Doctorate of Philosophy

Schrödinger's Catwalk

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LISTINGS

ACRONYMS

ML	machine learning. 11
QM	quantum mechanics. 2–4, 6, 7, 13, 23
QMLA	Quantum Model Learning Agent. vi

GLOSSARY

expectation value	Average outcome expected by measuring an observable of a quantum system many times, Section 1.2.1.. i, 2, 9
likelihood	Value that represents how likely a hypothesis is.. 9

Part I

CONTEXTUAL REVIEW

1 QUANTUM THEORY

Quantum mechanics (QM) – the study of nature's fundamental processes, manifest in its smallest particles – has been at the forefront of physics since the early 20$^{\text{th}}$ century [1]. Advances in theoretical understanding of quantum mechanical systems in the first half of the century [2, 11] led to novel technologies[1] in the second half [3], which came to underpin all modern information and communications technologies. The 21$^{\text{st}}$ century, on the other hand, is poised to see the development of technologies which *deliberately* exploit the most intricate quantum processes in order to yield some non-classical advantage. This thesis focuses on the application of machine learning to the characterisation of quantum mechanical systems through use of quantum simulators, so it is pertinent first to introduce the vocabulary of QM.

QM is central to the topics described in this thesis, however it is impossible to succinctly capture the entire discipline; in this chapter we will only introduce concepts utilised throughout. For completeness, we elucidate some fundamental topics of linear algebra and quantum theory in Appendix A, but consider them too cumbersome to include in the main text. For a more complete and general introduction to QM, the reader is referred to [4, 5]. Likewise, in this chapter we quickly summarise the key aspects of quantum computation, but for further details, we recommend unfamiliar readers to consult [6], while a more complete discussion is presented in [7].

1.1 QUANTUM MECHANICS

At any time, a quantum system, Q, can be described by its *wavefunction*, $\Psi(t)$, which contains all information about Q. In analogy with Newton's second law of motion, which allows for the determination of a particle's position at any time, $\vec{r}(t)$, given its conditions such as mass and acceleration as well as its initial position, $\vec{r}(t_0)$, quantum *equations of motion* can describe the evolution of Q through its wavefunction [8]. One proposal[2] for the equation of motion to describe the evolution of the wavefunction under known conditions, i.e. determining $\Psi(t)$ from $\Psi(t_0)\ \forall t > t_0$, is *Schrödinger 's equation* [4, 9, 10].

Although the Schrödinger equation is a *postulate* of QM (see Appendix A.2), let us introduce it in reverse order to elucidate its meaning, following [5]. We have yet to describe the structure of the wavefunction, which we will do in Section 1.2, but here we will represent wavefunctions using *Dirac notation* (Appendix A.6), and can think of them generically as vectors, i.e. $\Psi(t) \to |\psi(t)\rangle$. Suppose we have two such wavefunctions, $|\phi(t)\rangle, |\psi(t)\rangle$ which are functions of time $t > t_0$.

1 Colloquially referred to as *Quantum 1.0*.

2 The most noteworthy alternative formalism, due to Heisenberg [11], was shown equivalent to the Schrödinger picture described here.

We start with the assumption that *similarity* is conserved between two wavefunctions, if they undergo the same transformation (Susskind's *minus first* law of classical mehcanics [5])

$$\langle \phi(t)|\psi(t)\rangle = \langle \phi(t_0)|\psi(t_0)\rangle \tag{1.1}$$

Then, assuming some equations of motion capture the dynamics of Q, there exists some evolution operator, $\hat{U}(t)$, which deterministically maps $|\psi(t_o)\rangle$ to $|\psi(t)\rangle$.

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi(t_0)\rangle\,, \tag{1.2}$$

where we have not yet imposed any restrictions on $\hat{U}$. Combining Eqs. (1.1) to (1.2),

$$\begin{aligned} \langle \phi(t)|\psi(t)\rangle &= \langle \phi(t_0)|\hat{U}^\dagger\hat{U}|\psi(t_o)\rangle \\ \Rightarrow \langle \phi(t_0)|\hat{U}^\dagger(t)\hat{U}(t)|\psi(t_o)\rangle &= \langle \phi(t_0)|\psi(t_0)\rangle \\ \Rightarrow \hat{U}^\dagger(t)\hat{U}(t) &= \hat{\mathbb{1}} \quad \forall t, \end{aligned} \tag{1.3}$$

where the result $\hat{U}^\dagger(t)\hat{U}(t) = \hat{\mathbb{1}}$ is the condition for *unitarity* (Appendix A.5), so we can claim the quantum wavefunction evolves unitarily.

By construction, we require that after zero time, i.e. $t = t_0$, the wavefunction has not changed:

$$\begin{aligned} |\psi(t = t_0)\rangle = \hat{U}(t = t_0)\,|\psi(t_0)\rangle = |\psi(t_0)\rangle \\ \Rightarrow \hat{U}(t = t_0) = \hat{\mathbb{1}}. \end{aligned} \tag{1.4}$$

Without loss of generality we can set $t_0 = 0$, giving $\hat{H}(0) = \hat{\mathbb{1}}$. Then, let us consider an infintesimally small time increment $t_0 + \epsilon$: again, take $t_0 = 0$ so $t = \epsilon$, where $\epsilon \gg \epsilon^2$.

We can say

$$\hat{U}(\epsilon) = \hat{\mathbb{1}} + \mathcal{O}(\epsilon), \tag{1.5}$$

which merely suggests that the time evolution operator at very small time is very close to the identity, with some small displacement proportional to the time, which must be an operator to act on the wavefunction (vector). We suppose the form of the offset, so we can write

$$\hat{U}(\epsilon) = \hat{\mathbb{1}} - \epsilon\left(\frac{i}{\hbar}\hat{H}_0\right), \tag{1.6}$$

where the inclusion of the phase $-i$ is arbitrary, and we have named as $\hat{H}_0/\hbar$ the operator by which the time evolution differs from the identity. In other words, the operator $\hat{H}_0$ is generically the generator of the evolution/dynamics of Q: any difference between $|\psi(t_0)\rangle$ and $|\psi(t)\rangle$ arises

solely due to $\hat{H}_0$. So far there is no restriction on $\hat{H}_0$, except that it must be of the same dimension as the Hilbert space in question. Recalling the unitarity condition, however:

$$\begin{aligned} \hat{U}^\dagger(\epsilon)\hat{U}(\epsilon) &= \hat{\mathbb{1}} \\ \Rightarrow \left(\hat{\mathbb{1}} + \frac{i}{\hbar}\epsilon\hat{H}_0^\dagger\right)\left(\hat{\mathbb{1}} - \frac{i}{\hbar}\epsilon\hat{H}_0,\right) &= \hat{\mathbb{1}} \\ \Rightarrow \hat{\mathbb{1}} + \frac{i}{\hbar}\epsilon(\hat{H}_0^\dagger - \hat{H}_0) + \mathcal{O}(\epsilon^2) &= \hat{\mathbb{1}} \\ \Rightarrow (\hat{H}_0^\dagger - \hat{H}_0) &= 0 \\ \Rightarrow \hat{H}_0^\dagger &= \hat{H}_0. \end{aligned} \tag{1.7}$$

Eq. (1.7) results in the condition for *Hermiticity*, meaning that $\hat{H}_0$ is an observable of Q. In fact, this is the *Hamiltonian* of the system, described in the next section.

