces up to phases, which allows us to set $|\langle 0|z\rangle|^2 = e^{-\frac{1}{2}|z|^2}$. With this normalization, we have successfully produced the Glauber–Klauder–Sudarshan or Standard Coherent States. We note that we will use another version of (3.20), setting $\langle 0|z\rangle = 1$ in future sections (These are known as the Schrödinger coherent states).

Before we move on, the phase space representation of coherent states is worth mentioning. Choosing proper operators, we can define a phase space inside which each coherent state is represented by an ellipse (or circle, if we choose appropriately) of minimum area. This provides another step towards our attempt of describing quantum systems in a similar manner to their classic counterparts. After we introduce the generation through the displacement operator, an illuminating example will be given.

3.1.2 Important Properties

Overcompleteness

We proceed by examining the relationship between the elements of $\{|z\rangle\}$. Given two arbitrary states $|z_1\rangle, |z_2\rangle$, their inner product is given by,

$$\langle z_1|z_2\rangle = e^{-\frac{|z_1|^2}{2}} e^{-\frac{|z_2|^2}{2}} \sum_n \frac{(z_1^* z_2)^n}{n!} = e^{z_1^* z_2 - \frac{|z_1|^2}{2} - \frac{|z_2|^2}{2}}, \tag{3.22}$$

which is a continuous function of the two variables that never vanishes. This means that no two coherent states are orthogonal to each other. The specifics of this become more clear when we take the modulus squared,

$$|\langle z_1|z_2\rangle|^2 = e^{-|z_1 - z_2|^2}. \tag{3.23}$$

This relation shows us that as $|z_1 - z_2|$ grows, the states "come closer" to being orthogonal. Next, we will show that $\{|z\rangle\}$ resolve the unity, i.e. they produce a continuous equivalent of the completeness relations we encountered in equations (2.32), (1.45) and (3.18). This time, instead of a sum, we need to integrate over the whole complex plane. This approach implies that we've associated each

point of the complex plane with a coherent state, a detail that will become relevant later.

$$\begin{aligned}\int_{\mathbb{C}} |z\rangle \langle z| \, d^2z = \sum_n \frac{1}{n!} \int e^{-|z|^2} (|z|^2)^n \, |n\rangle \langle n| \, d(\text{Re } z) d(\text{Im } z) = \\ = \pi \sum_n |n\rangle \langle n| \int \frac{1}{n!} (|z|^2)^n e^{-|z|^2} \, d|z|^2 = \pi \sum_n |n\rangle \langle n| = \pi \hat{I}\end{aligned} \tag{3.24}$$

The combination of equations (3.23),(3.24) leads us to the conclusion that the canonical coherent states constitute an *overcomplete* basis of the Hilbert space $\mathcal{H}$. This means that any $|x\rangle \in \mathcal{H}$ can be decomposed into a, possibly infinite, linear combination of coherent states, but that decomposition is not *unique*. This important property is the one that conceptually survives to become part of the definition for any other family.

Stability under time evolution

One of the most important properties of coherent states arises when we study their evolution time. Namely, using (3.9) and (3.10) we can write[1]

$$\begin{aligned}\hat{U}_t |z\rangle = e^{-i\hat{H}t} |z\rangle = e^{-it\omega(\frac{1}{2}+\hat{N})} e^{-\frac{1}{2}|z|^2} \sum_n \frac{z^n}{\sqrt{n!}} |n\rangle = \\ = e^{-\frac{it\omega}{2}} e^{-\frac{1}{2}|z|^2} \sum_n \frac{z^n}{\sqrt{n!}} e^{-it\omega\hat{N}} |n\rangle = e^{-\frac{i\omega t}{2}} e^{-\frac{1}{2}|z|^2} \sum_n \frac{z^n}{\sqrt{n!}} e^{-it\omega n} |n\rangle = \\ = e^{-\frac{i\omega t}{2}} e^{-\frac{1}{2}|e^{-i\omega t}z|^2} \sum_n \frac{(e^{-i\omega t}z)^n}{\sqrt{n!}} |n\rangle = e^{-\frac{i\omega t}{2}} |e^{-i\omega t}z\rangle \, .\end{aligned} \tag{3.25}$$

Remembering that quantum states that differ only in phase form an equivalence class (we can ignore the $e^{-\frac{i\omega t}{2}}$ term), a crucial remark can be made here. As $e^{-i\omega t}z$ is just a rotation of z in the complex plane, we determine that coherent states always evolve into other coherent states by a time-dependent change in z which actually follows the classical oscillator solution.

In our analysis, we have successfully discerned the vital bridge coherent states offer between classical and quantum dynamics. A quantum system's evolution in phase space mirrors the trajectory of its classical counterpart. To avoid being sidetracked, we revisit this correspondence when it becomes relevant again in the next chapter.

Group Theoretical Approach

Starting from equation (3.20), we will show that there is an alternative way to construct the standard coherent states through the action of a *unitary displacement operator*. Given the governing symmetry group, this method is paramount to the concept of coherent states because it provides a way to generate any set of such states. Using (3.7) and (3.12), we can write,

$$\begin{aligned}|z\rangle = e^{-\frac{1}{2}|z|^2} \sum_n \frac{z^n}{\sqrt{n!}} |n\rangle = e^{-\frac{1}{2}|z|^2} \sum_n \frac{z^n (\hat{a}^\dagger)^n}{n!} |0\rangle = \\ = e^{-\frac{1}{2}|z|^2} e^{z\hat{a}^\dagger} * 1 * |0\rangle = e^{-\frac{1}{2}|z|^2} e^{z\hat{a}^\dagger} e^{-z^*\hat{a}} |0\rangle \, .\end{aligned} \tag{3.26}$$

[1] We have assumed the proper conditions for the validity of the property $f(\hat{a}) |z\rangle = f(z) |z\rangle$ for an analytic function of z. Also, we switch to $\hbar \equiv 1$.

To continue, we need to unify the exponentials above, which involve operators. Achieving that requires utilizing the *Baker-Campbell-Haussdorff* theorem [24],

Theorem 5 (BCH Formula) *Let G be a Lie group and denote the exponential map* $\exp\colon \mathfrak{g} \longrightarrow G$ *where $\mathfrak{g}$ is the Lie algebra of G. There exists a sufficiently small open subset $0 \in U \subset \mathfrak{g}$ so that the exponential map admits a local inverse, denoted log:* $\exp(U) \longrightarrow U$ *so that for all* $\exp(X)\exp(Y) \in \exp(U)$ *one has*

$$\log(\exp X \exp Y) = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}[X,[X,Y]] + \frac{1}{12}[Y,[X,Y]] + \dots \tag{3.27}$$

There exist many proofs for this theorem, but we will follow one using the lemma we presented in 1.1.2, see [23], which expedites the procedure in our case where

$$[\hat{a},[\hat{a},\hat{a}^\dagger]] = [\hat{a}^\dagger,[\hat{a},\hat{a}^\dagger]] = 0, \tag{3.28}$$

holds. Let us define an operator function $\hat{F}(x)$,

$$\hat{F}(x) = e^{x\hat{X}}e^{x\hat{Y}}, \tag{3.29}$$

and differentiate with respect to x in order to get

$$\begin{aligned} \frac{d}{dx}\hat{F}(x) &= \hat{X}e^{x\hat{X}}e^{x\hat{Y}} + e^{x\hat{X}}\hat{Y}e^{x\hat{Y}} = \\ &= (\hat{X} + e^{x\hat{X}}\hat{Y}e^{-x\hat{X}})e^{x\hat{X}}e^{x\hat{Y}} = (\hat{X} + e^{x\hat{X}}\hat{Y}e^{-x\hat{X}})\hat{F}(x). \end{aligned} \tag{3.30}$$

Using the BH-lemma and (3.28), the above relation reads

$$\frac{d}{dx}\hat{F}(x) = (\hat{X} + \hat{Y} + x[\hat{X},\hat{Y}])\hat{F}(x). \tag{3.31}$$

Integrating this equation and setting $x = 1$ gives us,

$$\hat{F}(1) = e^{\hat{X}}e^{\hat{Y}} = e^{\hat{X}+\hat{Y}}e^{\frac{1}{2}[\hat{X},\hat{Y}]}, \tag{3.32}$$

allowing us to reach the desired result,

$$e^{\hat{X}+\hat{Y}} = e^{-\frac{1}{2}[\hat{X},\hat{Y}]}e^{\hat{X}}e^{\hat{Y}}. \tag{3.33}$$

When applied to our case, we can finally write $|z\rangle$ as being generated by the "displacement" of $|0\rangle$ by quantity z through a unitary operator,

$$|z\rangle = e^{z\hat{a}^\dagger - z^*\hat{a}}\,|0\rangle = \hat{D}(z)\,|0\rangle\,. \tag{3.34}$$

Before we continue, building on our definition of an algebra (1) by introducing *Lie groups* G and their corresponding *Lie Algebras* $\mathfrak{g}$, will make understanding our discussion easier. Our treatment is by no means thorough (see Appendix B of [21] for more rigorous definitions).

Definition 6 *A Lie group G may be defined in several ways, for instance, as a smooth manifold with a group structure such that the group operations $(g_1, g_2) \to g_1 g_2$, $g \to g^{-1}$ are C^k [2], for some $k \geq 2$. This actually implies that all group operations are (real) analytical. A Lie group is said to be simple, or semisimple if it has no nontrivial invariant subgroup or Abelian invariant subgroup.*

A Lie algebra arises as the *tangent space at the identity* of its associated Lie group, capturing its infinitesimal structure. The bracket operation in the Lie algebra, if we assume associativity, corresponds to the usual commutator $[X, Y] = XY - YX$ (which implies the existence of the usual binary multiplication operation). We can formally use the definition,

Definition 7 *The term Lie algebra refers to an algebra $\mathfrak{g}$ over the real or complex numbers equipped with a binary operation called the Lie bracket, an antisymmetric bilinear [3] map denoted by $[\cdot, \cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ that satisfies the Jacobi identity,*

$$[[X, Y], Z] + [[Y, Z], X] + [[Z, X], Y] = 0, \text{ for any } X, Y, Z \in \mathfrak{g} \tag{3.35}$$

Given a Lie algebra associated with a Lie group, the elements of the algebra represent infinitesimal transformations or generators of the group. To transition from these infinitesimal actions to finite group actions, one uses the exponential map. Specifically, exponentiating any linear combination of Lie algebra elements produces an element of the associated Lie group.

The theory of Lie Algebras lets us see (3.34) in a different light. We start by pointing out that the commutation relations of $\{\hat{a}, \hat{a}^\dagger, \hat{I}\}$ show us that they *span* a Lie Algebra on the real numbers, also known as the *Weyl-Heisenberg* algebra $\mathfrak{w}$. The complex arguments we assign to the annihilation and creation operators in the exponential force us to use an alternate version, the $\mathfrak{w}_m$ algebra (we do not delve into further details here, but the core of the argument remains the same). Our aim is to understand $\hat{D}(z)$ as a unitary representation of an element of a group being generated by $\hat{a}, \hat{a}^\dagger$.

