Doctorate of Philosophy

Schrödinger's Catwalk

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January, 2021

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LISTINGS

ACRONYMS

AIC	Akaike information criterion. 84, 86
AICC	Akaike information criterion corrected. 84
BF	Bayes factor. 25–27, 33, 35, 48, 51, 55, 57, 61, 63, 64, 80, 81, 87, 89–91, 93–95
BFEER	Bayes factor enhanced Elo ratings. 80, 81, 93, 94, 96
BIC	Bayesian information criterion. 86
CLE	classical likelihood estimation. 13
EDH	experiment design heuristic. 18–23, 26, 35, 45, 55, 56, 83
ES	exploration strategy. 27–31, 33–35, 40, 43, 45, 49, 51, 61, 65, 67, 75, 79, 105, 108
ET	exploration tree. 28, 29, 31, 33–35, 45, 47, 75
FH	Fermi-Hubbard. 58
FP	false negatives. 78
FP	false positives. 78
GA	genetic algorithm. iii, 34, 67, 71, 74, 75, 80, 82, 83, 88, 90, 93, 96–98
GES	genetic exploration strategy. 67, 78, 93, 94, 97
HPD	high particle density. 18
IQLE	interactive quantum likelihood estimation. 13, 14, 93, 94
LTL	log total likelihood. 16
ML	machine learning. 6, 26, 27, 78
MS	model search. 27–29, 31, 35, 43, 45
MVEE	minimum volume enclosing ellipsoid. 18

NV nitrogen-vacancy. 9
NVC nitrogen-vacancy centre. 14

OF objective function. iii, 67, 68, 74, 75, 78, 80, 81, 83, 84, 88, 91–93

PGH particle guess heuristic. 19, 20, 45

QHL quantum Hamiltonian learning. 8–14, 16, 18, 20–22, 25–27, 31–35, 40, 43, 48, 55, 56, 75, 93, 94, 105
QL quadratic loss. 17
QLE quantum likelihood estimation. 13, 32
QMLA Quantum Model Learning Agent. ii, iii, vii, 8, 13, 24, 25, 27–31, 34, 35, 40, 43–49, 51, 52, 60, 61, 63–65, 67, 72, 74–77, 83, 87, 88, 90, 91, 93, 94, 96–98, 105

SMC sequential monte carlo. 11–13, 15, 18, 19, 22, 31

TLTL total log total likelihood. 16, 25–27, 35, 84, 91
TN true negatives. 78
TP true positives. 78

GLOSSARY

Jordan Wigner transformation (JWT)	Jordan Wigner transformation . 60, 61, 64
Loschmidt echo (LE)	Quantum chaotic effect described. . 14
chromosome	A single candidate in the space of valid solutions to the posed problem in a genetic algorithm. . 68
gene	Individual element within a chromosome. . 68
hyperparameter	Variable within an algorithm that determines how the algorithm itself proceeds.. 11
instance	a single implementation of the Quantum Model Learning Agent (QMLA) algorithm. iii, 48, 94, 97, 98, 105
likelihood	Value that represents how likely a hypothesis is.. 10, 13, 15, 18, 31, 33, 34, 36, 88
model	The mathematical description of some quantum system. 24
model space	Abstract space containing all descriptions (within defined constraints such as dimension) of the system as models. 29
probe	Input probe state, $\|\psi\rangle$, which the target system is initialised to, before unitary evolution. plural. 13, 15, 18–22, 54
results directory	Directory to which the data and analysis for a given run of QMLA are stored. . 49
run	collection of QMLA instances. iii, vii, 48, 49, 64, 65, 94, 96, 98, 105
spawn	Process by which new models are generated by combining previously considered models.. 29

success rate	. 48, 49
term	Individual constituent of a model, e.g. a single operator within a sum of operators, which in total describe a Hamiltonian. . 24
volume	Volume of a parameter distribution's credible region.. 18, 55, 56, 63
win rate	. 48, 49

Part I

CONTEXTUAL REVIEW

1 QUANTUM MECHANICS

The study of nature at the quantum level has been at the forefront of physics since the early 20^{th} century. ...

Here we will only introduce concepts utilised in this thesis. We elucidate some fundamental topics of linear algebra and quantum theory in Appendix A for completeness, but consider them too cumbersome to include in the main text. For a more complete and general introduction to quantum mechanics (QM), the reader is referred to [1].

