Lecture 1 Notes — Bones Quantum Introduction (May 11 2010)

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I. INTRODUCTION

In quantum theory, one predicts experiments by performing calculations involving the processes that transform the mathematical representative of a quantum system, such as operators on a state space or an observable. This mathematical structure has proven very rich, and consequently well studied. The premise of this course is to return to the basics of the field of 'Quantum Information' and to present this theory based on what we know now.

For instance, the theory of categories gives the precise description for the mathematical structures used in quantum information processing. We will use some ideas from Category Theory and Higher Algebra in the course, and it is assumed that those attending will have had no exposure to these topics.

Category Theory is useful for us as it allows one to study the mathematical structure formed by the composition of processes themselves. The wealth of information gained through this new viewpoint will be developed in this course — leading to the calculus of tensor networks states as a new description of the ground states of physical systems. In this new setting, states are viewed as linear maps, and states can be composed. States and observables themselves are typically not viewed in a way that emphasizes their own compositional structure, giving a categorical model of quantum computation the prospect of providing many new insights. To get a feeling for the types of insights possible, let's consider the following digression which will be made precise in the main text.

Consider the two classical single-bit operations: the identity operator, which is represented as a wire in a quantum circuit diagram, and the NOT operation, represented as a $\oplus$ on top of a wire. In quantum computation, the identity operator on a single qubit is given as a map: $\mathbf{1}_2 = |0\rangle\langle 0| + |1\rangle\langle 1|$, and NOT is given as $\sigma^x := |0\rangle\langle 1| + |1\rangle\langle 0|$. These are maps taking state vectors in the two-qubit Hilbert space $\mathbb{C}^2$ back to the two-qubit Hilbert space $\mathbb{C}^2$. Viewed in this way, both σ^x and $\mathbf{1}$ are arrows with the same domain and codomain, that is arrows: $\mathbb{C}^2 \xrightarrow{\sigma^x} \mathbb{C}^2$ and $\mathbb{C}^2 \xrightarrow{\mathbf{1}} \mathbb{C}^2$.

Now let's consider the states $\Phi^+ = |00\rangle + |11\rangle$ and $\Psi^+ = |01\rangle + |10\rangle$. In which ways are these states considered maps? It is claimed that in the most elementary case these states are maps from the complex numbers into the Hilbert space of two qubits $\mathbb{C}^2 \otimes \mathbb{C}^2$, that is they are arrows $\mathbb{C} \xrightarrow{\Phi^+} \mathbb{C}^2 \otimes \mathbb{C}^2$ and $\mathbb{C} \xrightarrow{\Psi^+} \mathbb{C}^2 \otimes \mathbb{C}^2$. To see this, simply pick a number $k \in \mathbb{C}$. Now Φ^+ acting on k is given as $\Phi^+(k) = k \cdot \Phi^+ \in \mathbb{C}^2 \otimes \mathbb{C}^2$, so Φ^+ took the arbitary number k into the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$, and is thus an arrow $\mathbb{C} \xrightarrow{\Phi^+} \mathbb{C}^2 \otimes \mathbb{C}^2$ (by linearity, $k = 1$ uniquely determines the state).

It turns out to be general (for states/maps etc.) that the following canonical isomorphisms are true (illustrated with the identity $\mathbf{1}$)

$$\begin{array}{ccccc} \mathbb{C}^2 \to \mathbb{C}^2 & \leftrightarrow & \mathbb{C} \to \mathbb{C}^2 \otimes \mathbb{C}^2 & \leftrightarrow & \mathbb{C}^2 \otimes \mathbb{C}^2 \to \mathbb{C} \\ |0\rangle\langle 0| + |1\rangle\langle 1| & \leftrightarrow & |00\rangle + |11\rangle & \leftrightarrow & \langle 00| + \langle 11|. \end{array}$$

meaning that every single map in a finite Hilbert space from $\mathbb{C}^2 \to \mathbb{C}^2$ gives rise to exactly one map $\mathbb{C} \to \mathbb{C}^2 \otimes \mathbb{C}^2$, but we already saw that maps from $\mathbb{C}$ into $\mathbb{C}^2 \otimes \mathbb{C}^2$ are themselves state vectors. (For a second, one might wrongly suspect that the left hand side above is the

result of a partial trace, but we could have equally well illustrated this isomorphism with $|000\rangle + |111\rangle \leftrightarrow |00\rangle\langle 0| + |11\rangle\langle 1|$, etc.)