To make our analysis more precise, we need to account for the non-commutative nature of the displacements caused by $\{\hat{D}(z)\}$, which become evident from the straightforward to prove relations,

$$\begin{aligned} \hat{D}(z_1)\hat{D}(z_2) &= e^{z_1 z_2^* - z_1^* z_2}\hat{D}(z_2)\hat{D}(z_1), \text{ or similarly,} \\ \hat{D}(z_2)\left|z_1\right\rangle = \hat{D}(z_2)\hat{D}(z_1)\left|0\right\rangle &= e^{\frac{z_1 z_2^* - z_1^* z_2}{2}}\hat{D}(z_1+z_2)\left|0\right\rangle = e^{\frac{z_1 z_2^* - z_1^* z_2}{2}}\left|z_1+z_2\right\rangle. \end{aligned} \tag{3.36}$$

This non-commutativity forces us to introduce an extra "phase term" $e^{is}, s \in \mathbb{R}$ to $\hat{D}(z)$ and to move to a wider set than the complex numbers, which is precisely the (Lie) Weyl-Heisenberg group,

$$\begin{aligned} W &\simeq \mathbb{R} \times \mathbb{C}, \\ W &\ni g = (s, z). \end{aligned} \tag{3.37}$$

We can finally say that the set of operators $e^{is}\hat{D}(z)$ form a unitary representation of the Weyl-Heisenberg group, generated by the elements of the Weyl-Heisenberg Lie algebra $\mathfrak{w}_m$ through the exponent map. This statement is a crucial motif universally used to construct *any* set of coherent states.

[2] C^k denotes the class of functions that are k-times continuously differentiable. That is, we can differentiate the function k times and each of those derivatives is continuous.

[3] Bilinearity refers to the property $[aX + bY, Z] = a[X, Z] + b[Y, Z]$ with a, b belonging to the real or complex numbers.

Phase space representation

Before we move on to provide a general definition and delve into other families of states, we show a schematic representation of the canonical coherent states as minimum area spheres inside a carefully selected phase space following [19]. In the context of the one-dimensional harmonic oscillator, we use the dimensionless position and momentum operators, generally referred to as quadratures, defined by

$$\hat{X}_1 = \frac{1}{\sqrt{2}}(\hat{a}^\dagger + \hat{a}), \;\; \hat{X}_2 = \frac{i}{\sqrt{2}}(\hat{a}^\dagger - \hat{a}), \tag{3.38}$$

and obeying the commutation relation,

$$\Delta\hat{X}_1 \Delta\hat{X}_2 \geq \frac{1}{2}. \tag{3.39}$$

With the inequality being saturated with $\Delta\hat{X}_1 = \Delta\hat{X}_2 = \frac{1}{\sqrt{2}}$ for the coherent states, which we denote as $\{|\alpha\rangle\}$ just in this paragraph to match the notation in Figure 3.1. Each $|\alpha\rangle$ is represented by a circle of radius $\frac{1}{2\sqrt{2}}$. Acting on the vacuum state $|0\rangle$ with $\hat{D}(\alpha)$, transfers the center of the circle to the point with coordinates (α_x,α_y)=(Re α,Im α).

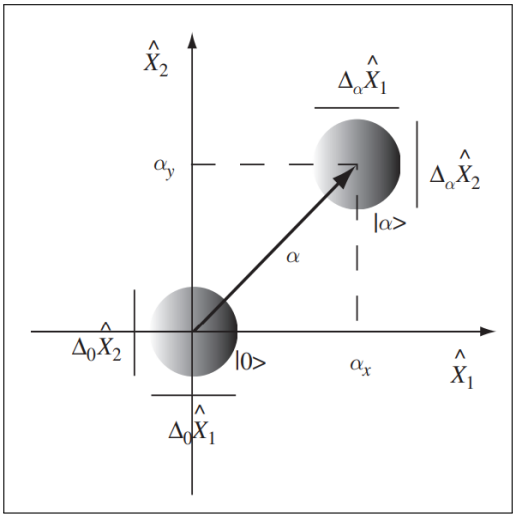

Figure 3.1: An instance of the phase space representation of the ground state and the coherent state $|\alpha\rangle$ using the quadrature operators.

3.2 A general definition

In our search for a definition that encompasses all sets of coherent states, we come to understand that for any specific example, there exists a corresponding set of properties that hold true. Some are shared among the different instances, some are unique. We define what constitutes a set of coherent states by pointing out the two main universal properties that survive in all cases. Though not a definition in the strictest sense, it serves as a good guideline to demonstrate the minimum requirements that must be met for a set of states to be called coherent. The two properties are *continuity* and *completeness*. We attempt to provide a clear picture of what these mean as outlined in [21] and use our study of the standard coherent states to provide concrete examples.

3.2.1 Continuity

We start by noting that regardless of the nature of the coherent states or their application, we always denote them by $\{|l\rangle\}$, where l is an element (generally multidimensional) of an appropriate label space Ω endowed with a notion of continuity (topology). Another way to express this property is that all finite-dimensional subspaces of Ω behave as manifolds, i.e. they are locally Euclidean. In the example we discussed, the set of all available parameters, i.e. the label space Ω, is the whole complex plane. Of course, it is endowed with the metric $d(z_1, z_2) = |z_1 - z_2|$, allowing for a definition of a distance between complex numbers, and subsequently a notion of continuity. Obviously, the complex plane is Euclidean everywhere.

We say that the coherent states are continuous when:

The vector $|l\rangle$ is a strongly continuous function of the label l.

Here, continuity refers to the property that for every convergent label set such that $l' \to l$ (which would refer to $d(z_1, z_2) \to 0$ in the previous example), it follows that $|||l'\rangle - |l\rangle\,|| \to 0$[4]. The important observation that any two coherent states are rarely, if ever, orthogonal can be made from this property. Thus, we immediately discern that the coherent states can never be the set of eigenstates of any self-adjoint operator.

We provide two brief examples to distinguish between the two continuities we have mentioned and to further drive the point about self-adjoint operators. The discrete spectrum of orthogonal energy eigenstates of a Hamiltonian $\hat{H}$, say $\{|n\rangle\}$, is immediately rejected as the label space are just the discrete natural numbers $\mathbb{N}$. On the other hand, the set of eigenstates of the position operator $\hat{x}$, $\{|x\rangle\}$ have the real number line as Ω, which is endowed with the metric $d(x_1, x_2) = |x_1 - x_2|$. However, the vectors are not strongly continuous in the label x, considering that regardless of the distance between two real numbers x_1, x_2, their inner product is $\langle x_1|x_2\rangle = \delta(x_1 - x_2)$.

3.2.2 Completeness

The completeness of coherent states is expressed by the following statement:

There exists a positive measure δl on Ω such that the unit operator $\hat{I}$ admits the resolution of unity,

$$\hat{I} = \int |l\rangle \langle l| \; \delta l, \tag{3.40}$$

when integrated over Ω.

We have encountered the resolution of unity as a property of complete orthonormal bases, for which it *always* holds, numerous times in this thesis. The main difference here is that $\{|l\rangle\}$ are not mutually orthogonal. This has the consequence that, unlike in orthonormal bases, the resolution of unity is not immediately implied and needs to be manually verified for any specific set of such states.

3.3 Spin Coherent States

The next set we examine are the spin coherent states, also referred to as Bloch or atomic coherent states in the literature, depending on the context and the chronology of their use. As we will see,

[4]The symbol $||\cdot||$ refers to the norm of a state.

they are generated by the action of a unitary representation of the elements of the *SU(2) group* or the *SO(3) group of rotations*, of which the former is a double cover, i.e. there exists a 2-to-1 homomorphism (map) from one to the other. The distinction depends on whether the system under study is of integer total angular momentum or not.

The group elements act on a state of the finite-dimensional Hilbert space $\mathcal{H}^j$ used to describe angular momentum in quantum mechanics. The superscript j refers to the total spin of the system ($j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$) and determines the dimension of $\mathcal{H}^j$, which is $2j + 1$.

3.3.1 Basics

We begin by reminding the essential properties of the well-known angular momentum operators $\{\hat{J}\}$, which will give us the elements of the $\mathfrak{su}(2)$ and $\mathfrak{so}(3)$ Lie Algebras (Unlike their respective groups, the algebras are isomorphic and we can refer to them interchangeably). We denote the angular momentum operator and its modulus squared by,

$$\begin{gathered}\hat{\vec{J}} = (\hat{J}_x, \hat{J}_y, \hat{J}_z) \to (\hat{J}_1, \hat{J}_2, \hat{J}_0), \\ \hat{\vec{J}}^2 \equiv \sum_{i=0}^{2} \hat{J}_i^2.\end{gathered} \tag{3.41}$$

In what follows, we drop the hats on the operators and set $\hbar \equiv 1$. The usual orthonormal basis $\{|j, n\rangle\}$ with $-j \leq n \leq j$ is the common set of eigenvectors of $\vec{J}^2$ and J_0 acting on the states as,

$$\begin{aligned}\vec{J}^2 |j, n\rangle &= j(j+1) |j, n\rangle , \\ J_0 |j, n\rangle &= n |j, n\rangle .\end{aligned} \tag{3.42}$$

Additionally, they form the algebra by obeying the commutation rules,

$$[J_1, J_2] = iJ_0, \ [J_0, J_1] = iJ_2, \ [J_2, J_0] = iJ_1. \tag{3.43}$$

Similar to the standard coherent states, we represent the closure of our algebra by the raising/lowering operators $\{J_\pm, J_0\}$. To maintain a correspondence with the notation we have adopted until now, we introduce a re-labeling of the basis vectors as $n \to n + j$, so that $n = 0, \ldots, 2j$. The operators are now defined by the following equations[5],

$$\begin{aligned}J_\pm &= J_1 \pm iJ_2, \\ J_0 |j, -j + n\rangle &= (-j + n) |-j + n\rangle , \\ J_+ |j, -j + n\rangle &= \sqrt{(n+1)(2j-n)} |j, -j + n + 1\rangle , \\ J_- |j, -j + n\rangle &= \sqrt{n(2j-n+1)} |j, -j + n - 1\rangle , \\ J_+ |j, j\rangle &= 0 |j, j\rangle , J_- |j, -j\rangle = 0 |j, -j\rangle .\end{aligned} \tag{3.44}$$

The algebra is closed by the commutation relations (similar to equation(3.6)),

$$[J_0, J_\pm] = \pm J_\pm, \ [J_+, J_-] = 2J_0. \tag{3.45}$$

[5]The normalization constants differ from the ones usually encountered due to our re-labeling. The eigenvalues of J_0 have been included so the comparison becomes easier.