We can also use the infintesimal evolution to see

$$\begin{aligned} |\psi(t)\rangle &= \hat{U}(t)\,|\psi(t_0)\rangle \\ \Rightarrow |\psi(\epsilon)\rangle &= \hat{U}(\epsilon)\,|\psi(t_0)\rangle \\ \Rightarrow |\psi(\epsilon)\rangle &= \left(\hat{\mathbb{1}} - \epsilon\frac{i}{\hbar}\hat{H}_0\right)|\psi(t_0)\rangle \\ \Rightarrow |\psi(\epsilon)\rangle &= |\psi(t_0)\rangle - \epsilon\frac{i}{\hbar}\hat{H}_0\,|\psi(t_0)\rangle \\ \Rightarrow \frac{|\psi(\epsilon)\rangle - |\psi(t_0)\rangle}{\epsilon} &= -\frac{i}{\hbar}\hat{H}_0\,|\psi(t_0)\rangle \end{aligned} \tag{1.8}$$

Taking the limit as $\epsilon \to 0$, the left hand side of the final line of Eq. (1.8) is the definition of the derivative of the wavefunction, $\frac{d|\psi(t)\rangle}{dt}$. Taken together, we have

$$\frac{d}{dt}\,|\psi(t)\rangle = \frac{-i}{\hbar}\hat{H}_0\,|\psi(t_0)\rangle\,, \tag{1.9}$$

where $|\psi(t)\rangle$ is the wavefunction at time t, $|\psi(t_0)\rangle$ is the wavefunction at t_0, such that $t > t_0$, $\hbar = 1.054 \times 10^{-34}$ is the reduced Planck constant and $\hat{H}_0$ is the *Hamiltonian* of Q. For brevity we generally refer to $t_0 = 0$, and absorb $\hbar$ into $\hat{H}_0$, which will later manifest in the Hamiltonian scalar parameters. Eq. (1.9) is the most general form of *Schrödinger equation*, otherwise known as the *time-dependent* Schrödinger equation; we include it as Postulate 6 when describing the fundamentals of QM (Appendix A.2), since it can be seen as an irreducible equation of motion which is essential to the description of quantum systems.

As mentioned, we presented this argument in a nonstandard order: we started with Eq. (1.2), which we can now consider the *solution* to the Schrödinger , specifically

$$\begin{aligned} |\psi(t)\rangle &= \hat{U}(t)\,|\psi(0)\rangle \\ \hat{U}(t) &= e^{-i\hat{H}_0 t} \end{aligned} \tag{1.10}$$

which describes the unitary evolution of the state according to the unitary evolution operator, $\hat{U}(t)$.

1.1.1 *Hamiltonians*

In the previous section we introduced the Hamiltonian[3] of Q as the generator of its time evolution dynamics; Hamiltonians are of primary importance in this thesis, so it is worth pausing to consider their physical meaning. We saw in Eq. (1.7) that $\hat{H}_0$ is Hermitian, meaning that the operator is physically observable according to Postulates 2 to 3 of quantum mechanics (Appendix A.2). The Hamiltonian operator captures the energy of Q: the eigenvalues of the observable $\hat{H}_0$ are the permitted energy levels of the system.

The quantum Hamiltonian, $\hat{H}_0$ is analogous to the classical Hamiltonian, insofar as it captures all the interactions of a given system which contribute to its time evolution. Knowing the classical Hamiltonian and the initial conditions – position and momentum – Hamilton's equations of motion allow for the calcaultion of those quantities for the particle in question an infintesimal time later [12]. Likewise, knowledge of the initial wavefunction, $|\psi(t_0)\rangle$, and the system's quantum Hamiltonian, $\hat{H}_0$, the quantum equations of motion – Schrödinger 's equation, Eq. (1.9) – permits the calculation of the wavefunction at later times. As such the Hamiltonian must consist of all processes which influence the evolution of Q; we will later break the Hamiltonian into independent *terms* which each correspond to unique physical interactions Q is subject to, **??**. We can think that each process/interaction Q undergoes contributes to its total energy, giving intuition as to why its eigenvalues are the energy levels.

Hamiltonians describe *closed* quantum systems, i.e. where *all* processes and interactions which influence Q are accounted for. Realistic quantum systems are influenced by a myriad of proximal systems, and it is therefore infeasible to analytically account for them all. Instead, *open* quantum systems' dynamics are described by Lindbladian operators, which encompass the Hamiltonian form. The Lindblad master equation is a generalisation of the Schrödinger equation, providing the equation of motion for open quantum systems [13, 14]. In this thesis we only consider closed models for quantum systems; for meaningful impact of the techniques presented here, it will be necessary to expand them to account for the open system dynamics of realistic experiments. We do, however, show initial progress towards this endeavour by modelling a physical system through a closed Hamiltonian, **??**.

1.2 QUANTUM INFORMATION

We have not yet described the structure of the wavefunction, instead performing the previous analysis with respect to some arbitrary objects. The wavefunction for a physical system, Q,

3 Aside: the author shares a hometown with the mathematician for whom it is named, William Rowan Hamilton. It is hoped that, after another 150 years, the next physicist from Trim, Co. Meath, Ireland might profitably use knowledge of Hamiltonians on a quantum computer (QC).

is also known as its *state*, a complete mathematical description of the system [15]. States are vectors[4], $|\psi\rangle \in \mathbb{C}$; the valid state space for Q is its *Hilbert space*, $\mathcal{H}$, which is a generalisation of Euclidean vector space, i.e. $|\psi\rangle \in \mathcal{H}$. The Hilbert space defines the overlap between any two vectors as the *inner product*, $\langle\psi|\phi\rangle$ (Appendix A.1). In general[5], a state can be seen as a *superposition* across its eigenstates, $\{|v_i\rangle\}$.

$$|\psi\rangle = \sum_i \alpha_i |v_i\rangle \tag{1.11a}$$

$$\text{subject to} \quad \sum_i |\alpha_i|^2 = 1, \quad \alpha_i \in \mathbb{C}. \tag{1.11b}$$

The cornerstone of QM is the effect of *measurement* on quantum systems: in general Q can be seen as occupying a multitude of eigenstates as in Eq. (1.11a), observing the system forces $|\psi\rangle$ into a definite occupation of a single eigenstate, where the *probability* that it is measured in each eigenstate $|v_i\rangle$ is given by $|\alpha_i|^2$, according to Born's rule [2]. α_i are hence named *probability amplitudes* since they inform the probability of measuring the corresponding eigenstate.

For an ideal[6] single particle, when the state, Eq. (1.11a), has two available eigenstates, e.g. the horizontal (H) and vertical (V) polarisation of a single photon, we can designate Q as a two-level computational platform, called a *qubit*, analogous to the workhorse of classical computation, the bit. A qubit's state vector can then be written as a sum over the two available eigenstates, where we assign vectors to the eigenstates as $|H\rangle = |v_1\rangle, |V\rangle = |v_2\rangle$.

$$|\psi\rangle = \alpha_1 |v_1\rangle + \alpha_2 |v_c\rangle, \tag{1.12}$$

where $\alpha_i \in \mathbb{C}$ and $|\alpha_1|^2 + |\alpha_2|^2 = 1$.