1.1 QM TODO

- states
  - qubits
- Hilbert space
  - pure/separable and mixed
- operators/gates
- Pauli matrices
- Bloch sphere
- measurement
  - projectors
- expectation value
- superposition/entanglement
- Hamiltonian
- Schrodinger equation
- Unitary evolution
- first/second quantisation
- quantum tech other than computation/simulation

1.2 QUANTUM MECHANICS AND INFORMATION

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 initial position, $\vec{r}(t_0)$, and

conditions such as mass and acceleration, quantum *equations of motion* can describe the evolution of Q through its wavefunction [2]. One proposal[1] for the equation of motion to describe the evolution of the wavefunction under known conditions, i.e. determining $\Psi(t)$ from $\Psi(t_0)\ \forall t$, is *Schrödinger 's equation* [1, 3, 4].

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 [6]. We consider wavefunctions using *Dirac notation* (Appendix A.6). Suppose we have two such wavefunctions, $|\phi(t)\rangle, |\psi(t)\rangle$ which are functions of time $t > t_0$. 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 [6])

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

Then, assuming some equations of motion capture the dynamics of Q, there exists some evolution operator, $\hat{U}(t)$, which deterministically maps $|\phi(t_o)\rangle$ 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 $\hat{U}^\dagger\hat{U} = \hat{\mathbb{1}}$ is the condition for *unitarity* (Appendix A.5), so we can claim the quantum wavefunction evolves unitarily.

By construction, we require

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

Without loss of generality we can set $t_0 = 0$. Then, let us consider an infintesimally small time increment $\epsilon = t_0 + \Delta t$, such that $\epsilon \gg \epsilon^2$.

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. We suppose the form of the offset, so we can write

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

1 The most noteworthy alternative formalism, due to Heisenberg [5], was shown equivalent to the Schrödinger picture described here.

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; 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

$$\frac{d}{dt}\,|\psi(t)\rangle = \frac{-i}{\hbar}\hat{H}_0\,|\psi(0)\rangle\,, \tag{1.9}$$

where $|\psi(t)\rangle$ is the wavefunction at time t, $|\psi(t_0)\rangle$ is the wavefunction at t, 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.

1.2.1 *Hamiltonians*

In the previous section we introduced the Hamiltonian[2] 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 (dynamics). 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 [7]. Likewise, knowledge of the initial wavefunction, $|\psi(t_0)\rangle$, and the system's quantum Hamiltonian, $\hat{H}_0$, the quantum equations of motion, i.e. 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 [8, 9] In this thesis we only consider closed models for quantum systems; it will be necessary to expand the techniques presented here to account for the open system dynamics of realistic experiments, however we do model a physical system through a closed Hamiltonian in **??**.

2 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 Hamiltonians on a quantum computer.

1.2.2 *States and qubits*

The wavefunction is also known as its *state*, which in general can be in superposition across its eigenstates, $|i\rangle$[3]. The valid state space for Q is its *Hilbert space*, $\mathcal{H}$, which is a generalisation of Euclidean vector space, i.e. $|\psi\rangle \in \mathcal{H}$.

$$|\psi\rangle = \sum_i \alpha_i |i\rangle \tag{1.10a}$$

$$\text{subject to} \quad \sum_i |\alpha_i|^2 = 1, \quad \alpha_x \in \mathbb{C}. \tag{1.10b}$$

For an ideal[4] single particle, when the state, Eq. (1.10a), 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. This is done by mapping each eigenstate to one of the orthogonal basis vectors, e.g. $|H\rangle = |0\rangle = |V\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

Then, a qubit's state can be written as

$$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle . \tag{1.11}$$

Qubits can then be interfaced together

1.3 QUANTUM COMPUTATION AND SIMULATION

- Algorithms
  - advantage
- Hardware

Supremacy proposals: [10]

Bringing together the concepts of the chapter so far, we can use qubits to represent the state of real quantum systems. This allows for efficient simuation of processes at the quantum level for the first time, facilitiating novel insights of nature's most intricate details.

3 We expand on this brief description in Appendix A.3, and the Dirac notation emplyed throughout in Appendix A.6.

4 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.

2 MACHINE LEARNING

machine learning (ML) is the application of statistics, algorithms and computing power to discover meaning and/or devise actions from data.

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
  - QNN, q svm,
- Remit of this thesis → 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

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 definition

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 [11].