The raising operator J_+ is used to generate the orthonormal basis (see (3.7)) by,

$$|j,-j+n\rangle = \sqrt{\frac{\Gamma(2j-n+1)}{n!\,\Gamma(2j+1)}} J_+^n |j,-j\rangle\,. \tag{3.46}$$

3.3.2 Derivation

As expected, there exist several parameterizations through which we can construct a unitary representation of SU(2) using $\{J_\pm, J_0\}$ as infinitesimal generators. The one we discuss is,

$$D(z,\psi) = N^{-\frac{1}{2}} e^{zJ_-} e^{-z^*J_+} e^{i\psi J_0}, \tag{3.47}$$

where $0 \leq \psi \leq 2\pi$ and z is an arbitrary complex number (N is a normalization constant). Taking into consideration the eigenequation of J_0 in (3.44), the last exponential in the above equation can be simply rewritten as $e^{i\psi(-j+n)}$, which constitutes a phase that can be ignored, whenever $D(z,\psi)$ acts on any $|j,-j+n\rangle$. This allows us to rewrite the displacement operator as,

$$D(z) = N^{-\frac{1}{2}} e^{zJ_-} e^{-z^*J_+}. \tag{3.48}$$

In theory, we are free to apply $D(z)$ on any of the orthogonal states to construct our set. We pick one of the highest-weight[6] states, $|j,j\rangle$, for two reasons. One, it greatly simplifies the calculating process as, the action of J_+ in (3.44) tells us that,

$$e^{-z^*J_+} |j,j\rangle = e^{e^{-z^*}0} |j,j\rangle = |j,j\rangle\,, \tag{3.49}$$

which means that the spin-coherent states are simply generated by the equation,

$$|z,j\rangle = D(z)\,|j,j\rangle = N^{-\frac{1}{2}} e^{zJ_-} |j,j\rangle \tag{3.50}$$

Remembering the Taylor expansion of the exponential of an operator, along with the action of J_- in (3.44), we notice that only the first $2j+1$ terms survive. Normalizing gives us the final expression for the spin coherent states,

$$|z,j\rangle = \frac{1}{(1+|z|^2)^j} \sum_{n=0}^{2j} z^n \sqrt{\frac{\Gamma(2j+1)}{n!\,\Gamma(2j-n+1)}}\, |j,-j+n\rangle \tag{3.51}$$

The second reason we choose the highest-weight states is that they are also minimum uncertainty states. The generalized uncertainty relation (3.13) for operators J_1 and J_2 reads,

$$\Delta J_1 \Delta J_2 \geq \frac{1}{2} |\langle J_0\rangle\,| \tag{3.52}$$

The process of proving that (3.52) is saturated for the highest weight states, as well as any other coherent state, is significantly lengthy but straightforward. This time, however, there exists a caveat preventing us from referring to the entire set of spin-coherent states as "minimum uncertainty". Unlike their canonical counterparts, these states cannot all be *simultaneously* of minimum uncertainty. For a thorough explanation, the reader is encouraged to see [21].

[6] The term "highest-weight" refers to the states that vanish upon application of one of the ladder operators.

Finally, the overlap between two states $|z\rangle, |z'\rangle$ is given by

$$\langle z|z'\rangle = \frac{(1+z^*z')^2 j}{(1+|z|^2)^j(1+|z'|^2)^j}, \tag{3.53}$$

which shows that there do in fact exist pairs of states that are orthogonal. Their relationship will become clear after we employ an alternative parameterization following [25]. Before we do that, we end this subsection by making sure that $\{|z,j\rangle\}$ resolve the unity. It turns out that a weight function is required for completeness when integrating, namely:

$$\frac{2j+1}{\pi}\int_{\mathbb{C}} \frac{|z\rangle\langle z|}{(1+|z|^2)^2}\, d^2z = I. \tag{3.54}$$

3.3.3 Important Parametrizations

Though all of our results can be obtained through the one parametrization we have been using, there exist two alternative choices that are of great use. We give a brief review before proceeding with the next set of coherent states.

$$z = \tan\left(\frac{\theta}{2}\right)e^{i\phi}, \tag{3.55}$$

where $0 \leq \theta < \pi$ and $0 \leq \phi < 2\pi$. This re-parameterization amounts to changing the label space Ω from the complex plane ($z = re^{i\phi'}$) to the *Riemann* sphere. This process is achieved through a *stereographic projection*. Drawing the z-plane tangentially to the south pole of the unit sphere, as seen in Figure (3.2), a line is drawn from every point on the complex plane to the north pole. The point where each line intersects the sphere is the point of projection with coordinates (θ, ϕ).

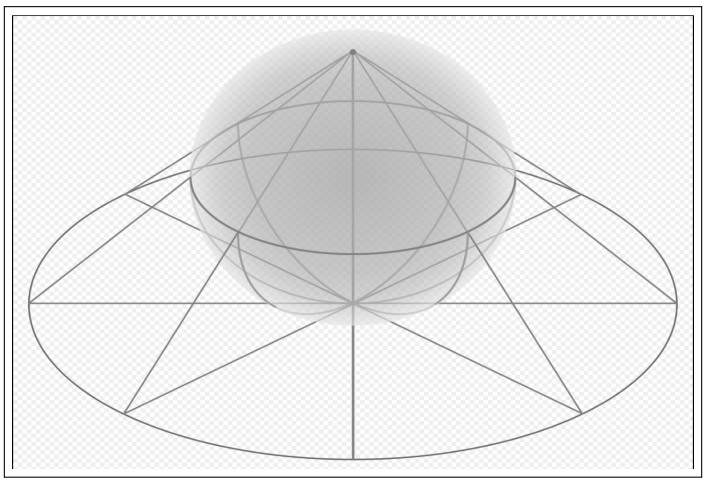

Figure 3.2: Schematic representation of a stereographic projection from the north pole of the sphere. Notice that circles on the plane get projected as circles on the sphere.

With some imagination, one can discern that $\phi = \phi'$ and $r = \tan(\frac{\theta}{2})$. This parameterization of spherical geometry is, in a way, the "right fit" for the spin-coherent states. One reason for that will become clear when we discuss the associated Fubini-Study Metric. This parametrization also allows us to understand the orthogonal states we detected in (3.53), they represent antipodal points on the sphere.

We conclude by making the remark that it is of paramount importance to our argument in the next chapter that we can write our displacement operator in the form (3.34). Here, due to the more complicated nature of the commutation relation, ($\hat{a}, \hat{a}^\dagger$ commute with $\hat{I}$ but $J_\pm$ do not commute with J_0) we require another parametrization by introducing a new complex variable ξ, which is related to z and (θ, ϕ) by

$$\xi = -\frac{\theta}{2} e^{-i\phi}, \; z = -\frac{\xi^*}{|\xi|} \tan(|\xi|). \tag{3.56}$$

With this, using what is called a *disentangling formula* (a specific instance of the BCH formula), we can write,

$$|z, j\rangle = D(\xi)\,|j, j\rangle = e^{\xi J_+ - \xi^* J_-}\,|j, j\rangle\,. \tag{3.57}$$

3.4 SU(1,1) or SL(2,R) Coherent states

The last set of coherent states we examine will be used when we study systems whose operator evolution is governed by the *SL(2,R) group* (We will return to what this means in the next chapter). As is evident from the title, we refer to the associated coherent states as those of the SU(1,1) group, following the literature. Again, the reason being that the $\mathfrak{su}(1,1)$ and $\mathfrak{sl}(2,R)$ Lie Algebras are isomorphic, with the respective groups only being "locally isomorphic"[7].

The group SL(2,R) and its representations play pivotal roles across multiple areas of theoretical physics. It is central to two-dimensional conformal field theories. The AdS/CFT correspondence in string theory, which bridges gravity theories in Anti-de Sitter space with conformal field theories, also sees SL(2,R) as key due to its connection to AdS isometries. Furthermore, the symmetries of SL(2,R) emerge in the near-horizon geometries of certain black holes, in quantum cosmological models of the early universe, and in various aspects of string theory beyond AdS/CFT. The advanced topics usually tackled by this group make it clear that it often remains less emphasized in undergraduate studies. Hence, a brief introduction is provided for clarity.

The special linear group of degree 2 over the real numbers consists of all the 2×2 real matrices with determinant 1. These matrices describe area-preserving transformations in the real plane. Just as in Section 3.3, we start by constructing the Hilbert space on which the group elements will act, using a label h, with the difference being that this time the space is infinite-dimensional. The discrete orthonormal basis $\{|h, n\rangle\}$ we use, along with the action of the algebra generators gives us the "discrete series" representation of SL(2,R). Namely, we use three operators $L_0, L_{\pm 1}$ obeying the commutation relations,

$$[L_0, L_{\pm 1}] = \mp L_{\pm 1}, \; [L_1, L_{-1}] = 2L_0, \tag{3.58}$$

further demonstrating the similarities with $\mathfrak{su}(2)$. The orthonormal basis is the common set of eigenvectors of L_0 and $C_2 = L_0^2 - \frac{1}{2}(L_{-1}L_1 + L_1 L_{-1})$, called the Casimir operator[8]. The full action

[7] Locally isomorphic implies that, in the vicinity of the identity element, two groups behave identically with respect to their group operations

[8] In general, the term Casimir operator refers to an operator that commutes with all generators of an algebra. $\vec{J}^2$ and J_0 are such examples.

of the elements of $\mathfrak{sl}(2,R)$ is given below.

$$\begin{aligned} L_0 \left|h,n\right\rangle &= (h+n)\left|h,n\right\rangle, \\ C_2 \left|h,n\right\rangle &= h(h-1)\left|h,n\right\rangle, \\ L_{-1}\left|h,n\right\rangle &= \sqrt{(n+1)(2h+n)}\left|h,n+1\right\rangle, \\ L_1 \left|h,n\right\rangle &= \sqrt{n(2h+n-1)}\left|h,n-1\right\rangle. \end{aligned} \tag{3.59}$$

The correspondence between (3.44) and (3.59) is clear, with L_{-1} and L_1 acting as the raising and lowering operators respectively. Before we proceed with the coherent states, we present the final member of the family consisting of equations (3.7) and (3.46),

$$\left|h,n\right\rangle = \sqrt{\frac{\Gamma(2h)}{n!\,\Gamma(2h+n)}} L_{-1}^n \left|h,0\right\rangle. \tag{3.60}$$

Deriving the expression for the SL(2,R) coherent states using the means we have employed thus far is impractical, if not impossible (consider, for example, that an exponential operator of L_{-1} would not have any vanishing terms). As such, we do not show any proof, but give the results based on Perelomov's approach to generalized coherent states for an arbitrary Lie Group in [22]. The normalized states read

$$\left|z,h\right\rangle = (1-|z|^2)^h \sum_{n=0}^{\infty} z^n \sqrt{\frac{\Gamma(2h+n)}{n!\,\Gamma(2h)}}\left|h,n\right\rangle, \tag{3.61}$$

where our label space is now the upper complex half-plane $P_+ = \{z \in \mathbb{C}, \mathrm{Im}\ z > 1\}$. An equivalent parametrization is the (unbounded) unit complex disc $\mathcal{D} = \{z \in \mathbb{C}, |z| < 1\}$, which can be achieved starting from the former through a *Möbius transformation*. Both of these representations are commonly used in 2-dimensional hyperbolic geometry. This geometry will re-appear when we associate a metric with each set of coherent states. The resolution of unity by $\{|z,h\rangle\}$ bears resemblance to (3.54), namely

$$\frac{2h-1}{\pi}\int_{\mathcal{D}} \frac{\left|z\right\rangle\left\langle z\right|}{(1-|z|^2)^2}\, d^2z = I. \tag{3.62}$$

Our presentation of the basic of these states is completed with inner product between any two $\left|z\right\rangle, \left|z'\right\rangle$ which is also similar to (3.53),

$$\langle z,h|z',h\rangle = (1-z^*z')^{-2h}(1-|z|^2)^h(1-|z'|^2)^h. \tag{3.63}$$

We end this chapter by repeating the process in the end of subsection 3.3.3. Requiring an expression of the form (3.57),(3.34), we associate each element z of the unit disk $\mathcal{D}$ a complex variable ξ,

$$\begin{aligned} \xi = \frac{\rho}{2}e^{i\phi},\ \ z = \frac{\xi}{|\xi|}\tanh(|\xi|), \\ z = \tanh(\frac{\rho}{2})e^{i\phi}, |z|<1 \end{aligned} \tag{3.64}$$

finally allowing us to write

$$\left|z,h\right\rangle = D(\xi)\left|h,0\right\rangle = e^{\xi L_{-1} - \xi^* L_1}\left|h,0\right\rangle. \tag{3.65}$$

3.5 Geometry of Hilbert Spaces

The geometric view of quantum states has numerous applications, especially in, but not limited to, quantum information theory. Concepts like quantum channels, quantum state transformations, and most importantly entanglement can often be given a geometric interpretation, which can be useful in deriving certain results and offering novel ways to study and understand them.