Every map of *type* $\mathbb{C}^2 \to \mathbb{C}^2$ gives rise to one state in $\mathbb{C}^2 \otimes \mathbb{C}^2$ and likewise, every map $\mathbb{C}^2 \to \mathbb{C}^2$ gives rise to exactly one costate, which is a map of type $\mathbb{C}^2 \otimes \mathbb{C}^2 \to \mathbb{C}$. This was named *braket-duality* during a talk in Clarendon Laboratory.

Although the Categorical Algebra gives rigorous justification to statements of map-state and braket-duality, depending on one's own background, readers may wish to first see the power and beauty behind these methods, before devoting the needed time to understand the details of the proofs. On the other hand, readers who have traditionally worked in Categorical Quantum Theory will be interested to see how the appropriate changes and additions to their approach can produce a tool applicable to quantum information science.

A. Quantum Theory Notation and Background

- We are attempting to write across disciplines, so our presentation attempts to be minimal but also complete.
- Those attending the course who would like to go over more details related to any part of this document are encouraged to contact us.

We do assume readers to be familiar with qubit states ψ which are equivalently represented as state vectors $|\psi\rangle$, where the bracket $|\ \rangle$ is linear in ψ (e.g. $|c\psi\rangle = c|\psi\rangle$ and $|\psi + \phi\rangle = |\psi\rangle + |\phi\rangle$), and one defines an inner product conjugate linear in it's first argument as $\langle\psi, \phi\rangle = \sum_{i=1}^{n} \overline{\psi_i}\phi_i$ — called a *Hermitian form*. In the physics literature, $|\phi\rangle|\psi\rangle$, $|\phi, \psi\rangle$, $|\phi\rangle \otimes |\psi\rangle$, $|\phi\psi\rangle$ and $\phi \otimes \psi$ are used to mean the same thing. Unitary maps U, such that $UU^\dagger = \mathbf{1}$, transform states leaving inner products and hence angles between states $|\psi\rangle$, $|\phi\rangle$ and $|U\psi\rangle$, $|U\phi\rangle$ unchanged. These statements become a special case of something more general when given precise Categorical meaning.

Each unitary map acting on a qubit state space can be represented by the complex image under the exponential map (exp) of a Hermitian matrix generated by linear real sums of tensor products of Pauli matrices (see below) — this Hermitian matrix is called the Hamiltonian.

The time dependence of state $|\psi\rangle$ is given by Schrodinger's equation: $i\hbar\dfrac{d}{dt}|\psi\rangle = H|\psi\rangle$, where the (real valued) spectrum of the Hamiltonian operator $H = H^\dagger$ is the set of possible outcomes when one measures the systems total energy. Some Hamiltonian is always acting on the state of a quantum system, and so Schrodinger's equation must be solved to find the time-dependence of the evolution.

For instance, if one prepares a system into an energy eigenstate of H, such that $H|\psi_0\rangle = E_0|\psi_0\rangle$, then $|\psi_0(t)\rangle = \exp[-iE_0t]|\psi_0(0)\rangle$ and the evolution of the state makes a circle in the Argand plane with angular frequency $2\pi E_0$. In what follows, we let $\hbar = 1$ making $\exp[-itH]$ dimensionless for H in units of angular frequency.

Typically, in quantum information theory, we consider an idealised Hamiltonian such as

the Ising Model with Transverse Field

$$H = \sum_i h^i(t)\sigma_i^z + \sum_i \Delta^i(t)\sigma_i^x + \frac{1}{2}\sum_{i,j} J_{ij}(t)\sigma_i^z\sigma_j^z \tag{1}$$

where each $h^i(t)$, $\Delta^i(t)$ and $J_{ij}(t)$ is any function of time we choose. Under the Lie braket $[A, B] = AB - BA$, (1) forms a basis for a real vector space, and hence the terms in H generate the full Lie algebra $\mathbf{u}(2^n)$ and the complex image under exp generates the full Unitary group $\mathbf{U}(2^n)$. We will provide explicit examples of this when we time Hamiltonians to generate quantum circuit representations of the string diagrams possible in Monoidal Categories.