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 $|1\rangle$

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

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

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:

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

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

$$\begin{aligned} &\Rightarrow a = \pm b \quad \text{but also} \quad |a|^2 + |b|^2 = 1 \\ \Rightarrow \quad &a = \frac{1}{\sqrt{2}} \quad ; \quad b = \pm\frac{1}{\sqrt{2}} \\ &\Rightarrow |\psi\rangle = \frac{1}{\sqrt{2}}\,|\leftrightarrow\rangle \pm \frac{1}{\sqrt{2}}\,|\updownarrow\rangle \\ &\Rightarrow ket\psi = \frac{1}{\sqrt{2}}\,|0\rangle \pm \frac{1}{\sqrt{2}}\,|1\rangle \end{aligned} \tag{A.9}$$

These particular superpositions are of significance:

$$|+\rangle = \frac{1}{\sqrt{2}}\,(|0\rangle + |1\rangle) \tag{A.10a}$$

$$|-\rangle = \frac{1}{\sqrt{2}}\,(|0\rangle - |1\rangle) \tag{A.10b}$$

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 $|\psi_B\rangle$:

$$|\psi\rangle = |\psi_A\rangle\,|\psi_B\rangle = |\psi_A\psi_B\rangle = |\psi_A\rangle \otimes |\psi_B\rangle \tag{A.11}$$

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 $|-\rangle$

$$\begin{aligned}
|\psi\rangle &= |+\rangle \otimes |-\rangle \\
|\psi\rangle &= \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right) \\
&= \frac{1}{2}\left[|00\rangle - |01\rangle + |10\rangle - |11\rangle\right] \\
&= \frac{1}{2}\left[\begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} - \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix}\right] \\
&= \frac{1}{2}\left[\begin{pmatrix}1\\0\\0\\0\end{pmatrix} - \begin{pmatrix}0\\1\\0\\0\end{pmatrix} + \begin{pmatrix}0\\0\\1\\0\end{pmatrix} - \begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right]. \\
\Rightarrow |\psi\rangle &= \frac{1}{2}\begin{pmatrix}1\\-1\\-1\\1\end{pmatrix}
\end{aligned} \tag{A.12}$$

That is, the system is given by a linear combination of the four basis vectors

$$\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\0\\1\end{pmatrix}. \tag{A.13}$$

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,

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right), \tag{A.14}$$

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.11),

$$\begin{aligned} |\Phi^+\rangle &= |\psi_1\rangle \otimes |\psi_2\rangle \\ &= (a_1|0\rangle + b_1|1\rangle) \otimes (a_2|0\rangle + b_2|1\rangle) \\ &= a_1a_2|00\rangle + a_1b_2|01\rangle + b_1a_2|10\rangle + b_1b_2|11\rangle \end{aligned} \tag{A.15}$$

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

$$U(a_1|\psi_1\rangle + a_2|\psi_2\rangle + \ldots a_k|\psi_k\rangle) = a_1(U|\psi_1\rangle) + a_2(U|\psi_2\rangle) + \cdots + a_k(U|\psi_k\rangle). \tag{A.16}$$

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*:

$$UU^\dagger = I \Rightarrow U^\dagger = U^{-1} \tag{A.17}$$

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

$$(U_1 \otimes U_2)\left(|\psi_1\rangle \otimes |\psi_2\rangle\right) = \left(U_1 |\psi_1\rangle\right) \otimes \left(U_2 |\psi_2\rangle\right) \tag{A.18}$$

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,

$$\begin{aligned} |x\rangle = |0\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ |y\rangle = |1\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned} \tag{A.19}$$

We saw above 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,

$$\begin{aligned} \langle\psi|^\dagger &= |\psi\rangle \\ |\psi\rangle^\dagger &= \langle\psi| \end{aligned} \tag{A.20}$$

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} \Rightarrow \langle\psi| = \begin{pmatrix} \psi_1^* & \psi_2^* & \dots & \psi_n^* \end{pmatrix} \tag{A.21}$$

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

$$\begin{aligned} |\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_n \end{pmatrix} \quad ; \quad |\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_n \end{pmatrix} \\ \Rightarrow \langle\phi| = \begin{pmatrix} \phi_1^* & \phi_2^* & \phi_3^* & \cdots & \phi_n^* \end{pmatrix} \\ \Rightarrow \langle\phi|\,|\psi\rangle = \begin{pmatrix} \phi_1^* & \phi_2^* & \phi_3^* & \cdots & \phi_n^* \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_n \end{pmatrix} \\ \Rightarrow \langle\phi|\,|\psi\rangle = \phi_1^*\psi_1 + \phi_2^*\psi_2 + \phi_3^*\psi_3 + \cdots + \phi_n^*\psi_n \end{aligned} \tag{A.22}$$