This chapter's final section is dedicated to one approach to geometric quantum mechanics, producing a *Riemannian metric structure* with which the manifolds of quantum states are endowed. To do that, we briefly discuss the concepts of *rays* and *projective Hilbert spaces* before we can finally reach the so-called *Fubini-Study metric* for pure states. We will also briefly talk about the relationship between this metric and coherent states. We mainly follow ([26],[27],[28]).

3.5.1 A first attempt

Given the complete metric space requirement (see A.1), every Hilbert space $\mathcal{H}$ has the structure of a differentiable manifold, allowing for the definition of a "local chart" on $\mathcal{H}$, where two states that are "close" to each other live. This means that, in theory, after defining what "close" states mean and calculating their distance, we can define a *line element*, which in turn allows us to derive a *metric tensor* and the desired Riemannian structure. After briefly going over this process, we will discuss why the result is not satisfactory, providing motivation for an alternative methodology.

The distance D between any two states can be defined thanks to the hermitian inner product of $\mathcal{H}$. More precisely, given two normalized states $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}$, we write,

$$D(|\psi_1\rangle, |\psi_2\rangle) = \| |\psi_1\rangle - |\psi_2\rangle \| = \langle\psi|\psi\rangle^{\frac{1}{2}} = \ldots = [2(1 - \text{Re}\,(\langle\psi_1|\psi_2\rangle))]^{\frac{1}{2}}, \tag{3.66}$$

where $|\psi\rangle = |\psi_1\rangle - |\psi_2\rangle$. We understand "close states" in the following way. Consider a set of normalized kets $\{|\psi(s)\rangle\}$ in $\mathcal{H}$ whose elements depend smoothly on a n-dimensional parameter $\xi = (\xi_1, \xi_2, \ldots, \xi_n) \in \mathbb{R}^n$. A small difference in the parameter $d\xi$ defines close states $|\psi(\xi)\rangle$ and $|\psi(\xi + d\xi)\rangle$. The latter's Taylor expansion with respect to ξ in first-order approximation is

$$|\psi(\xi + d\xi\rangle = |\psi(\xi)\rangle + \sum_{\mu=1}^{n} |\partial_\mu \psi\rangle \, d\xi^\mu \equiv |\psi(\xi)\rangle + |d\psi(\xi)\rangle, \tag{3.67}$$

where $\partial_\mu \psi = \frac{\partial \psi}{\partial \xi^\mu}$. This, allows us to write up to second order the square of (3.66), i.e. the line element as,

$$ds^2 = \langle d\psi | d\psi\rangle = \sum_{\mu\nu} \langle \partial_\mu \psi | \partial_\nu \psi\rangle \, d\xi^\mu d\xi^\nu = g'_{\mu\nu} d\xi^\mu d\xi^\nu. \tag{3.68}$$

In this context, the term 'second-order' refers to the differential 2-form on the manifold, indicative of the bilinear structure of the metric, arising from terms quadratic in ds. This should not be confused with a second-order Taylor expansion. Given the symmetric nature of (3.68), and metric tensors in general, it is easy to see that the real parts of the inner products $\langle \partial_\mu \psi | \partial_\nu \psi\rangle$ turn out to be the entries of the metric tensor $g'_{\mu\nu}$ associated to our Hilbert space.

It turns out that this metric tensor holds no physical meaning in the context of ordinary quantum mechanics. The reason is the redundant description of quantum states Hilbert spaces provide. As we have already pointed out numerous times throughout this thesis, states differing by a phase

$e^{i\phi}, \phi \in \mathbb{R}$ (or a complex number in general, if we are referring to unnormalized states as well) represent the same physical state. However, using the terms Re $(\langle \partial_\mu \psi | \partial_\nu \psi \rangle)$, we can show that the metric tensors associated with the families $\{|\psi'(\xi)\rangle\}$ and $\{|\psi(\xi)\rangle\}$ where

$$|\psi'(\xi)\rangle = e^{ia(\xi)} |\psi(\xi)\rangle, a(\xi) \in \mathbb{R}, \tag{3.69}$$

are not identical (see [27] for a derivation). As such, we need to account for this redundancy and construct a new metric that is invariant under the gauge transformation defined by (3.69).

3.5.2 Fubini Study Metric

This new metric can be thought of as defined using not the quantum states, but rather the set of equivalence classes, created by the sets of physically equivalent non-zero vectors in $\mathcal{H}$, called *rays*. Formally, a ray is defined as

$$\begin{aligned} R_\psi &= \{|\phi\rangle \in \mathcal{H} | \exists \alpha \in (\mathbb{C} \setminus \{0\}) : |\phi\rangle = e^{i\alpha} |\psi\rangle\}, \\ R_\psi &= \{|\phi\rangle \in \mathcal{H} | \exists c \in (\mathbb{C} \setminus \{0\}) : |\phi\rangle = c |\psi\rangle\}, \end{aligned} \tag{3.70}$$

if we are referring to normalized states or unnormalized vectors respectively. It is worth mentioning that the physical equivalence we have been talking about originates from the Born rule, stating that the transition probability between two states, the only observable quantity in Quantum Mechanics, $|\psi_1\rangle, |\psi_2\rangle$ is given by the equation

$$P(\psi_1, \psi_2) = \frac{|\langle \psi_1 | \psi_2 \rangle|^2}{|\langle \psi_1 | \psi_1 \rangle| |\langle \psi_2 | \psi_2 \rangle|}. \tag{3.71}$$

Now, we can define the said space (manifold) of rays, called the Projective Hilbert Space by,

$$\mathcal{P}(\mathcal{H}) := (\mathcal{H} - \{0\}) / \sim, \tag{3.72}$$

where $\sim$ denotes the equivalence relation between two vectors in the same ray, i.e.

$$\phi \sim \psi \Leftrightarrow \phi \in R_\psi. \tag{3.73}$$

It is important to mention that $\mathcal{P}(\mathcal{H})$ is not a vector space, which means we are not necessarily allowed to explicitly write two neighboring rays as $|\psi\rangle, |\psi\rangle + |d\psi\rangle$. Following the same procedure that lead us to (3.68) (this time we need a second-order Taylor expansion, for more details, see [26], the line element between to neighboring rays is given by,

$$ds^2_{FS} = \langle d\psi | d\psi \rangle - \langle \psi | d\psi \rangle \langle d\psi | \psi \rangle, \tag{3.74}$$

assuming that the states are normalized. If not, the appropriate denominators are added, as we will see in the next chapter. This line element corresponds to the metric tensor

$$g_{\mu\nu} = \langle \partial_\mu \psi | \partial_\nu \psi \rangle - \langle \partial_\mu \psi | \psi \rangle \langle \psi | \partial_\nu \psi \rangle. \tag{3.75}$$

Before we continue with the relation to coherent states, we mention that the Fubini-Study distances have been used in a different proposal of complexity. Here, the metric is used for different purposes.

Chapter 4

A method for analytical calculations

In theory, our work in Chapters 1 and 2 has provided a framework to solve the operator or state dynamics of many-body systems accurately. Beginning with the auto-correlation function and an initial operator, it's possible to construct the Krylov Basis and solve the discrete Schrödinger equations to finally determine the corresponding probability amplitudes. Furthermore, we introduced a complexity measure, as given by (2.2), for a more refined characterization of the behavior of systems, distinguishing beyond merely chaotic and non-chaotic distinctions. However, in practice, these setups often deviate from the ideal scenario, necessitating computational and numerical approaches. Thus, identifying methods to provide analytical solutions for such problems is crucial for deepening our understanding of them. We present a two-fold example of such a method, which relies on coherent states and the displacement operators generating them.

This approach rests on one powerful observation— the interesting similarity in structure between the Liouvillian and its action on the Krylov basis in equation (1.55) and the exponential of the displacement operator acting on a reference state we worked to craft in the triplet of equations {(3.34),(3.57),(3.65)}. As we have mentioned, this type of displacement operator can be obtained as the unitary representation of any arbitrary Lie group, these three examples are simply the ones we will discuss. In fact, the similarity grows even stronger when we consider that the Liouvillian gets exponentiated when we calculate the time evolution of an operator in (1.51). We will attempt to provide a clear picture of the specifics of this correspondence and what it entails.

The crux of our argument is to interpret the Liouvillian $\mathcal{L}$ as the sum of abstract raising and lowering operators,

$$\mathcal{L} = \alpha(A_+ + A_-), \tag{4.1}$$

with α being a system-dependent proportionality factor whose meaning will become clear when we delve into specific examples (Section 2.2 provides a strong hint). Essentially, we are referring to Liouvillians which are elements of the algebra of a certain symmetry group, i.e. the subset of quantum systems which are governed by symmetry. Of course, there exist many examples of such systems. When we apply our procedure to the SL(2,R) group, we anticipate reproducing the large N SYK-model results[1], given our comment in the last paragraph of section 2.2. The SU(2) and Weyl-Heisenberg cases are not directly related to physical examples and we will refer to those systems as "particles moving on a group".

[1]In general, the Hamiltonians in QFT and CFT belong to the Lie Algebras of the Poincare group (group of translations and Lorentz transformations) and the conformal group (group of angle preserving transformations) respectively[1].

Let's examine the effects of (4.1). Firstly, it allows us to establish an isomorphism between the Krylov Basis $\{|\mathcal{O}_n)\}$ and the discrete series representation of the symmetry group A_+, A_- generate, i.e. the orthonormal basis upon which the unitary representation of the group acts. This immediately relieves us of the heavy, if not impossible, burden of computing the quantities associated with the Lanczos recursion method. After associating our initial operator $|\mathcal{O})$ with the highest-weight state of the orthonormal basis, we have obtained the whole Krylov basis. With this, we can write

$$\alpha A_+ = b_{n+1}|\mathcal{O}_n), \ \alpha A_- = b_n|\mathcal{O}_{n-1}), \tag{4.2}$$

allowing us to read off the Lanczos coefficients without any calculations, leaving only the probability amplitudes $\{\phi_n(t)\}$. Combining (4.1) with the above, we reach the most important conclusion of this approach. *The time evolution of the initial operator $|O)$ can be thought of as a coherent state generated by a displacement operator with complex variable $\xi = i\alpha t$.* This means that the operator's dynamics are really an orbit in the phase space of coherent states i.e. a motion in classical phase space. The details of this observation will not be analyzed here, but a description is given in [1]. Finally, thanks to the completeness requirement we have set and $|\mathcal{O}(t)$ being a coherent state, we can decompose it using the orthonormal basis and read out the coefficients, which turn out to be $\{\phi_n(t)\}$.