In general, a qubit requires two orthogonal state vectors to define a *basis*; we list a number of the usual special cases:

$$X\text{-basis} = \begin{cases} |+\rangle = \dfrac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ |-\rangle = \dfrac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \end{cases} \tag{1.13a}$$

$$Y\text{-basis} = \begin{cases} |i\rangle = \dfrac{1}{\sqrt{2}}(|0\rangle + i|1\rangle) \\ |-i\rangle = \dfrac{1}{\sqrt{2}}(|0\rangle - i|1\rangle) \end{cases} \tag{1.13b}$$

4 We immediately use Dirac notation to represent the state; it is defined in Appendix A.6.
5 We expand on this brief description in Appendix A.3.
6 Here we restrict to the space of ideal, *logical* qubits. In reality, physical qubits are beset by errors, demanding error correction routines such that multiple particles are needed attain a single logical qubit.

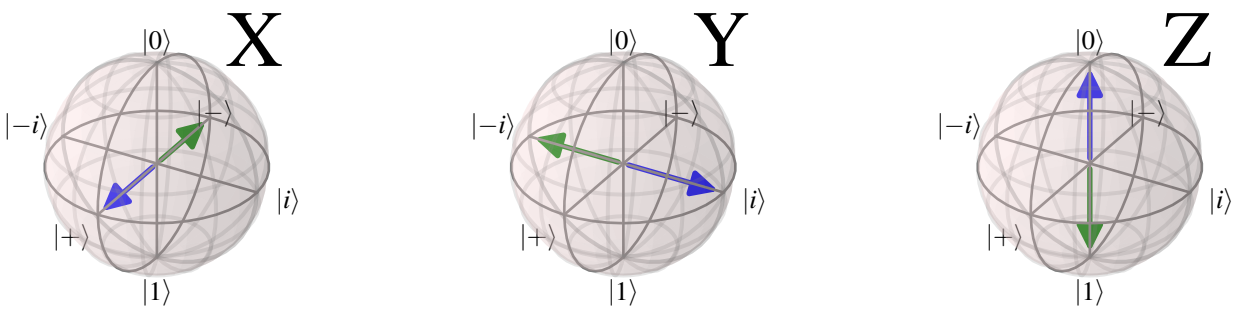

Figure 1.1: Bloch sphere representation of bases, where each pair of basis states are shown by blue and green vectors. The X-basis has basis vectors $\{|+\rangle, |-\rangle\}$; Y-basis has $\{|i\rangle, |-i\rangle\}$ and Z-basis has $\{|0\rangle, |1\rangle\}$.

$$Z\text{-basis} = \begin{cases} |0\rangle \\ |1\rangle \end{cases} \tag{1.13c}$$

A visual tool for representing qubits is the *Bloch sphere*, which presents orthogonal basis states as parallel unit vectors of opposite direction: we show each of the bases of Eq. (1.13) in Fig. 1.1.

We can make two remarks about basis states for a single qubit:

- Basis states from one basis can be seen as superpositions with respect to alternative bases
  - e.g. in the X-basis, $|+\rangle$ is a basis vector, but in the Z-basis, $|+\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$ is a superposition over basis vectors.
- Bases are local rotations of each other
  - rotating the X-basis through an angle $\pi/2$ about the Y-axis results in the Z-axis.

As we alluded to in Section 1.1: by imposing mathematical structure on quantum systems' states, i.e. representing Q as a state vector at any time, then operations which alter the state of the system must be matrices. In general an n-dimensional vector is rotated by an $n \times n$ matrix; here one-qubit oeprators have the effect of rotating the state vector, which we can again visualise on the Bloch sphere. By thinking of qubits generically with respect to any basis, we can encode information in the qubit's amplitudes, by performing operations (or gates) upon the qubit, we change the information, i.e. we can design information processing techniques leveraging the infrastructure – states, operators and measurement – of QM.

We introduce a set of speical one-qubit operators, the *Pauli matrices*,

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{1.14a}$$

$$\hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{1.14b}$$

$$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.14c}$$

The Pauli matrices are used to define rotation operators about their respective axes, and hence are very useful: we can break *any* rotation of a qubit into rotations of various angles, θ, about the three axes of the Bloch sphere. Any single qubit operation can therefore be expressed as a product of the *rotation operators*, $\hat{R}_x, \hat{R}_y, \hat{R}_z$, exemplified in Fig. 1.2 and defined as

$$\hat{R}_w(\theta) = e^{-i\frac{\theta}{2}\hat{\sigma}_w} = \cos(\theta/2)\,\hat{\mathbb{1}} - i\sin(\theta/2)\,\hat{\sigma}_w. \tag{1.15}$$

The Pauli matrices are Hermitian, meaning they are observable. We can see that the eigenstates of $\hat{\sigma}_z$ are the Z-basis states: $\hat{\sigma}_z|0\rangle = |0\rangle$; $\hat{\sigma}_z|1\rangle = -|1\rangle$. Recalling the earlier claim that the two-level quantum system (e.g. H and V polarisation of a photon) can be mapped to eigenvectors[7] of an obserable operator to form a qubit, we term the Z-basis the *computational* basis. By defining the computational basis, we ground abstract computational reasoning in the physical realisation: anywhere throughout this thesis where the basis states $|0\rangle, |1\rangle$ are referenced, we mean the eigenstates of the physical axis which is defined as the Z-axis for the system in question. In the computational basis, then, a qubit can be specified as

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle. \tag{1.16}$$

The concepts of qubits representing quantum systems, as well as operators altering their states and measurement collapsing those states, extend straightforwardly to multipartite systems, by merging Hilbert spaces through tensor products, as we show in Appendix A.3.1. The cases where this is a simple mathematical exercise represent *pure* states; of course this leads to the more intricate topic of *mixed* states and entanglement, briefly described in **??**. In this thesis, however, we are concerned only with pure states, i.e. separable qubits. While single qubit states are spanned by the Pauli opeartors, multi-qubit states are spanned by the Pauli group, $\mathbb{G}$: n-qubit states are spanned by $\mathbb{G}_n = \left(\mathbb{C}^2\right)^{\otimes n}$.

1.2.1 *Expectation value*

Upon measurement, the state vector of Q has amplitude associated with only one eigenvector. On average, however, the eigenvector to which it would collapse encodes statistical insight on the state prior to measurement. In other words, if we prepared ψ and measured it – via some

7 The terms *eigenstate* and *eigenvector* are interchangeable, although it may be helpful to think of eigenstate as the physical manifestation (horizontal photon), and think of eigenvector as the logical manifestions ($|0\rangle$).