Definition I.1. *Recall from angular momentum representation the familiar Pauli Matrices. We let $\sigma_1 \equiv \sigma_x$, $\sigma_2 \equiv \sigma^y$ and $\sigma_3 \equiv \sigma^z$ which satisfy (i) $[\sigma_i, \sigma_j] = 2i\epsilon^{ijk}\sigma_k$, (ii) complex conjugation is generated by σ_j $\forall w \in \{i, j, k\}$ as $\sigma_j\sigma_w^*\sigma_j = -\sigma_w$ for $i \neq j$ and (iii) $Tr(\sigma_i\sigma_j) = 2\delta_{ij}$. Note that it is common to change subscripts to superscripts $\sigma_x \equiv \sigma^x$ to distinguish powers of operators σ_x^2 from operators acting on specific indices σ_3^x — that is, σ_x acting on the third qubit and not σ_x cubed. This should be evident from context.*

These familiar operators from quantum mechanics form a Geometric Algebra (a.k.a. Clifford Algebra — here this algebra arises as a property of the basis). Consider $\{\sigma_i^l\}$ as a basis for a real left and right distributive vector space (that is, a left and right $\mathbb{C}$-module): such that

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \mathbf{1} = -i\sigma_x\sigma_y\sigma_z \tag{2}$$

Then consider the product

$$\sigma_i\sigma_j = \delta_{ij}\mathbf{1} + i\epsilon^{ijk}\sigma_k \quad \text{(Geometric product of vectors).} \tag{3}$$

It is clear that for $i \neq j$

$$\{\sigma_i^l, \sigma_j^l\} = 0 \tag{4}$$

meaning that the vectors anti-commute viz.

$$\sigma_i^l\sigma_j^l = -\sigma_j^l\sigma_i^l. \tag{5}$$

We also note that

$$\{\sigma^i, \sigma^j\} = 2\delta_{ij}\mathbf{1}. \tag{6}$$

Exercise I.2. *Verify Equations 3, 4, 5 and 6.*

Up to an energy scale, the Hamiltonians acting on the Hilbert space $\mathbb{C}^2$ can be expanded in terms of a dot product of a polarisation vector $\underline{P} := (p_1, p_2, p_3)$, $\forall i, p_i \in \mathbb{R}$, and a sigma vector $\underline{\sigma} := (\sigma_1, \sigma_2, \sigma_3)$ as

$$\underline{\sigma}.\underline{P} = p_i\sigma^i = p_1\sigma^1 + p_2\sigma^2 + p_3\sigma^3. \tag{7}$$

This is of course not a complete basis for the space of linear operators $L : \mathbb{C}^2 \to \mathbb{C}^2$ since we left out the span of the centre of the algebra $\mathbf{1}_2$.

Clearly the vectors $\underline{P}$ are in the vector space $\mathbb{R}^3$. We can elevate this vector space to a Hilbert space by defining an inner product between vectors — that is a map $(-,-)$ taking two elements from the vector space (in this case Hamiltonians on $\mathbb{C}^2$) and producing a scalar in the underlining field $\mathbb{C}$.

$$(-,-) : (\mathbb{C}^2 \to \mathbb{C}^2) \times (\mathbb{C}^2 \to \mathbb{C}^2) \to \mathbb{C} :: (\underline{\sigma}.\underline{A}, \underline{\sigma}.\underline{B}) \mapsto Tr[(\underline{\sigma}.\underline{A}).(\underline{\sigma}.\underline{B})] = \underline{A}.\underline{B}. \tag{8}$$

Straight forward calculation also yields

$$(\underline{\sigma}.\underline{A}, \underline{\sigma}.\underline{B}) = A_i B_i + i\epsilon_{ijk}\sigma^k = \underline{A}.\underline{B} + i\underline{\sigma}(\underline{A} \wedge \underline{B}). \tag{9}$$

which readers should check as an exercise.