Before we proceed to the second part of this method, we make two important remarks. Firstly, this part of our argument is sufficient to perform the desired analytical calculations. We have successfully found a way to overcome the computational hurdles of the Lanczos method. Recent literature, in fact, mainly utilizes this part only. Additionally, this whole process can be applied to the Krylov state complexity and the Hamiltonian, with the addition of the set of coefficients $\{a_n\}$. The displacement operators become more complicated and the resulting Complexity is potentially different. Considering that our aim with this thesis was to explicitly reproduce some of the results in [1], we do not examine this avenue but mention the findings in [14] for comparison's sake.

The Fubini-Study metric associated with each set of coherent states allows us to search for geometric tools with which we can examine Krylov Complexity. In our case, we examine the relation between operator growth and the geodesic curves of the metric space, the proportionality between $K_\mathcal{O}$ and the volume enclosed by the orbit as well as the relation between the mean curvature of the information metric and the complexity growth/potential for chaotic behavior of the system. The geometry of Krylov complexity has not been exhaustively researched leaving room for future findings.

4.1 Weyl-Heisenberg Group

We start by examining the dynamics of "a particle moving in the Weyl-Heisenberg group". By that, we mean that the Liouvillian is an element of the Weyl-Heisenberg algebra (we are allowed to adjoin the number operator to our algebra by including its commutation relations with the other operators, see [20]) we mentioned in (3.1.2), having the following form,

$$\mathcal{L} = \alpha(a^\dagger + a). \tag{4.3}$$

Our first step is associating our initial operator with one state from the orthonormal basis,

$$|\mathcal{O}) \leftrightarrow |0\rangle\,, \tag{4.4}$$

and by combining (4.3) with (3.5) we complete the identification between the Krylov Basis and $\{|n\rangle\}$, obtaining the Lanczos coefficients along the way,

$$|\mathcal{O}_n) \leftrightarrow |n\rangle\,,\ b_n = \alpha\sqrt{n}. \tag{4.5}$$

Remembering how the standard coherent states $\{|z\rangle\}$ get generated in (3.34), we observe that the operator's time evolution through the Liouvillian is just a displacement operator with $z = i\alpha t$,

$$\begin{aligned} |\mathcal{O}(t)) = e^{i\alpha(a^\dagger + a)t}\,|0\rangle = \\ = |z = i\alpha t\rangle = . \end{aligned} \tag{4.6}$$

This allows us to read off the probability amplitudes by decomposing $|z\rangle$ using (3.20) and $|\mathcal{O}(t))$ using (1.57),

$$\begin{aligned} |z = i\alpha t\rangle = e^{-\alpha^2 t^2/2}\sum_{n=0}^{\infty} i^n \frac{\alpha^n t^n}{\sqrt{n!}}\,|n\rangle\,, \\ \phi_n(t) = e^{-\alpha^2 t^2/2}\frac{\alpha^n t^n}{\sqrt{n!}}. \end{aligned} \tag{4.7}$$

The probabilities corresponding to the obtained $\{\phi_n(t)\}$ form the Poisson distribution. We observe that the Lanczos coefficients do not grow linearly and thus expect the complexity to not grow exponentially. Also, the starting point of our approach, the auto-correlation function is simply ϕ_0, i.e.

$$C(t) = e^{-\alpha^2 t^2/2}. \tag{4.8}$$

It is important to point out that, thus far, we have not solved any equations, differential or algebraic, to obtain our results. As such, it is not obvious that our Lanczos coefficients solve the Schrödinger equations in (1.58) with the obtained $\{\phi_n(t)\}$. We provide verification for this and the following examples. Starting from the partial time derivative of $\phi_n(t)$ we get the following expression,

$$\begin{aligned} \partial_t\phi_n(t) = -\alpha^2 t\phi_n(t) + n\frac{\phi_n(t)}{t} = \\ \alpha^2 t\sqrt{n+1}\frac{\phi_n(t)}{\sqrt{n+1}} + \frac{(\sqrt{n})^2\alpha}{\alpha t}\phi_n(t) = -\alpha\sqrt{n+1}\phi_{n+1}(t) + \alpha\sqrt{n}\phi_{n-1}(t) = \\ b_n\phi_{n-1}(t) - b_{n+1}\phi_{n+1}(t), \end{aligned} \tag{4.9}$$

which confirms our results. We proceed with the calculation of Krylov complexity for this system,

$$\begin{aligned} K_{\mathcal{O}} = \sum_{n=0}^{\infty} n|\phi_n(t)|^2 = e^{-\alpha^2 t^2}\sum_{n=0}^{\infty}\frac{n(\alpha^n t^n)^2}{n!} = \\ = e^{-\alpha^2 t^2}\sum_{n=1}^{\infty}\frac{(\alpha^n t^n)^2}{(n-1)!} = e^{-\alpha^2 t^2}\alpha^2 t^2\sum_{n=1}^{\infty}\frac{(\alpha^{n-1} t^{n-1})^2}{(n-1)!} = e^{-\alpha^2 t^2}\alpha^2 t^2\sum_{n=0}^{\infty}\frac{n(\alpha^n t^n)^2}{n!} = \alpha^2 t^2. \end{aligned} \tag{4.10}$$

We observe a non-maximal, quadratic growth to complexity for this system. This behavior will re-appear when examining the other systems, albeit for a short duration. Moving to Krylov state complexity, to include the a_n coefficients, the Hamiltonian requires some extra terms that won't be explored here (see [14]),

$$H = \alpha(a^\dagger + a) + \omega N + \delta I, \tag{4.11}$$

where ω, δ are constants and N is the number operator. The resulting coefficients and complexity are,

$$\begin{aligned} a_n &= \omega n + \delta, b_n = \alpha\sqrt{n}, \\ K_\psi &= \frac{4\alpha^2}{\omega^2}\sin^2(\frac{\omega t}{2}). \end{aligned} \tag{4.12}$$

In this case, even though $\{b_n\}$ remain the same and the Hilbert space is infinite-dimensional, the existence of $\{a_n\}$ bounds the system resulting in oscillating complexity. In fact, it is easy to see, considering the Taylor expansion of $f(\omega) = a^{\frac{\sin^2(\omega t)}{\omega^2}}$, that for $a_n \to 0$, the complexity grows quadratically in time.

Finally, we calculate the Fubini-Study metric associated with the rays of the canonical coherent states $\{|z\rangle\}$. We will derive the metric using the non-normalized version of the states and equation (3.74) (To be more precise, we use the normalization $\langle z|z\rangle = e^{-|z|^2}$. We start with $\langle dz|dz\rangle$ and use the orthonormality of $\{|n\rangle\}$,

$$\begin{aligned} |dz\rangle = \sum_{n=1}^{\infty}\frac{nz^{n-1}dz}{\sqrt{n!}}|n\rangle, \langle dz|dz\rangle = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{nm(z^*)^{n-1}(z)^{n-1}dzdz^*}{\sqrt{n!}\sqrt{m!}}\langle m|n\rangle = \\ = \sum_{n=1}^{\infty}\frac{n^2}{n!}(|z|^2)^{n-1}dzdz^* = \sum_{n=1}^{\infty}\frac{n}{(n-1)!}(|z|^2)^{n-1}dzdz^*. \end{aligned} \tag{4.13}$$

Re-indexing the above sum to $n-1 \to n$ and splitting the sum into two, we get,

$$\begin{aligned} \langle dz|dz\rangle = (\sum_{n=0}^{\infty}\frac{(|z|^2)^n}{n!}dzdz^* + \sum_{n=0}^{\infty}\frac{n(|z|^2)^n}{n!}dzdz^*) = \\ (e^{|z|^2} + |z|^2\sum_{n=1}^{\infty}\frac{(|z|^2)^{n-1}}{(n-1)!})dzdz^* = e^{|z|^2}(|z|^2+1)dzdz^*. \end{aligned} \tag{4.14}$$

The terms $\langle dz|z\rangle, \langle z|dz\rangle$ are complex conjugates of each other and only one needs to be calculated. We write,

$$\begin{aligned} \langle dz|z\rangle = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{m(z^*)^{m-1}z^n dz^*}{\sqrt{m!}\sqrt{n!}}\langle m|n\rangle = \sum_{n=1}^{\infty}\frac{z(|z|^2)^{n-1}}{(n-1)!}dz^* = e^{|z|^2}zdz^*, \\ \langle z|dz\rangle = e^{|z|^2}z^*dz. \end{aligned} \tag{4.15}$$

Combining the above and taking into account the chosen normalization, we obtain the Fubini-Study line element,

$$ds^2_{FS} = dzdz^*, \tag{4.16}$$

which shows that the associated geometry is that of the plane (as we expected from our label space Ω). To make this clearer, we introduce the polar coordinates $z = re^{i\phi}$ to get,

$$\begin{aligned} dz = \frac{\partial z}{\partial r}dr + \frac{\partial z}{\partial \phi}d\phi = e^{i\phi}dr + ire^{i\phi}d\phi = e^{i\phi}(dr + id\phi), \\ dz^* = \frac{\partial z^*}{\partial r}dr + \frac{\partial z^*}{\partial \phi}d\phi = e^{-i\phi}dr - ire^{-i\phi}d\phi = e^{-i\phi}(dr - id\phi), \\ ds^2_{FS} = dzdz^* = dr^2 + r^2d\phi^2 \end{aligned} \tag{4.17}$$

We make three remarks based on this result. Firstly, the flat information geometry, corresponding to quadratic complexity growth, has zero mean curvature, i.e. $R = 0$. Second, the trajectory $z = i\alpha t$ in the coherent state phase space corresponds to a linear trajectory, which is a geodesic on this manifold, with $r = \alpha t, \phi = \frac{\pi}{2}$. Third, as we will show, the "volume" (surface in this case) V_t covered by this trajectory is proportional to $K_{\mathcal{O}}$,

$$V_t = \int_0^{r(t)} \int_0^{2\pi} \sqrt{det(ds_{FS})}\, d\phi\, dr' = \int_0^{\alpha t} \int_0^{2\pi} r'\, d\phi\, dr' = 2\pi \frac{(\alpha t)^2}{2} = \pi K_{\mathcal{O}}. \tag{4.18}$$

The purpose of these three 3 geometric observations is to search for properties that will be shared among all systems. As such, we will study the behavior of the associated quantities in the other two examples as well and attempt to draw some general conclusions.