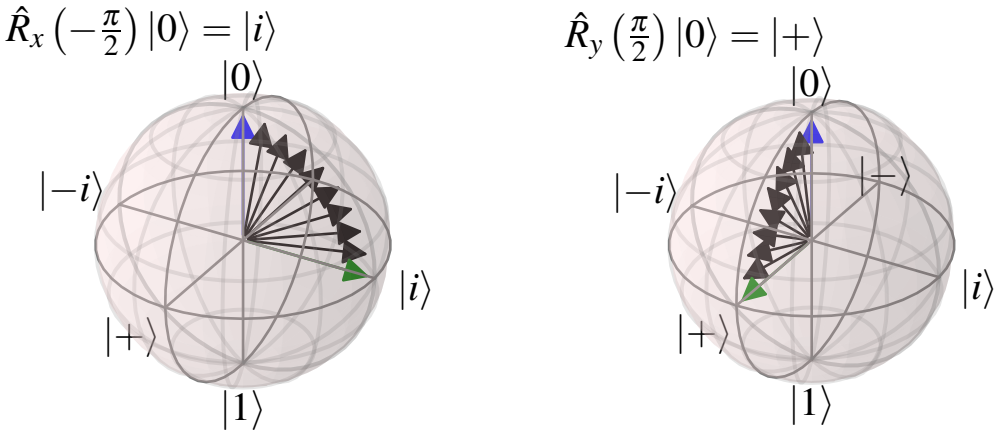

Figure 1.2: Rotations on Bloch sphere. The initial and final state are shown in blue and green respectively, while intermediate states are shown in black. **Left**, The Z-basis unit vector, $|0\rangle$, is rotated about the X-axis, resulting in the unit vector along the Y-axis. **Right**, The Z-basis unit vector, $|0\rangle$, is rotated about the Y-axis, resulting in the unit vector along the X-axis.

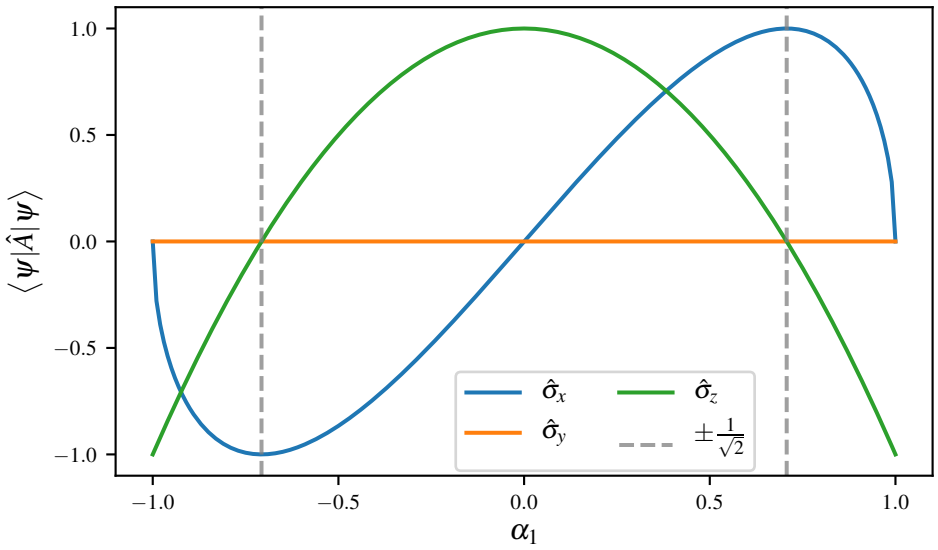

Figure 1.3: Expectation values of the observable $\hat{A}$ – here the Pauli matrices – for $|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle$. Coefficients are real, varying $\alpha_1 \in (-1, 1)$, such that $\alpha_0 = \sqrt{1-\alpha_1^2}$.

observable, $\hat{A}$ – and repeat the procedure N times, then as $N \to \infty$, the average outcome is the *expecatation value* for the system,

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = \sum_i \alpha_i \langle v_i | \hat{A} | v_i \rangle , \tag{1.17}$$

where $\langle \hat{A} \rangle$ is the expectation value (average) for the observable, A; $|v_i\rangle$ are the eigenvectors of $\hat{A}$, and $\alpha_i \in \mathbb{C}$ are the proability amplitudes associated with each $|v_i\rangle$ when the state ψ is represented as in Eq. (1.11a). We show some examples of expectation values for the observable Pauli matrices in Section 1.2.1.

An underlying theme of this thesis is to flip the usual logic: instead of using knowledge of the system to derive the expectation value, per Eq. (1.17), we will *estimate* expectation values, either through experiment or simulation, and use them to infer the structure of the observable. This trick enables machine learning routines to reverse engineer the processes Q is subject to, as we will describe in **??**. There is a subtlety to be aware of, however: in later chapters, we will make reference to the expectation value and *likelihood* almost interchangeably – these are distinct concepts that *sometimes* overlap, but not in all cases, as we explain in **??**.

1.3 QUANTUM SIMULATION AND COMPUTATION

Relying on the premise and language of quantum information processing – states, qubits, operators, measurements and expectation values – the growing field of *quantum technology* aims to exploit the non-classical statistics yielded by quantum systems in order to retrieve outcomes beyond the capability of their classical counterparts [16]. Applications range from enhanced sensing and metrology [17, 18], to highly-secure communication and cryptography protocols [19, 20, 21]. The initial motivation for the development of quantum technologies, however, was the observation that simulating nature at a quantum level would require exponential resources and is therefore only feasible given controllable quantum systems, which can accurately emulate the true dynamics [22, 23, 24, 25].

The notion of controlling quantum systems to mimic the dynamics of real quantum systems is tantamount to *quantum simulation* [26, 27]. In particular, simulating quantum systems is believed to be of interest for quantum chemistry [28, 29, 30], for example leading to advances in the simulation of molecular dynamics [31, 32]. More generally, however, this led to research into a wider domain of calculations called *quantum computation* which considers the information processing capability of controllable quantum systems beyond merely simulating quantum systems. Then, *universal quantum computers* (or, *quantum Turing machines*), assume access to *logical* qubits and operations (or *gates*) for the implementation of quantum circuits [33]. This ignited interest in *quantum algorithms* which provide some provable advantage [34, 35, 36, 37, 38]. Indeed, it was found that the space of problems addressible by such devices goes beyond the classical counterpart, suggesting there exists a class of quatum algorithms which can offer significant advantage over any feasible algorithm on classical hardware [39].

Of course, while the advances in algorithmic quantum computation promise huge impact, they are tempered by contemporary experimental constraints, which must deal with the reality that construction and control of quantum devices is a significant challenge. In constructing QCs and dealing with their output, we must account for physical effects which lead to errors, requiring expensive error mitigation schemes to be reliable [40, 41]. Furthermore, there are a number of criteria required before a QC can be deemed functional [42].

Any two-level quantum system can be used as a qubit; a range of platforms have emerged in attempts to fulfil the potential of quantum computation [43], among the most popular[8]:

- Photonic qubits (linear optical QCs) [44]
  - existing infrastructure for commercial production of photonics-based technologies suggests the relatively straightforward fabrication of integrated photonic devices at the scale of millions of degrees of freedom [45];
  - photons do not decohere so are useful for encoding information [46];
  - photons do not interfere [8, 47], so information processing must be mediated by non-trivial measurement schemes [48];
  - they are liable to a unique error mechanism – photon loss – necessitating novel quantum error correcting codes [49];
  - on-demand single photon generation has not yet been demonstrated, although there is significant progress in the area of photon generation [50].
- Superconducting qubits [51, 52]
  - relatively straightforward to control and couple with each other, enabling high-fidelity two-qubit gates, e.g. 99.7% reached in [53];
  - difficult to engineer substantial coherence times, although there has been significant recent progress [54, 55], e.g. $T_1 \sim \mathcal{O}(\text{ms})$ in [56];
  - require cryogenic temperatures [51];
  - arbitrary qubit connectivity at scale is yet to be demonstrated [52];
  - methods for the fabrication of medium-to-large scale devices required for fault tolerant quantum computation are not yet known [57].
- Ion traps [58, 59]
  - high two qubit gate fidelities, e.g. 99.9% in [60];
  - very high coherence times, e.g. $\mathcal{O}(10\ \text{min})$ in [61];
  - straightforward state preparation and readout, e.g. 99.99% readout fidelity in [62];
  - long gate-times, e.g. $\mathcal{O}(\mu\text{s})$ in [63];
  - uncertain scalability [64].