Exercise I.3. *Verify that for $\underline{A} = \underline{B}$ the (geometric) wedge product vanishes and so we note that the eigenvalues of $(\underline{A}.\underline{\sigma})$ are $\pm|\underline{A}|$, where both roots appear as $\underline{A}.\underline{\sigma}$ is traceless.*

It is standard to express a quantum state in terms of observables, by expanding in a basis of measurement outcomes (e.g. the eigenvalues of a Hermitian operator such as $\underline{A}.\underline{\sigma}$). We consider the complex amplitudes c_0 and c_1 and any state ψ in $\mathbb{C}^2$ can be written as

$$\psi = c_0| + |A|\rangle + c_1| - |A|\rangle, \tag{10}$$

where for normalized $\underline{A}$ one recovers $\psi = c_0| + 1\rangle + c_1| - 1\rangle$. For a bipartite system formed from $\mathbb{C}^2 \otimes \mathbb{C}^2$. Here the possible values the spin variable s_i can take after measurement is inside the ket. If we then introduce binary indicator variables x_i (in this case a single indicator variable will do), we can relate them to spin variables as $s_i = 1 - 2x_i$. In the standard basis, s_i is replaced with the matrix σ_z and x_i is a projector onto $|0\rangle$, and the state becomes $\psi = c_0|0\rangle + c_1|1\rangle$.

Consider the expansion of an arbitrary Hamiltonian acting on a single qubit state space, that is the complex Hilbert space $\mathbb{C}^2$. Here $H_2 = p_0\mathbf{1} + \underline{P}.\underline{\sigma}$ gives a general form where

$$\exp[-it/\hbar H_2] = \exp[-ip_0 t/\hbar]\exp[-it/\hbar \underline{P}.\underline{\sigma}]. \tag{11}$$

The term $p_0\mathbf{1}$ corresponds to an energy reference. Mathematically it is the centre of the algebra: $-it\mathbf{1}$ maps under exp to the centre of the Unitary group. It thus corresponds to the so called *global phase* and is safely ignored for our purposes. Now the complex image of $\underline{P}$ under exp becomes

$$R_{\underline{P}}(\theta) := e^{-i\theta \underline{P}.\underline{\sigma}} = \mathbf{1}\cos(\theta) - i\underline{P}.\underline{\sigma}\sin(\theta) \tag{12}$$

which is understood as a rotation about the unit vector $\underline{P}$.

Exercise I.4. *Show that whenever* $A^2 = 1$, $\exp[-iA\theta] = \mathbf{1}\cos\theta - iA\sin\theta$ *by using*

$$\exp(A) = \sum_{k=0}^{\infty} \frac{1}{k} A^k \tag{13}$$

Remark I.5. *(Projective nature of Hilbert space) As measurements on quantum states are projections in Hilbert space, normalization constants are only used when they aid in the presentation. In the present paper, most often they are safely omitted.*

Remark I.6. *(Basis) Whenever we talk about a basis* $\{|i\rangle\}$ *we mean a finite set of kets* $|i\rangle$ *with index* i *such that* $\langle i|j\rangle = \delta_{ij}$.

II. FROM ABSTRACT HAMILTONIAN MECHANICS TO GRAPHICAL CALCULUS

The first lecture deals in part with constructing implementable quantum processes. We will continue by showing the pictures to represent quantum states as follows:

Other states are represented by changing the internal label inside the triangle, and costates (e.g. $\langle 0|$, $\langle +|$ etc.) are represented by reflecting across the vertical of the page (using the $\dagger$ functor), so the triangle instead points to the right.

Because we have included what would be considered as atemporal quantum networks, we will consider the direction of the states important when trying to implement them as a quantum process, but when doing reasoning and calculation the direction of circuit components is relaxed.

By considering the duality between states and maps, we will see that one can consider composition of not just maps, but states as well. This allows us to take advantage of more than just the isomorphism $|00\rangle + |11\rangle \leftrightarrow |0\rangle\langle 0| + |1\rangle\langle 1| \leftrightarrow \langle 00| + \langle 11|$. In fact, we are able to consider this bijection for any quantum state and any quantum map—see Table II.