4.2 SU(2) Group

In the case of a Liouvillian being an element of $\mathfrak{su}(2)$, the Hilbert space in which the states of the system live is finite-dimensional. As such, keeping in mind the definition of $K_{\mathcal{O}}$, we expect the existence of a bound on complexity growth (and of course the Lanczos coefficients). As we will see, the system does not reach a maximum and form a plateau in time but rather, it oscillates similarly to (4.12). The Liouvillian this time is

$$\mathcal{L} = \alpha(J_+ + J_-) \tag{4.19}$$

Here, for a spin-j system, we have two choices of highest weight states in $|j, j\rangle$ and $|j, -j\rangle$ being annihilated by J_+, J_- respectively. In our initial derivation, we started from the former to make our calculations easier. Now, we make the association

$$|\mathcal{O}) \leftrightarrow |j, -j\rangle\,, \tag{4.20}$$

which, using (3.44), allows us to identify each element of the Krylov Basis and read the Lanczos coefficients b_n as

$$|\mathcal{O}_n) = |j, -j + n\rangle\,,\ b_n = \alpha\sqrt{(n(2j - n + 1)}, n = 0, \ldots, 2j, \tag{4.21}$$

which already shows the bound on complexity. Besides their non-maximal growth, they also show decreasing behavior for higher n. Remembering that $\{b_n\}$ represent hopping amplitudes, a decreasing sequence of Lanczos coefficients means that the average position in the Krylov chain does not necessarily always grow. To make things more specific, the coefficients follow a symmetric distribution (except for b_0) around a maximum value,

$$n_{b_{max}} = j + \frac{1}{2},\ b_{j+\frac{1}{2}} = \alpha(j + \frac{1}{2}). \tag{4.22}$$

The minimum values are

$$b_1 = b_{2j} = \alpha\sqrt{2j}. \tag{4.23}$$

Again, we can find $|\mathcal{O}(t))$ by generating the spin-coherent state from (3.57) (starting from $|j,-j\rangle$) and setting the complex variable $\xi = i\alpha t$,

$$|\mathcal{O}(t)) = |z = i\tan(\alpha t), j\rangle = e^{i\alpha(J_+ + J_-)t}\,|j,-j\rangle\,. \tag{4.24}$$

Equation (3.51) allows us to write the coherent state as a linear combination of $\{|j,-j+n\rangle\}$ and obtain the probability amplitudes by comparing with (1.57),

$$\begin{aligned} |z = i\tan(\alpha t), j\rangle &= \frac{1}{(1+\tan^2(\alpha t))^2}\sum_{n=0}^{2j} i^n \tan^n(\alpha t)\sqrt{\frac{\Gamma(2j+1)}{n!\,\Gamma(2j-n+1)}}\,|j,-j+n\rangle\,, \\ \phi_n(t) &= \cos^{2j}(\alpha t)\tan^n(at)\frac{\sqrt{(2j)!}}{\sqrt{n!}\sqrt{(2j-n)!}} \end{aligned} \tag{4.25}$$

The process of verifying that $\{\phi_n(t)\}$ and $\{b_n\}$ are compatible is a bit more involved in this case. We need to prove that

$$\partial_t\phi_n(t) = \alpha\sqrt{n(2j-n+1)}\phi_{n-1}(t) - \alpha\sqrt{(n+1)(2j-n)}\phi_{n+1}(t). \tag{4.26}$$

We start by re-writing $\phi_{n+1}(t), \phi_{n-1}(t)$,

$$\begin{aligned} \phi_{n-1}(t) = \cos^{2j}(\alpha t)\tan^{n-1}(\alpha t)\sqrt{\frac{(2j)!}{(n-1)!\,(2j-n+1)!}} &= \frac{\phi_n}{\tan(\alpha t)}\frac{\sqrt{n}}{\sqrt{(2j-n+1)}}, \\ \phi_{n+1}(t) = \ldots = \phi_n\frac{\tan(\alpha t)}{\sqrt{n+1}}\sqrt{2j-n} & \end{aligned} \tag{4.27}$$

Adding these two with proper coefficients and re-arranging, we get,

$$\begin{aligned} &\alpha\sqrt{n(2j-n+1)}\phi_{n-1}(t) - \alpha\sqrt{(n+1)(2j-n)}\phi_{n+1}(t) = \\ &= \alpha\phi_n[\frac{n}{\tan(\alpha t)} - \tan(\alpha t)(2j-n)] = \alpha\phi_n[\frac{n}{\cos^2(\alpha t)\tan(\alpha t)} - 2j\tan(\alpha t)]. \end{aligned} \tag{4.28}$$

Our aim is to reach the same expression by differentiating $\phi_n(t)$ with respect to time. Carefully re-writing some terms, we reach

$$\begin{aligned} \partial_t\phi_n(t) = \tan^n(\alpha t)cos^{2j}(\alpha t)\frac{\sqrt{(2j)!}}{\sqrt{n!}\sqrt{(2j-n)!}}[\frac{n}{\cos^2(\alpha t)\tan(\alpha t)} - \frac{2j}{\cos(\alpha t)}\sin(\alpha t)] = \\ = \alpha\phi_n[\frac{n}{cos^2(\alpha t)\tan(\alpha t)} - 2j\tan(\alpha t)], \end{aligned} \tag{4.29}$$

which completes our proof. Unlike in (4.7), the distribution of the probabilities of $\{\phi_n(t)\}$ in this case is not obvious at first sight. As such, we need to show a brief derivation of their form.

$$\begin{aligned} p_n(t) = |\phi_n(t)|^2 = \tan^{2n}(\alpha t)\cos^{4j}(\alpha t)\frac{(2j)!}{n!\,(2j-n)!} = \\ = \binom{2j}{n}(\sin^2(\alpha t))^n(1-\sin^2(\alpha t))^{(2j-n)}, \end{aligned} \tag{4.30}$$

which is of course the binomial distribution with probability of success equal to $\sin^2(\alpha t)$. Following the same steps, we mention that the correlation function is given by

$$C(t) = \frac{1}{\cos^{2j}(\alpha t)}. \tag{4.31}$$

This correlation function allows us to assign physical importance to the study of this system as it appears when analyzing free harmonic oscillators at finite temperature. Setting $\lambda = \sin^2(\alpha t)$,we proceed with the calculation of $K_{\mathcal{O}}$

$$\begin{aligned} K_{\mathcal{O}} &= \sum_{n=0}^{2j} n \binom{2j}{n} \lambda^n (1-\lambda)^{(2j-n)} = \sum_{n=1}^{2j} n \binom{2j}{n} \lambda^n (1-\lambda)^{(2j-n)} = \\ &= 2j\lambda \sum_{n=0}^{2j-1} \binom{2j-1}{n} \lambda^n (1-\lambda)^{(2j-1-n)} = 2j \sin^2(\alpha t). \end{aligned} \tag{4.32}$$

As we expected, there is no exponential growth to complexity. However, we do observe a quadratic growth of the form $K_{\mathcal{O}} \sim 2j\alpha^2 t^2$, at early times, just as in the previous example. Here, the complexity is periodic in time, reaching its maximum $K_{\mathcal{O}}^{max} = 2j$ at $t = (2k+1)\frac{\pi}{2\alpha}$ and going back to zero at times $t = \frac{k\pi}{\alpha}$, $k \in \mathbb{Z}$. It is interesting to examine how the complexity changes when generalizing to K_ψ. In that case, the Hamiltonian is of the form

$$H = \alpha(J_+ + J_-) + \gamma J_0 + \delta I. \tag{4.33}$$

Skipping the (more complicated than its operator counterpart) derivation, the Lanczos coefficients and the complexity read,

$$\begin{aligned} a_n = \gamma(-j+n) + \delta,\ b_n = \alpha\sqrt{n(2j-n+1)}, \\ K_\psi = \frac{2j}{1+\frac{\gamma^2}{4\alpha^2}} \sin^2(\alpha t \sqrt{1+\frac{\gamma^2}{4\alpha^2}}). \end{aligned} \tag{4.34}$$

We see that here the difference is only quantitative to $K_{\mathcal{O}}$, with a new factor being added which vanishes when $\gamma \to 0$.

Calculating the associated metric to our set of spin-coherent states will justify calling the Rieman sphere (θ, ϕ) parametrization a "natural choice". Again, we calculate using the unnormalized version $|z, j\rangle$, i.e. $\langle z|z\rangle = (1+z\bar{z})^{2j}$. We follow the same steps as before but do not present the calculation in its entirety,

$$\begin{aligned} |dz\rangle &= \sum_{n=0}^{2j} n z^{n-1} \sqrt{\frac{\Gamma(2j+1)}{n!\,\Gamma(2j-n+1)}}\, |j, -j+n\rangle\, dz, \\ \langle dz|dz\rangle &= \sum_{n=0}^{2j}\sum_{m=0}^{2j} mn z^{n-1}(z^*)^{m-1} \sqrt{\binom{2j}{n}\binom{2j}{m}}\, \langle -j+m|-j+n\rangle\, dz dz^* = \\ &= 2j dz dz^* \Big(\sum_{n=0}^{2j-1} (|z|^2)^n \frac{(2j-1)!}{n!\,(2j-1-n)!} + \sum_{n=0}^{2j-1} n(|z|^2)^n \frac{(2j-1)!}{n!\,(2j-1-n)!}\Big) = \\ &\ldots = 2j dz dz^* [(1+|z|^2)^{2j-1} + A], \end{aligned} \tag{4.35}$$

where,

$$A = \sum_{n=1}^{2j-1} n(|z|^2)^n \frac{(2j-1)!}{n!\,(2j-1-n)!} = \sum_{n=0}^{2j-2}(n+1)(|z|^2)^{n+1}\frac{(2j-1)!}{(n+1)!\,(2j-2-n)!} = \\ = 2j(1+|z|^2)^{2j-1}. \tag{4.36}$$

Combining (4.35),(4.36) and the normalization condition, we finally get,

$$\frac{\langle dz|dz\rangle}{\langle z|z\rangle} = (\frac{2j}{1+|z|^2} + \frac{|z|^2(2j-1)2j}{(1+|z|^2)^2})dzdz^* \tag{4.37}$$

The two remaining terms are calculated using similar arguments,

$$\begin{aligned} \langle dz|z\rangle &= \sum_{n=0}^{2j}\binom{2j}{n} n(|z|^2)^{n-1} z dz^* = \dots \\ &= 2j\sum_{n=0}^{2j-1}(|z|^2)^n \binom{2j-1}{n} z dz^* = 2j(1+|z|^2)^{2j-1} z dz^*, \\ \langle z|dz\rangle &= 2j\sum_{n=0}^{2j-1}(|z|^2)^n \binom{2j-1}{n} z dz^* = 2j(1+|z|^2)^{2j-1} z^* dz. \end{aligned} \tag{4.38}$$

We can finally calculate the Fubini-Study line element, which turns out to be

$$ds^2_{FS} = \frac{\langle dz|dz\rangle}{\langle z|z\rangle} - \frac{\langle dz|z\rangle\,\langle z|dz\rangle}{\langle z|z\rangle^2} = \dots = \frac{2j}{(1+|z|^2)^2} dzdz^*, \tag{4.39}$$

which is of course the complex sphere metric, demonstrating why the Riemann sphere parametrization of the label space was a natural choice. To make this more clear, we switch to the (θ, ϕ) parametrization using the change of variable in (3.55),

$$\begin{aligned} dz &= \frac{\partial z}{\partial\theta}d\theta + \frac{\partial z}{\partial\phi}d\phi = \dots = e^{i\phi}\left(\frac{d\theta}{2\cos^2(\frac{\theta}{2})} + i\tan\left(\frac{\theta}{2}\right)d\phi\right), \\ dz^* &= \frac{\partial z^*}{\partial\theta}d\theta + \frac{\partial z^*}{\partial\phi}d\phi = \dots = e^{-i\phi}\left(\frac{d\theta}{2\cos^2(\frac{\theta}{2})} - i\tan\left(\frac{\theta}{2}\right)d\phi\right), \end{aligned} \tag{4.40}$$

allowing us to rewrite (4.39) in a more appropriate form,

$$ds^2_{FS} = \frac{j}{2}(d\theta^2 + \sin^2(\theta)d\phi^2), \tag{4.41}$$

that clearly corresponds to the surface of a sphere of radius $\sqrt{\frac{j}{2}}$, a metric with constant positive curvature. Knowing the Ricci scalar for the surface of a sphere (see **??**), we see that in this case, it becomes,

$$R = \frac{4}{j}. \tag{4.42}$$

Keeping in mind that we have set $\xi = i\alpha t$ and using (3.56), we see that again, the evolution in time of $|\mathcal{O}(t))$ gets mapped to a geodesic curve on the associated metric with $\theta = 2\alpha t, \phi = \frac{\pi}{2}$. Finally, the "volume" in this geometry is given by,

$$V_t = \int_0^{\theta}\int_0^{2\pi} \sqrt{det(ds_{FS})}\, d\phi\, d\theta' = \int_0^{2at}\int_0^{2\pi} \sin(\theta)\, d\phi\, d\theta = 2\pi j \sin^2(at) = \pi K_{\mathcal{O}}, \tag{4.43}$$

adding more evidence to our observation of the proportionality between Krylov complexity and volume in the information metric.