8 listed with their primary advantages and limitations.

The ever-increasing space of contenders has led to a growing eco-system for quantum software [65], promising a wide range of applications in the era of noisy intermediate scale quantum devices [66]. Following numerous proposoals [67], recent efforts have married state-of-the-art hardware with bespoke algorithms in order to achieve quantum advantage [68, 69]. Evidently there is vast effort in bringing quantum computational resources to reality; in this thesis, however, we are not concerned with the architecture underlying our presumed quantum simulator – we perform simulations only on classical hardware. In principle, however, any quantum simulator – universal or otherwise – capable of implementing the time evolution operator, Eq. (1.10), can be called upon as a co-processor by the algorithms presented.

Our restriction to classical resrouces leads to a few remarks:

- given access to a fault-tolerant QC/simulator, the algorithms described would enjoy an automatic exponential speedup:
  - the classical bottleneck is the calculation of the time evolution dynamics, Eq. (1.10), according to the matrix exponential, of dimension 2^n, where n is the dimension of the system;
  - it is believed that the same calculation can be performed in polynomial time on a QC [26].
- the results achieved in this thesis are limited by the capability of classical computers in simulating quantum systems
  - we study only up to 8-qubit systems, whereas it would be of interest to extend these methods to higher dimensions, which is expected to be feasible when reliable quantum simulators/computers are available.

The remit of this thesis – given these limitations – is therefore to robustly test the presented algorithms, and provide a benchmark achieved through classical facilities, against which the same algorithm can be run in conjunction with quantum hardware.

2

MACHINE LEARNING

Machine learning (ML) is the application of statistics, algorithms and computing power to discover meaning and/or devise actions from data. ML has become an umbrella term, encompassing the family of algorithms which aim to leverage computaters to learn without being explicitly programmed, as opposed to the more general , which seeks to make computers behave intelligently, admitting explicit programs to achieve tasks [70]. Its history is therefore imprecise since a number of early, apparently unrelated algorithms were proposed independently, which now constitute ML routines [71, 72]. Nevertheless, the field of ML has been advancing rapidly since the second half of the 20$^{\text{th}}$ century [73], especially recently due to the availability of advanced hardware such as graphics processing units (GPUs), facilitating significant progress through an ever-increasing aresnal of powerful open source software [74, 75, 76].

Throughout this thesis, we endeavour to combine known methods from the ML literature with capabilities of QCs[1]. Typical ML algorithms, which rely on central processing units (CPUs) or GPUs, are deemed *classical* machine learning, in contrast with quantum machine learning (QML), where QCs are central to processing the data. Similarly to the remit of Chapter 1, here we do not provide an exhaustive account of ML algorithms: rather, we describe only the algorithms which are used in later chapters, referring readers to standard texts for a wider discussion [73, 77]

2.1 CLASSICAL MACHINE LEARNING

- definition and aim(s)
- supervised
- unsupervised
- example algorithms and applications

2.2 QUANTUM MACHINE LEARNING

- distinctions
  - q data q hardware → pure QML
  - q data classical hardware → ml for q physics
  - classical data q hardware → q enhanced ml
  - classical data c hardware → wrong thesis (Section 2.1)
- examples/applications of QML

1 Or simulated QCs, in this thesis.

  - QNN, q svm,
- Remit of this thesis $\rightarrow$ ml for q physics
  - i.e. using data from quantum system and/or hardware but in conjunction with classical co-processor, for the study of quantum systems

[78]

APPENDIX

A

FUNDAMENTALS

There are a number of concepts which are fundamental to any discussion of QM, but are likely to be known to most readers, and are therefore cumbersome to include in the main body of the thesis. We include them here for completeness[1].

A.1 LINEAR ALGEBRA

Here we review the language of linear algebra and summarise the basic mathematical techniques used throughout this thesis. We will briefly recall some definitions for reference.

- Notation

Definition of	Representation
Vector (or *ket*)	$\|\psi\rangle$
Dual Vector (or *bra*)	$\langle\psi\|$
Tensor Product	$\|\psi\rangle \otimes \|\phi\rangle$
Complex conjugate	$\|\psi^*\rangle$
Transpose	$\|\psi\rangle^T$
Adjoint	$\|\psi\rangle^\dagger = (\|\psi\rangle^*)^T$

Table A.1: Linear algebra definitions.

The dual vector of a vector (ket) $|\psi\rangle$ is given by $\langle\psi| = |\psi\rangle^\dagger$.

The *adjoint* of a matrix replaces each matrix element with its own complex conjugate, and then switches its columns with rows.

$$M^\dagger = \begin{pmatrix} M_{0,0} & M_{0,1} \\ M_{1,0} & M_{1,1} \end{pmatrix}^\dagger = \begin{pmatrix} M^*_{0,0} & M^*_{0,1} \\ M^*_{1,0} & M^*_{1,1} \end{pmatrix}^T = \begin{pmatrix} M^*_{0,0} & M^*_{1,0} \\ M^*_{0,1} & M^*_{1,1} \end{pmatrix} \tag{A.1}$$

1 Much of this description is reproduced from my undergraduate thesis [79].

The *inner product* of two vectors, $|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix}$ and $|\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{pmatrix}$ is given by

$$\langle\phi|\psi\rangle = (|\phi\rangle^\dagger)\,|\psi\rangle = (\phi_1^* \ \phi_2^* \ \dots \ \phi_n^*) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} = \phi_1^*\psi_1 + \phi_2^*\psi_2 + \cdots + \phi_n^*\psi_n \tag{A.2}$$

$|\psi\rangle_i, |\phi\rangle_i$ are complex numbers, and therefore the above is simply a sum of products of complex numbers. The inner product is often called the scalar product, which is in general complex.

A.2 POSTULATES OF QUANTUM MECHANICS

There are numerous statements of the postulates of quantum mechanics. Each version of the statements aims to achieve the same foundation, so we endeavour to explain them in the simplest terms.

1 Every moving particle in a conservative force field has an associated wave-function, $|\psi\rangle$. From this wave-function, it is possible to determine all physical information about the system.

2 All particles have physical properties called observables (denoted q). In order to determine a value, q, for a particular observable, there is an associated *operator* $\hat{Q}$, which, when acting on the particles wavefunction, yields the value times the wavefunction. The observable q is then the eigenvalue of the operator $\hat{Q}$.

$$\hat{Q}\,|\psi\rangle = q|\psi\rangle \tag{A.3}$$

3 Any such operator $\hat{Q}$ is Hermitian

$$\hat{Q}^\dagger = \hat{Q} \tag{A.4}$$

4 The set of eigenfunctions for any operator $\hat{Q}$ forms a complete set of linearly independent functions.

5 For a system with wavefunction $|\psi\rangle$, the expectation value of an observable q with respect to an operator $\hat{Q}$ is denoted by $\langle q\rangle$ and is given by

$$\langle q\rangle = \langle\psi|\hat{Q}|\psi\rangle \tag{A.5}$$

6 The time evolution of $|\psi\rangle$ is given by the time dependent *Schrodinger Equation*

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi, \tag{A.6}$$

where $\hat{H}$ is the system's Hamiltonian.