$\psi \in \mathbb{C}^2 \otimes \mathbb{C}^2$	$\leftrightarrow$	$\psi \in \mathbb{C}^2 \to \mathbb{C}^2$	$\leftrightarrow$	$\psi \in (\mathbb{C}^2 \otimes \mathbb{C}^2)^\dagger$
$\lvert 00\rangle + \lvert 11\rangle$	$\leftrightarrow$	$\mathbf{1} = \lvert 0\rangle\langle 0\rvert + \lvert 1\rangle\langle 1\rvert$	$\leftrightarrow$	$\langle 00\rvert + \langle 11\rvert$
$\lvert 01\rangle + \lvert 10\rangle$	$\leftrightarrow$	$\sigma^x = \lvert 0\rangle\langle 1\rvert + \lvert 1\rangle\langle 0\rvert$	$\leftrightarrow$	$\langle 01\rvert + \langle 10\rvert$
$\lvert 01\rangle - \lvert 10\rangle$	$\leftrightarrow$	$i\sigma^z\sigma^x = \lvert 0\rangle\langle 1\rvert - \lvert 1\rangle\langle 0\rvert$	$\leftrightarrow$	$\langle 01\rvert - \langle 10\rvert$
$\lvert 00\rangle - \lvert 11\rangle$	$\leftrightarrow$	$\sigma^z = \lvert 0\rangle\langle 0\rvert - \lvert 1\rangle\langle 1\rvert$	$\leftrightarrow$	$\langle 00\rvert - \langle 11\rvert$
$\lvert 00\rangle + \lvert 01\rangle + \lvert 10\rangle - \lvert 11\rangle$	$\leftrightarrow$	$H = \frac{1}{\sqrt{2}}(\sigma^x + \sigma^z)$	$\leftrightarrow$	$\langle 00\rvert + \langle 01\rvert + \langle 10\rvert - \langle 11\rvert$

FIG. 1. Illustrates the bijection between states, maps and costates for the Bell basis and the Hadamard gate. Normalisation constants are omitted.

In the sections that follow, we will outline different aspects of our model by building on examples. The examples will help build intuition into how a categorical model of quantum circuits can be used.

1. Identity wires revisited

In the Introduction, we already mentioned by example how states are maps, and how maps are states. We have also seen how identity wires relate to Bell states. There is still much room for further abstraction.

Remark II.1. *(Defining identity as a composition of linear maps) More formally, we consider a Hilbert space $\mathcal{H}$ with orthonomal basis $\{|i\rangle\}$ and introduce the linear operators to prove the following theorem (II.2)*

$$\eta := \sum_i |i\rangle \otimes |i\rangle \tag{14}$$

$$\epsilon := \sum_i \langle i| \otimes \langle i| \tag{15}$$

Theorem II.2. *(Bracket-Duality) There exists an isomorphism Ω sending*

$$|\psi\rangle \longleftrightarrow \langle\psi| \tag{16}$$

Proof. We first provide a map between a state/map $|\psi\rangle$ and its transpose.

$$\epsilon(\mathbf{1} \otimes |\psi\rangle) = \sum_i \langle i|\mathbf{1}^\dagger \otimes \langle i|\psi\rangle = \sum_i \langle i|\psi\rangle\langle i| = \langle\psi| \tag{17}$$

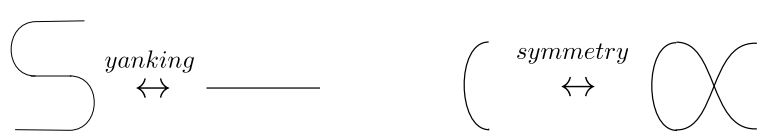
$$(\langle\psi| \otimes \mathbf{1})\eta = \sum_i \langle\psi|i\rangle \otimes |i\rangle = |\psi\rangle \tag{18}$$

Now we consider linear extension of the invertable map

$$\text{overline}(-) : \mathbb{C} \to \mathbb{C}^* :: k \mapsto \overline{k} \tag{19}$$

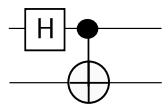
now using this map which defines complex conjugation together with the maps defined above gives Ω, (note that they commute) which establishes the isomorphism we call bracket-duality. □

This so-called bra-ket duality, allows one to define the identity morphism by considering duality of the appropriate bra/ket of ϵ/η.