4.3 SL(2,R) Group

We finish our thesis with one last example which in some ways holds the most physical importance. Firstly, our aim here is, as we have said, to obtain the results presented in 2.2. Additionally, it will be interesting to see what our geometric quantities will look like, considering that this example is an instance of a chaotic quantum system. Operator evolution is now governed by the SL(2,R) group with the Liouvillian taking the form

$$\mathcal{L} = \alpha(L_{-1} + L_1). \tag{4.44}$$

The initial operator is associated with the highest weight state of the discrete series representation of the group labeled by h,

$$|\mathcal{O}) \leftrightarrow |h, 0\rangle\,. \tag{4.45}$$

The action of L_{-1} in (3.59) and this association allows us to read the Lanczos coefficients and identify all elements of the Krylov basis,

$$|\mathcal{O}_n) = |h, n\rangle\,,\ b_n = \alpha\sqrt{n(2h+n-1)},\ n \in \mathbb{N}. \tag{4.46}$$

Properly adjusting the temperature-dependent parameter α and setting $\eta = 2h$, these coefficients are equivalent to the ones in (2.11), saturating the growth limit as desired. Generating the SU(1,1) coherent states using (3.65) with $\xi = i\alpha t$, the relation between ξ and z in (3.64) allows us to write

$$|\mathcal{O}(t)) = |z = i\tanh(\alpha t), h\rangle = e^{i\alpha(L_{-1}+L_1)t}\,|h, 0\rangle\,. \tag{4.47}$$

The set $\{|z\rangle\}$ being an overcomplete basis, we can expand any single coherent state according to (3.61) and obtain the probability amplitudes,

$$\begin{aligned} |z = i\tanh(\alpha t), h\rangle &= (1-\tanh^2(\alpha t))^2 \sum_{n=0}^{\infty} i^n \tanh^n(\alpha t)\sqrt{\frac{\Gamma(2h+n)}{n!\,\Gamma(2h)}}\,|h, n\rangle\,, \\ \phi_n(t) &= \sqrt{\frac{\Gamma(2h+n)}{n!\,\Gamma(2h)}}\frac{\tanh^n(\alpha t)}{\cosh^{2h}(\alpha t)}, \end{aligned} \tag{4.48}$$

matching the ones in (2.12), assuming $\eta = 2h$. Given how $\{\phi_n(t)\}$ match the ones obtained by solving the Schrödinger equation using the above $\{b_n\}$, we do not need to verify their validity. We

provide a brief outline of the procedure for completeness purposes. Starting from the time derivative of any ϕ_n, we write

$$\begin{aligned}\partial_t\phi_n(t) = \ldots = \frac{\tanh^n(\alpha t)}{\cosh^{2h}(\alpha t)}\sqrt{\frac{\Gamma(2h+n)}{n!\,\Gamma(2h)}}[\frac{n\alpha}{\tanh(\alpha t)\cosh^2(\alpha t)} - 2h\alpha\tanh\alpha t] = \\ = \phi_n\alpha[\frac{n}{\cosh(r)\sinh(r)} - 2h\tanh(r)],\end{aligned} \tag{4.49}$$

where we have set $\alpha t = r$. It is straightforward to show that the two terms in (1.1) can be written as

$$\begin{aligned}b_n\phi_{n-1}(t) = \frac{\alpha\phi_n}{\tanh(r)}n, \quad -b_{n+1}\phi_{n+1}(t) = \alpha\phi_n\tanh(r)(2h+n), \\ b_n\phi_{n-1}(t) - b_{n+1}\phi_{n+1}(t) = \alpha\phi_n(t)[\frac{n}{\tanh(r)} - n\tanh(r) - 2h\tanh(r)] = \\ = \ldots = \phi_n\alpha[\frac{n}{\sinh(r)\cosh(r)} - 2h\tanh(r)],\end{aligned} \tag{4.50}$$

completing the verification. These probability amplitudes, when squared, form the negative binomial distribution with probability of success $\frac{1}{\cosh^2(\alpha t)}$,

$$\begin{aligned}p_n(t) = |\phi_n(t)|^2 = \frac{(2h+n-1)!}{n!\,(2h-1)!}\frac{\tanh^{2n}(\alpha t)}{\cosh^{4h}(\alpha t)} = \\ = \frac{(2h+n-1)!}{n!\,(2h-1)!}(1 - \frac{1}{\cosh^2(\alpha t)})^n(\frac{1}{\cosh^2(\alpha t)})^{2h}.\end{aligned} \tag{4.51}$$

We retrieved the correct auto-correlation function with $\phi_0(t)$ in

$$C(t) = \frac{1}{\cosh^{2h}(\alpha t)}. \tag{4.52}$$

Calculating the complexity here requires a few slightly more intricate steps than before. The process goes as follows,

$$\begin{aligned}K_{\mathcal{O}} = \sum_{n=0}^{\infty} n|\phi_n(t)|^2 = \sum_{n=0}^{\infty} n\frac{(2h+n-1)!}{n!\,(2h-1)!}\frac{\tanh^{2n}(\alpha t)}{\cosh^{4h}\alpha t} = \ldots = \\ = \frac{\tanh^2(\alpha t)}{\cosh^{4h}(\alpha t)}\sum_{n=0}^{\infty} n\frac{(2h+n-1)!}{n!\,(2h-1)!}x^{n-1} = \frac{\tanh^2(\alpha t)}{\cosh^{4h}(\alpha t)}\frac{d}{dx}(f(x)),\end{aligned} \tag{4.53}$$

where we have defined $x = \tanh^2(\alpha t)$ and

$$f(x) = \sum_{n=1}^{\infty}\frac{(2h+n-1)!}{n!\,(2h-1)!}x^n = \sum_{n=0}^{\infty}\frac{(2h+n-1)!}{n!\,(2h-1)!}x^n - 1 = \frac{1}{(1-x)^{2h}} - 1, \tag{4.54}$$

thanks to the generalized binomial theorem. With this, we can finally write,

$$\begin{aligned}K_{\mathcal{O}} = \frac{\tanh^2(\alpha t)}{\cosh^{4h}(\alpha t)}2h(1-\tanh^2(\alpha t))^{-2h-1} = \\ 2h\frac{\tanh^2(\alpha t)}{\cosh^{4h}(\alpha t)}(\cosh^{4h+2}(\alpha t)) = 2h\sinh^2(\alpha t).\end{aligned} \tag{4.55}$$

We have managed to reach the result in (2.13) through this alternative approach. Generalizing to state complexity produces interesting results. The Hamiltonian in this case becomes

$$H = \alpha(L_{-1} + L_1) + \gamma L_0 + \delta I, \tag{4.56}$$

with the final result for the complexity reading

$$K_\psi = \frac{2h}{\sqrt{1 - \frac{\gamma^2}{4\alpha^2}}} \sinh^2(\alpha t \sqrt{1 - \frac{\gamma^2}{4\alpha^2}}). \tag{4.57}$$

Comparing with (4.34), we observe the similarity in the inclusion of a multiplication factor in the same place. However, the existence of the minus sign here implies that the effect of including a_n is not simply quantitative. Specifically, for $\gamma > 2\alpha$, the square root is imaginary making the complexity periodic in time. A real root gives a result similar to (4.55) while $\gamma = 2\alpha$ is an edge case for which we obtain quadratic growth of K_ψ in time. This analysis requires detailed manipulations to be properly defined and these results can be correlated to the TFD state of the harmonic oscillator. The reader is referred to the original source of these results, [14].

All that remains is examining the behavior of the geometric aforementioned quantities for this system. We start by determining the Fubini-Study metric, assuming the normalization condition $\langle z|z\rangle = (1 - |z|^2)^{-2h}$ to make our calculations easier.

$$\begin{aligned} |dz, h\rangle &= \sum_{n=0}^{\infty} n z^{n-1} \sqrt{\frac{\Gamma(2h+n)}{n!\,\Gamma(2h)}}\, |h, n\rangle\, dz, \\ \langle dz|dz\rangle = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} n z^{n-1} m z^{*m-1} &\sqrt{\frac{\Gamma(2h+n)}{n!\,\Gamma(2h)}} \sqrt{\frac{\Gamma(2h+m)}{m!\,\Gamma(2h)}}\, \langle h, m|h, n\rangle\, dz dz^* = \\ &= \cdots = \frac{2h dz dz^*}{(1-|z|^2)^{2h+1}} [\frac{|z|^2(2h+1)}{(1-|z|^2)} + 1]. \end{aligned} \tag{4.58}$$

The complex conjugate parts are derived in a similar manner,

$$\begin{aligned} \langle dz|z\rangle = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} m (z^*)^{m-1} z^n &\sqrt{\frac{\Gamma(2h+n)}{n!\,\Gamma(2h)}} \sqrt{\frac{\Gamma(2h+m)}{m!\,\Gamma(2h)}}\, \langle h, m|h, n\rangle\, dz^* = \ldots = \\ &= \frac{2h z dz^*}{(1-|z|^2)^{2h+1}}, \\ \langle z|dz\rangle &= \frac{2h z^* dz}{(1-|z|^2)^{2h+1}}. \end{aligned} \tag{4.59}$$