Using these building blocks, we can begin to construct a language to describe quantum systems.

A.3 STATES

An orhthonormal basis consists of vectors of unit length which do not overlap, e.g. $|x_1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, |x_2\rangle = \begin{pmatrix}0\\1\end{pmatrix} \Rightarrow \langle x_1|x_2\rangle = 0$. In general, if $\{|x\rangle\}$ are the eigenstates of a system, then the system can be written as some state vector, $|\psi\rangle$, in general a superposition over the basis-vectors:

$$|\psi\rangle = \sum_x a_x|x\rangle \tag{A.7a}$$

$$\text{subject to} \quad \sum_x |a_x|^2 = 1, \quad a_x \in \mathbb{C} \tag{A.7b}$$

The *state space* of a physical system (classical or quantum) is then the set of all possible states the system can exist in, i.e the set of all possible values for $|\psi\rangle$ such that Eq. (A.7b) are satisfied.

For example, photons can be polarised horizontally ($\leftrightarrow$) or vertically ($\updownarrow$); take those two conditions as observable states to define the eigenstates of a two-level system, so we can designate the photon as a qubit. Then we can map the two states to a 2-dimensional, x-y plane: a general vector on such a plane can be represented by a vector with coordinates $\begin{pmatrix}x\\y\end{pmatrix}$. These polarisations can then be thought of as standard basis vectors in linear algebra. Denote $\leftrightarrow$ as the eigenstate $|0\rangle$ and $\updownarrow$ as $|1\rangle$

$$|\leftrightarrow\rangle = |0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \qquad \text{A unit vector along x-axis} \tag{A.8a}$$

$$|\updownarrow\rangle = |1\rangle = \begin{pmatrix}0\\1\end{pmatrix} \qquad \text{A unit vector along y-axis} \tag{A.8b}$$

Now, in relation to the concept of superposition, we can consider, for example, a photon in an even superposition of the vertical and horizontal polarisations, evenly splitting the two basis vectors. As such, we would require that, upon measurement, it is equally likely that the

photon will *collapse* into the polarised state along x as it is to collapse along y. That is, we want $\Pr(\updownarrow) = \Pr(\leftrightarrow)$ so assign equal modulus amplitudes to the two possibilities:

$$|\psi\rangle = a\,|\leftrightarrow\rangle + b\,|\updownarrow\rangle\,, \quad \text{with} \quad \Pr(\updownarrow) = \Pr(\leftrightarrow) \Rightarrow |a|^2 = |b|^2 \tag{A.9}$$

We consider here a particular case, due to the significance of the resultant basis, where $\leftrightarrow$-polarisation and $\updownarrow$-polarisation have real amplitudes $a, b \in \mathbb{R}$.

$$\begin{aligned} &\Rightarrow a = \pm b \quad \text{but also} \quad |a|^2 + |b|^2 = 1 \\ \Rightarrow \quad &a = \frac{1}{\sqrt{2}} \quad ; \quad b = \pm\frac{1}{\sqrt{2}} \\ &\Rightarrow |\psi\rangle = \frac{1}{\sqrt{2}}\,|\leftrightarrow\rangle \pm \frac{1}{\sqrt{2}}\,|\updownarrow\rangle \\ &\Rightarrow |\psi\rangle = \frac{1}{\sqrt{2}}\,|0\rangle \pm \frac{1}{\sqrt{2}}\,|1\rangle \end{aligned} \tag{A.10}$$

These particular superpositions are of significance:

$$|+\rangle = \frac{1}{\sqrt{2}}\,(|0\rangle + |1\rangle) \tag{A.11a}$$

$$|-\rangle = \frac{1}{\sqrt{2}}\,(|0\rangle - |1\rangle) \tag{A.11b}$$

This is called the Hadamard basis: it is an equally valid vector space as the standard basis which is spanned by $\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$, as it is simply a rotation of the standard basis.

A.3.1 *Mulitpartite systems*

In reality, we often deal with systems of multiple particles, represented by multiple qubits. Mathematically, we consider the state vector of a system containing n qubits as being the tensor product of the n qubits' individual state vectors[2]. For instance, suppose a 2-qubit system, $|\psi\rangle$ consisting of two independent qubits $|\psi_A\rangle$ and $|\psi_B\rangle$:

$$|\psi\rangle = |\psi_A\rangle\,|\psi_B\rangle = |\psi_A\psi_B\rangle = |\psi_A\rangle \otimes |\psi_B\rangle \tag{A.12}$$

Consider first a simple system of 2 qubits. Measuring in the standard basis, these qubits will have to collapse in to one of the basis states $|0,0\rangle, |0,1\rangle, |1,0\rangle, |1,1\rangle$. Thus, for such a 2-qubit system, we have the general superposition

$$|\psi\rangle = \alpha_{0,0}|0,0\rangle + \alpha_{0,1}|0,1\rangle + \alpha_{1,0}|1,0\rangle + \alpha_{1,1}|1,1\rangle$$

2 We will later discuss entangled states, which can not be described thus.

where $\alpha_{i,j}$ is the amplitude for measuring the system as the state $|i,j\rangle$. This is perfectly analogous to a classical 2-bit system necessarily occupying one of the four possibilities $\{(0,0),(0,1),(1,0),(1,1)\}$.

Hence, for example, if we wanted to concoct a two-qubit system composed of one qubit in the state $|+\rangle$ and one in $|-\rangle$

$$\begin{aligned}
|\psi\rangle &= |+\rangle \otimes |-\rangle \\
|\psi\rangle &= \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right) \\
&= \frac{1}{2}\left[|00\rangle - |01\rangle + |10\rangle - |11\rangle\right] \\
&= \frac{1}{2}\left[\begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} - \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix}\right] \\
&= \frac{1}{2}\left[\begin{pmatrix}1\\0\\0\\0\end{pmatrix} - \begin{pmatrix}0\\1\\0\\0\end{pmatrix} + \begin{pmatrix}0\\0\\1\\0\end{pmatrix} - \begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right]. \\
\Rightarrow |\psi\rangle &= \frac{1}{2}\begin{pmatrix}1\\-1\\-1\\1\end{pmatrix}
\end{aligned} \tag{A.13}$$

That is, the two qubit system – and indeed any two qubit system – is given by a linear combination of the four basis vectors

$$\{|00\rangle, |0,1\rangle, |10\rangle, |11\rangle\} = \left\{\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right\}. \tag{A.14}$$

We can notice that a single qubit system can be described by a linear combination of two basis vectors, and that a two qubit system requires four basis vectors to describe it. In general we can say that an n-qubit system is represented by a linear combination of 2^n basis vectors.

A.3.2 *Registers*

A *register* is generally the name given to an array of controllable quantum systems; here we invoke it to mean a system of multiple qubits, specifically a subset of the total number of available qubits. For example, a register of ten qubits can be denoted $|x[10]\rangle$, and we can think of the system as a register of six qubits together with a register of three and another register of one qubit.

$$|x[10]\rangle = |x_1[6]\rangle \otimes |x_2[3]\rangle \otimes |x_3[1]\rangle$$

A.4 ENTANGLEMENT

?? Another unique property of quantum systems is that of *entanglement*: when two or more particles interact in such a way that their individual quantum states can not be described independent of the other particles. A quantum state then exists for the system as a whole instead. Mathematically, we consider such entangled states as those whose state can not be expressed as a tensor product of the states of the individual qubits it's composed of: they are dependent upon the other.