Example A.6.1.

$$\begin{aligned} |\psi\rangle = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \quad ; \quad |\phi\rangle = \begin{pmatrix} 4 \\ 5 \\ 6 \end{pmatrix} \\ \Rightarrow \langle\phi|\,|\psi\rangle = \begin{pmatrix} 4 & 5 & 6 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \\ = (4)(1) + (5)(2) + (6)(3) = 32 \end{aligned} \tag{A.23}$$

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.

$$\begin{pmatrix} 1 \\ 2 \end{pmatrix} \begin{pmatrix} 3 & 4 \end{pmatrix} = \begin{pmatrix} 3 & 4 \\ 6 & 8 \end{pmatrix} \tag{A.24}$$

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

$$|0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{A.25a}$$

$$|0\rangle\langle 1| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{A.25b}$$

$$|1\rangle\langle 0| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{A.25c}$$

$$|1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{A.25d}$$

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

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

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,

$$\begin{aligned}\hat{Q}\left|0\right\rangle &= \left|0\right\rangle(0) + \left|1\right\rangle(1) \\ \Rightarrow \hat{Q}\left|0\right\rangle &= \left|1\right\rangle\end{aligned} \tag{A.27}$$

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*

$$\hat{Q} = \left|00\right\rangle\left\langle 11\right| + \left|11\right\rangle\left\langle 00\right| + \left|10\right\rangle\left\langle 10\right| + \left|01\right\rangle\left\langle 01\right| \tag{A.28}$$

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:

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

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

$$\begin{aligned}&= \left|00\right\rangle\left\langle 11\left|00\right.\right\rangle + \left|11\right\rangle\left\langle 00\left|00\right.\right\rangle + \left|10\right\rangle\left\langle 10\left|00\right.\right\rangle + \left|01\right\rangle\left\langle 01\left|00\right.\right\rangle \\ &= \left|00\right\rangle(0) + \left|11\right\rangle(1) + \left|10\right\rangle(0) + \left|01\right\rangle(0) \\ \Rightarrow &\hat{Q}\left|00\right\rangle = \left|11\right\rangle\end{aligned} \tag{A.30}$$

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,

$$\begin{aligned}\left|\psi\right\rangle =& a\left|10\right\rangle + b\left|01\right\rangle \\ \hat{Q}\left|\psi\right\rangle =& \Big(\left|00\right\rangle\left\langle 11\right| + \left|11\right\rangle\left\langle 00\right| + \left|10\right\rangle\left\langle 10\right| + \left|01\right\rangle\left\langle 01\right|\Big)\Big(a\left|10\right\rangle + b\left|01\right\rangle\Big) \\ =& a\Big(\left|00\right\rangle\left\langle 11\left|10\right.\right\rangle + \left|11\right\rangle\left\langle 00\left|10\right.\right\rangle + \left|10\right\rangle\left\langle 10\left|10\right.\right\rangle + \left|01\right\rangle\left\langle 01\left|10\right.\right\rangle\Big) \\ &+ b\Big(\left|00\right\rangle\left\langle 11\left|01\right.\right\rangle + \left|11\right\rangle\left\langle 00\left|01\right.\right\rangle + \left|10\right\rangle\left\langle 10\left|01\right.\right\rangle + \left|01\right\rangle\left\langle 01\left|01\right.\right\rangle\Big)\end{aligned} \tag{A.31}$$

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*

$$\begin{aligned} \langle 11|10\rangle = \langle 00|10\rangle = \langle 01|10\rangle = \langle 11|01\rangle = \langle 00|01\rangle = \langle 10|01\rangle = 0 \\ \langle 10|10\rangle = \langle 01|01\rangle = 1 \end{aligned} \tag{A.32}$$

We can express the above as

$$\begin{aligned} \hat{Q}\,|\psi\rangle = a\Big((0)\,|00\rangle + (0)\,|11\rangle + (1)\,|10\rangle + (0)\,|01\rangle\Big) \\ +b\Big((0)\,|00\rangle + (0)\,|11\rangle + (0)\,|10\rangle + (1)|01\rangle\Big) \\ =a\,|10\rangle\,| + b|01\rangle \\ =|\psi\rangle \end{aligned} \tag{A.33}$$

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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