Combining equations (4.58) and (4.59) and taking into account the normalization condition, we finally get the line element,

$$\begin{aligned} ds^2_{FS} = \ldots &= \frac{2h}{(1-|z|^2)} [1 + \frac{|z|^2(2h+1)}{(1-|z|^2)} - \frac{2h|z|^2}{(1-|z|^2)}] dz dz^* = \\ &= \frac{2h dz dz^*}{(1-|z|^2)^2}, \end{aligned} \tag{4.60}$$

which is the usual Poincare metric on the hyperbolic disc, used to model two-dimensional hyperbolic geometry. This result does not surprise us, given our analysis in 3.4. We can write the line element using the re-parametrization in (3.64),

$$\begin{aligned} dz &= \frac{\partial z}{\partial \rho} d\rho + \frac{\partial z}{\partial \phi} d\phi = \ldots = e^{i\phi}\left(\frac{1}{2\cosh^2\left(\frac{\rho}{2}\right)} d\rho + i \tanh\left(\frac{\rho}{2}\right) d\phi\right), \\ dz^* &= \frac{\partial z^*}{\partial \rho} d\rho + \frac{\partial z^*}{\partial \phi} d\phi = \ldots = e^{-i\phi}\left(\frac{1}{2\cosh^2\left(\frac{\rho}{2}\right)} d\rho - i \tanh\left(\frac{\rho}{2}\right) d\phi\right). \end{aligned} \tag{4.61}$$

allowing us to rewrite (4.60) as

$$ds^2_{FS} = \frac{h}{2}(d\rho^2 + \sinh^2 \rho d\phi^2). \tag{4.62}$$

This form of the metric, though less recognizable in the literature, will help us in the calculations. For starters, the complex variable ξ corresponds to $\rho = 2\alpha t, \phi = \frac{\pi}{2}$, which is a geodesic in this metric, completing the observation for the time evolution of $|O(t))$ and the orbit in the coherent state phase space in all of our examples. Additionally, the volume traced by this orbit is given by,

$$V_t = \int_0^{\rho} \int_0^{2\pi} \sqrt{det(ds_{FS})}\, d\phi\, d\rho' = \int_0^{2\alpha t} \int_0^{2\pi} \frac{h}{2} \sinh(\rho)\, d\phi\, d\rho = \pi h(-1 + \cosh(2\alpha t)) = \pi K_{\mathcal{O}}, \tag{4.63}$$

adding further evidence to our claim. Finally, the Ricci scalar for this metric turns out to be

$$R = -\frac{4}{h}. \tag{4.64}$$

This result is important for two main reasons. Firstly, we can see that, at least in the context of our examples, negative curvature in the Riemannian manifold associated with the states appeared when we were studying a chaotic system, thus providing a potential way to distinguish systems with such properties. Also, this correlation between negative curvature in the information metric and chaos has already been studied in a notable body of work.

Appendix A

GNS Construction Details

A.1 Linear algebra and functional analysis aspects

Handling abstract algebra constructs such as von Neumann algebras, factors, etc. in the analysis of subsection 1.3.1 requires thorough knowledge of some foundational concepts of Vector Spaces, Hilbert Spaces and Group Representation Theory. A brief rundown is given below.

In the language of Quantum Mechanics, systems are described by vectors belonging to Hilbert Spaces. To understand those, we first define a Vector space[9],

Definition 8 *A set* $\{|x\rangle, |y\rangle, ...etc\}$*, on which two operations* $+$ *(addition) and* $\cdot$ *(multiplication) are defined is called a Linear Vector Space* $\mathcal{V}$ *if the following axioms hold:*

(i) it is closed under linear combination over the complex or real numbers, i.e. for any $|x\rangle, |x\rangle \in \mathcal{V}$ *and* $\alpha, \beta \in \mathbb{C}$ *or* $\mathbb{R}$ *then*

$$\alpha |x\rangle + \beta |y\rangle \in \mathcal{V} \tag{A.1}$$

(ii) There exists a null vector $|0\rangle$*, such that*

$$|x\rangle + |0\rangle = |x\rangle \in \mathcal{V} \tag{A.2}$$

(iii) For every $|x\rangle \in \mathcal{V}$*, there exists a* $|-x\rangle \in \mathbb{V}$ *such that*

$$|x\rangle + |-x\rangle = |0\rangle \tag{A.3}$$

(iv) The operation x *commutative and associative, i.e.*

$$|x\rangle + |y\rangle = |y\rangle + |x\rangle$$

$$(|x\rangle + |y\rangle) + |z\rangle = |x\rangle + (|y\rangle + |z\rangle) \equiv |x\rangle + |y\rangle + |z\rangle \tag{A.4}$$

(v) $1 \cdot |x\rangle = |x\rangle$

(vi) Multiplication by a number is associative, i.e.

$$\alpha \cdot |\beta x\rangle = (\alpha\beta)\, |x\rangle \equiv |x\rangle\, (\alpha\beta) \tag{A.5}$$

(vii) The two operations satisfy the distributive properties:

$$\alpha \cdot (|x\rangle + |y\rangle) = |x\rangle \alpha + |y\rangle \beta and$$

$$(\alpha + \beta) \cdot |x\rangle = |x\rangle \alpha + |x\rangle \beta \tag{A.6}$$

A very important concept that enriches Vector Spaces with a plethora of important properties is that of the *inner (scalar) product.*

Definition 9 *A vector space endowed with an inner product mapping any pair of elements* $|x\rangle, |y\rangle \in \mathcal{V}$ *satisfying the following properties*

(i)

$$\langle x|y\rangle = \langle y|x\rangle^*$$

(ii)

$$\langle ax_1 + bx_2|y\rangle = a^* \langle x_1|y\rangle + b^* \langle x_2|y\rangle \tag{A.7}$$

(iii)

$$|\langle x|x\rangle|^2 \geq 0,$$

(the equation holding iff $|x\rangle = 0$*)*

is called an inner product space.

The inner product on a Vector Space $\mathcal{V}$ is a special type of *linear functional*, i.e. a linear transformation from $\mathcal{V}$ to $\mathbb{C}$. The fact that every element in the space of linear functionals on $\mathcal{V}$, usually denoted as $\tilde{\mathcal{V}}$ and called the *Dual Space*, can be associated with the inner product with a vector $|x\rangle$ on $\mathcal{V}$ allows for the establishment of an isomorphism between a Vector Space and its Dual. This one-to-one correspondence between the two spaces is of great significance for the foundations of state representation, observable quantities, transformations, measurements, etc.

This finally leads us to the definition of the Hilbert Space,

Definition 10 *A Hilbert space is a real or complex inner product space that is also complete with respect to the norm defined by the inner product.*

A metric space is "complete" if every Cauchy sequence of points in the space converges to a point in the space. A Cauchy sequence is a sequence of points such that the distance between any two points later in the sequence can be made as small as desired[1]. See [4] for a more rigorous treatment.

[1] finite-dimensional vector spaces automatically satisfy the completeness requirement.

A.2 Density Matrix Formalism in Quantum Mechanics

The *Density Operator* constitutes an alternative but mathematically equivalent formalism for Quantum Mechanics which generalizes the notion of the state of a quantum system (This part of the appendix was written using ([19],[29],[30]). Instead of the state vector $|\boldsymbol{\psi}\rangle$, one can instead use a Hermitian Operator $\hat{\boldsymbol{\rho}}$ from the corresponding Hilbert Space to extract the maximum amount of information about the system. The Density Matrix provides a more convenient and in many cases natural way to describe the characteristics of certain systems such as, but not limited to, those where the exact state of the system is not known. A brief overview is provided below

A core aspect of the density matrix formalism is the existence of *mixed states*. Mixed states, on the other hand, describe a quantum system with an ensemble of pure states say p_i,$|\psi_i\rangle$. The system itself of course is described by a single state. We, however, only have a probability distribution due to our ignorance of the system.

It is crucial to understand that the p_i's are not the usual probability amplitudes c_i used when describing a state as a linear combination of other states (coherent superposition), but they represent the "classical" probabilities (incoherent superposition), obviously obeying the condition

$$\sum_i p_i = 1 \tag{A.8}$$

Definition 11 *Initially, we define the Density Operator for a system in mixed state p_i,$|\psi_i\rangle$ as*

$$\hat{\tilde{\rho}} \equiv \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right| = \sum_i p_i \hat{P}_i \tag{A.9}$$

Obviously, the respective operator for a pure state is simply the Projection operator of the $|\psi\rangle$ which describes the system,

$$\hat{\rho} = \left|\psi\right\rangle \left\langle\psi\right| \tag{A.10}$$

The most important properties of these operators are listed below. These are not only useful for making calculations with the density matrix but also provide the bedrock for an independent reformulation of the definition.

- Density Matrices which belong to pure states are idempotent whereas it is fairly straightforward to show that their mixed counterparts are not,

$$\hat{\rho}^2 = \hat{\rho}, \hat{\tilde{\rho}}^2 = (..) = \sum_i p_i^2 \hat{P}_i \neq \hat{\tilde{\rho}} \tag{A.11}$$

- The Trace of a Density Operator is necessarily equal to 1. This property is a reflection of the normalization[2] of a state and of the conservation of probability as aforementioned.

$$Tr(\hat{\tilde{\rho}}) = Tr(\hat{\rho}) = 1 \tag{A.12}$$

- The Trace of the square of a Density Operator is necessarily less than or equal to 1. The equality holds strictly for pure states.

$$Tr(\hat{\tilde{\rho}}^2) < 1, Tr(\hat{\rho}^2) = Tr(\hat{\rho}) = 1 \tag{A.13}$$

[2]Omitting normalization requires dividing the expression for expectation values etc. with a factor $\mathrm{Tr}(\hat{\rho})$

This differentiation is crucial for studying systems using the Density Matrix Formulation as it acts as a criterion to determine the purity of a state.

- Density Matrices are always positive (and thus Hermitian) Operators.The following equality holds for any $|\varphi\rangle$,

$$\langle\varphi|\hat{\hat{\rho}}|\varphi\rangle \geq 0 \tag{A.14}$$

This property, along with the Trace of the Density Matrix gives rise to the following crucial theorem

Theorem 12 (Characterization of density operators) *An operator $\hat{\hat{\rho}}$ is the density operator associated to some ensemble $\{p_i,|\psi_i\rangle\}$ if and only if it satisfies the conditions:*

(i) $\hat{\hat{\rho}}$ has a trace equal to one

(ii) $\hat{\hat{\rho}}$ is a positive operator

With this, the Density Operator is given a characterization intrinsic to itself. Any operator that is positive and has Trace equal to one is defined to be a Density Operator. The time evolution of a Density Matrix can be shown to be

$$i\hbar\frac{\partial\hat{\hat{\rho}}}{\partial t} = [\hat{H}, \hat{\hat{\rho}}] \tag{A.15}$$

Where $\hat{H}$ is the corresponding system's Hamiltonian. This equation is known as the *von Neumann* equation and can be easily identified as the quantum analogue of Liouville's Theorem regarding the evolution of a Hamiltonian flow of states (rEEf melet). The Density Operator owes its name to the apparent similarities between the classical phase space density and itself.

The expectation value of a given observable represented by a Hermitian operator, say $\hat{A}$, is given by the following formula,

$$\langle\hat{A}\rangle = \mathrm{Tr}(\hat{\hat{\rho}}\hat{A}) \tag{A.16}$$

This general expression for the expectation value can also be set as the state vector-independent definition of the Density Matrix. Accordingly, the total probability of measuring a system at an eigenstate a_n is given by

$$P(a_n) = \mathrm{Tr}(\hat{\hat{\rho}}\hat{P}_n) \tag{A.17}$$

This brief section is not an exhaustive overview by any means, we simply reach a few important needed results given by the equations (A.15) and (A.16). Following the *correspondence principle* of Quantum Mechanics, both these equations are the quantum counterparts of the classical equations in Hamiltonian mechanics, replacing Poisson Brackets with Commutators and adding the multiplicative factor $i\hbar$ and Integration over the phase space with taking the Trace. (see [19] for more information).

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