To understand what we mean by this dependence, consider a counter-example. Consider the Bell state,

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right), \tag{A.15}$$

if we measure this state, we expect that it will be observed in either eigenstate $|00\rangle$ or $|11\rangle$, with equal probability due to their amplitudes' equal magnitudes. The bases for this state are simply the standard bases, $|0\rangle$ and $|1\rangle$. Thus, according to our previous definition of systems of multiple qubits, we would say this state can be given as a combination of two states, like Eq. (A.12),

$$\begin{aligned} |\Phi^+\rangle &= |\psi_1\rangle \otimes |\psi_2\rangle \\ &= (a_1|0\rangle + b_1|1\rangle) \otimes (a_2|0\rangle + b_2|1\rangle) \\ &= a_1a_2|00\rangle + a_1b_2|01\rangle + b_1a_2|10\rangle + b_1b_2|11\rangle \end{aligned} \tag{A.16}$$

However we require $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, which would imply $a_1b_2 = 0$ and $b_1a_2 = 0$. These imply that either $a_1 = 0$ or $b_2 = 0$, and also that $b_1 = 0$ or a_2=0, which are obviously invalid since we require that $a_1a_2 = b_1b_2 = \frac{1}{\sqrt{2}}$. Thus, we cannot express $|\Phi^+\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$; this inability to separate the first and second qubits is what we term *entanglement*.

A.5 UNITARY TRANSFORMATIONS

A fundamental concept in quantum mechanics is that of performing transformations on states. *Quantum transformations*, or *quantum operators*, map a quantum state into a new state within the same Hilbert space. There are certain restrictions on a physically possible quantum transformation: in order that U is a valid transformation acting on some superposition $|\psi\rangle = a_1|\psi_1\rangle + a_2|\psi_2\rangle + \ldots a_k|\psi_k\rangle$, U must be linear

$$U(a_1|\psi_1\rangle + a_2|\psi_2\rangle + \ldots a_k|\psi_k\rangle) = a_1(U|\psi_1\rangle) + a_2(U|\psi_2\rangle) + \cdots + a_k(U|\psi_k\rangle). \tag{A.17}$$

To fulfil these properties, we require that U *preserve the inner product*:

$$\langle\psi_0|U^\dagger U|\psi\rangle = \langle\psi_0|\psi\rangle$$

That is, we require that any such transformation be *unitary*:

$$UU^\dagger = I \Rightarrow U^\dagger = U^{-1} \tag{A.18}$$

Unitarity is a sufficient condition to describe any valid quantum operation: any quantum transformation can be described by a unitary transformation, and any unitary transformation corresponds to a physically implementable quantum transformation.

Then, if U_1 is a unitary transformation that acts on the space $\mathcal{H}_1$ and U_2 acts on $\mathcal{H}_2$, the product of the two unitary transformations is also unitary. The tensor product $U_1 \otimes U_2$ acts on the space $\mathcal{H}_1 \otimes \mathcal{H}_2$. So, then, supposing a system of two separable qubits, $|\psi_1\rangle$ and $|\psi_2\rangle$ where we wish to act on $|\psi_1\rangle$ with operator U_1 and on $|\psi_2\rangle$ with U_2, we perform it as

$$(U_1 \otimes U_2)\left(|\psi_1\rangle \otimes |\psi_2\rangle\right) = \left(U_1 |\psi_1\rangle\right) \otimes \left(U_2 |\psi_2\rangle\right) \tag{A.19}$$

A.6 DIRAC NOTATION

In keeping with standard practice, we employ *Dirac notation* throughout this thesis. Vectors are denoted by *kets* of the form $|a\rangle$. For example, the standard basis is represented by,

$$\begin{aligned} |x\rangle = |0\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ |y\rangle = |1\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned} \tag{A.20}$$

We saw in Table A.1 that for every such ket, $|\psi\rangle$, there exists a *dual vector*: its complex conjugate transpose, called the *bra* of such a vector, denoted $\langle\psi|$. That is,

$$\begin{aligned} \langle\psi|^\dagger &= |\psi\rangle \\ |\psi\rangle^\dagger &= \langle\psi| \end{aligned} \tag{A.21}$$

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} \Rightarrow \langle\psi| = \begin{pmatrix} \psi_1^* & \psi_2^* & \dots & \psi_n^* \end{pmatrix} \tag{A.22}$$

Then if we have two vectors $|\psi\rangle$ and $|\phi\rangle$, their *inner product* is given as $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle$.

$$\begin{aligned} |\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_n \end{pmatrix} \quad ; \quad |\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_n \end{pmatrix} \\ \Rightarrow \langle\phi| = \begin{pmatrix} \phi_1^* & \phi_2^* & \phi_3^* & \cdots & \phi_n^* \end{pmatrix} \\ \Rightarrow \langle\phi|\,|\psi\rangle = \begin{pmatrix} \phi_1^* & \phi_2^* & \phi_3^* & \cdots & \phi_n^* \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_n \end{pmatrix} \\ \Rightarrow \langle\phi|\,|\psi\rangle = \phi_1^*\psi_1 + \phi_2^*\psi_2 + \phi_3^*\psi_3 + \cdots + \phi_n^*\psi_n \end{aligned} \tag{A.23}$$

Example A.6.1.

$$\begin{aligned} |\psi\rangle = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \quad ; \quad |\phi\rangle = \begin{pmatrix} 4 \\ 5 \\ 6 \end{pmatrix} \\ \Rightarrow \langle\phi|\,|\psi\rangle = \begin{pmatrix} 4 & 5 & 6 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \\ = (4)(1) + (5)(2) + (6)(3) = 32 \end{aligned} \tag{A.24}$$

Similarly, their *outer product* is given as $|\phi\rangle\langle\psi|$. Multiplying a column vector by a row vector thus gives a matrix. Matrices generated by a outer products then define operators:

Example A.6.2.

$$\begin{pmatrix} 1 \\ 2 \end{pmatrix} \begin{pmatrix} 3 & 4 \end{pmatrix} = \begin{pmatrix} 3 & 4 \\ 6 & 8 \end{pmatrix} \tag{A.25}$$

Then we can say, for $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$|0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{A.26a}$$

$$|0\rangle\langle 1| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{A.26b}$$

$$|1\rangle\langle 0| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{A.26c}$$

$$|1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{A.26d}$$

And so any 2-dimensional linear transformation in the standard basis $|0\rangle, |1\rangle$ can be given as a sum

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = a|0\rangle\langle 0| + b|0\rangle\langle 1| + c|1\rangle\langle 0| + d|1\rangle\langle 1| \tag{A.27}$$

This is a common method of representing operators as outer products of vectors. A transformation that *exchanges* a particle between two states, say $|0\rangle \leftrightarrow |1\rangle$ is given by the operation

$$\hat{Q} : \begin{cases} |0\rangle \to |1\rangle \\ |1\rangle \to |0\rangle \end{cases}$$

Which is equivalent to the outer product representation

$$\hat{Q} = |0\rangle\langle 1| + |1\rangle\langle 0|$$

For clarity, here we will prove this operation

Example A.6.3.

$$\begin{aligned} \hat{Q} &= |0\rangle\langle 1| + |1\rangle\langle 0| \\ &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

So then, acting on $|0\rangle$ *and* $|1\rangle$ *gives*

$$\hat{Q}|0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$$

$$\hat{Q}|1\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle$$

To demonstrate how Dirac notation simplifies this:

$$\begin{aligned}\hat{Q}\left|0\right\rangle &= \left(\left|0\right\rangle\left\langle 1\right| + \left|1\right\rangle\left\langle 0\right|\right)\left|0\right\rangle \\ &= \left|0\right\rangle\left\langle 1\right|\left|0\right\rangle + \left|1\right\rangle\left\langle 0|0\right\rangle \\ &= \left|0\right\rangle\left\langle 1|0\right\rangle + \left|1\right\rangle\left\langle 0|0\right\rangle\end{aligned}$$

Then, since $|0\rangle$ and $|1\rangle$ are orthogonal basis, their inner product is 0 and the inner product of a vector with itself is 1, ($\langle 1|1\rangle = \langle 0|0\rangle = 1, \langle 0|1\rangle = \langle 1|0\rangle = 0$). So,

$$\begin{aligned}\hat{Q}\left|0\right\rangle &= \left|0\right\rangle(0) + \left|1\right\rangle(1) \\ \Rightarrow \hat{Q}\left|0\right\rangle &= \left|1\right\rangle\end{aligned} \tag{A.28}$$

And similarly for $\hat{Q}\left|1\right\rangle$. This simple example then shows why Dirac notation can significantly simplify calculations across quantum mechanics, compared to standard matrix and vector notation. To see this more clearly, we will examine a simple 2-qubit state under such operations. The method generalises to operating on two or more qubits generically: we can define any operator which acts on two qubits as a sum of outer products of the basis vectors $\left|00\right\rangle, \left|01\right\rangle, \left|10\right\rangle$ and $\left|11\right\rangle$. We can similarly define any operator which acts on an n qubit state as a linear combination of the 2^n basis states generated by the n qubits.

Example A.6.4. *To define a transformation that will exchange basis vectors $|00\rangle$ and $|11\rangle$, while leaving $|01\rangle$ and $|10\rangle$ unchanged (ie exchanging $|01\rangle \leftrightarrow |01\rangle, |10\rangle \leftrightarrow |10\rangle$) we define an operator*

$$\hat{Q} = \left|00\right\rangle\left\langle 11\right| + \left|11\right\rangle\left\langle 00\right| + \left|10\right\rangle\left\langle 10\right| + \left|01\right\rangle\left\langle 01\right| \tag{A.29}$$

Then, using matrix calculations this would require separately calculating the four outer products in the above sum and adding them to find a 4×4 matrix to represent $\hat{Q}$, which then acts on a state $|\psi\rangle$. Instead, consider first that $|\psi\rangle = |00\rangle$, ie one of the basis vectors our transformation is to change:

$$\hat{Q}\left|00\right\rangle = \left(\left|00\right\rangle\left\langle 11\right| + \left|11\right\rangle\left\langle 00\right| + \left|10\right\rangle\left\langle 10\right| + \left|01\right\rangle\left\langle 01\right|\right)\ \left|00\right\rangle \tag{A.30}$$

And as before, only the inner products of a vector with itself remains:

$$\begin{aligned}&= \left|00\right\rangle\left\langle 11\left|00\right.\right\rangle + \left|11\right\rangle\left\langle 00\left|00\right.\right\rangle + \left|10\right\rangle\left\langle 10\left|00\right.\right\rangle + \left|01\right\rangle\left\langle 01\left|00\right.\right\rangle \\ &= \left|00\right\rangle(0) + \left|11\right\rangle(1) + \left|10\right\rangle(0) + \left|01\right\rangle(0) \\ \Rightarrow &\hat{Q}\left|00\right\rangle = \left|11\right\rangle\end{aligned} \tag{A.31}$$

i.e the transformation has performed $\hat{Q} : |00\rangle \rightarrow |11\rangle$ as expected. Then, if we apply the same transformation to a state which does not depend on one of the target states, eg,

$$\begin{aligned}\left|\psi\right\rangle =& a\left|10\right\rangle + b\left|01\right\rangle \\ \hat{Q}\left|\psi\right\rangle =& \Big(\left|00\right\rangle\left\langle 11\right| + \left|11\right\rangle\left\langle 00\right| + \left|10\right\rangle\left\langle 10\right| + \left|01\right\rangle\left\langle 01\right|\Big)\Big(a\left|10\right\rangle + b\left|01\right\rangle\Big) \\ =& a\Big(\left|00\right\rangle\left\langle 11\left|10\right.\right\rangle + \left|11\right\rangle\left\langle 00\left|10\right.\right\rangle + \left|10\right\rangle\left\langle 10\left|10\right.\right\rangle + \left|01\right\rangle\left\langle 01\left|10\right.\right\rangle\Big) \\ &+ b\Big(\left|00\right\rangle\left\langle 11\left|01\right.\right\rangle + \left|11\right\rangle\left\langle 00\left|01\right.\right\rangle + \left|10\right\rangle\left\langle 10\left|01\right.\right\rangle + \left|01\right\rangle\left\langle 01\left|01\right.\right\rangle\Big)\end{aligned} \tag{A.32}$$

And since the inner product is a scalar, we can factor terms such as $\langle 11|10\rangle$ *to the beginning of expressions, eg* $|00\rangle \langle 11| |10\rangle = \langle 11 |10\rangle |00\rangle$*, and we also know*

$$\begin{aligned} \langle 11|10\rangle = \langle 00|10\rangle = \langle 01|10\rangle = \langle 11|01\rangle = \langle 00|01\rangle = \langle 10|01\rangle = 0 \\ \langle 10|10\rangle = \langle 01|01\rangle = 1 \end{aligned} \tag{A.33}$$

We can express the above as

$$\begin{aligned} \hat{Q}\,|\psi\rangle = a\Big((0)\,|00\rangle + (0)\,|11\rangle + (1)\,|10\rangle + (0)\,|01\rangle\Big) \\ +b\Big((0)\,|00\rangle + (0)\,|11\rangle + (0)\,|10\rangle + (1)|01\rangle\Big) \\ =a\,|10\rangle\,| + b|01\rangle \\ =|\psi\rangle \end{aligned} \tag{A.34}$$

Then it is clear that, when $|\psi\rangle$ *is a superposition of states unaffected by transformation* $\hat{Q}$*, then* $\hat{Q}\,|\psi\rangle = |\psi\rangle$*.*

This method generalises to systems with greater numbers of particles (qubits). If we briefly consider a 3 qubit system - and initialise all qubits in the standard basis state $|0\rangle$ - then the system is represented by $|000\rangle = |0\rangle \otimes |0\rangle \otimes |0\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix}$. This quantity is an 8-row vector. To calculate the outer product $\langle 000|000\rangle$, we would be multiplying an 8-column bra $\langle 000|$ by an 8-row ket $|000\rangle$. Clearly then we will be working with 8×8 matrices, which will become quite difficult to maintain effectively and efficiently quite fast. As we move to systems of larger size, standard matrix multiplication becomes impractical for hand-written analysis, although of course remains tractable computationally up to $n \sim 10$ qubits. It is obvious that Dirac's bra/ket notation is a helpful, pathematically precise tool for QM.

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