2. *Compactness: From identity wires to Bell states as cups and caps*

We have already mentioned in the last Section (II 1) that identity wires are in 1-1 correspondence with the Bell states (e.g. $|00\rangle + |11\rangle$), and costates ($\langle 00| + \langle 11|$), where we again note that the relation to identity is not by considering the reduced density matrix. Typically any Bell state is realised by letting the circuit



act on the complete basis $\{|0\rangle, |1\rangle\}^2$, where

$$\mathsf{H} := \underline{\sigma}.\underline{P} = (\sigma^1, \sigma^2, \sigma^3).(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}) = \frac{1}{\sqrt{2}}(\sigma^x + \sigma^z), \tag{20}$$

and the Controlled NOT-gate maps $|a, b\rangle \mapsto |a, a \oplus b\rangle$ for $a, b \in \{0, 1\}$. The standard symmetric Bell state is thus given by letting this circuit act on $|00\rangle$. One of our goals is to examine each component of a quantum circuit, and hence to examine these different two (e.g. maps and wires) and three-legged (e.g. dots) parts under map-state duality. We will soon justify that:

(i): The copy operation given by a black dot ($\bullet$) in a circuit with three connected wires can, under map-state duality be viewed as a multiplication taking elements from $\mathbb{C}^2 \to \mathbb{C}^2 \otimes \mathbb{C}^2$ or equivalently as a GHZ-state.

(ii): The unit (identity) of the multiplication $\bullet$ is given as $|+\rangle := \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and for the multiplication $\oplus$ as $|0\rangle$.

(iii): Likewise from (ii), the dot ($\oplus$) meant to represent XOR addition, under map state duality, defines a multiplication as well a GHZ-state, but this time in the $|\pm\rangle$ basis, instead of the $|0/1\rangle$ basis for $\bullet$.

It is easy to verify in the circuit language that, under map state duality, the unit for the multiplication for $\oplus$ generates the Bell-state when applied to $\bullet$ and vise-versa (see Figure 2). Likewise, when considering the unit for $\bullet$ under map-state duality, one generates the same Bell state. This is called a *compact structure* in category theory, and hence these multiplications, $\bullet$ and $\oplus$, share the same compact structure, and so the categorical quantum circuit algebra has the following graphical rewrites shown in Figure 2:

Remark II.3. *(Bell Basis) Using compactness and single qubit gate operations one is able to generate diagrammatic representations of the remaining three states in the Bell basis (the forth state is generated by acting on the top with a* NOT*-gate, or by acting on the bottom with a* Z*-gate).*

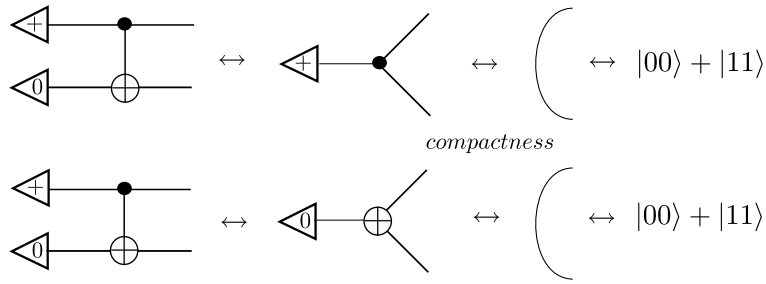
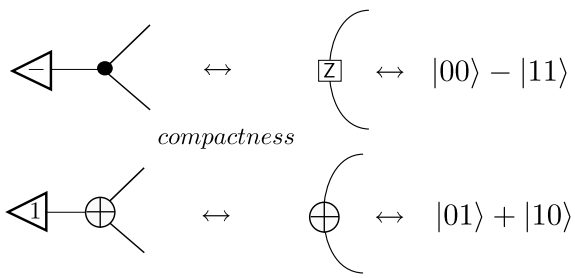


FIG. 2. Showing that the compact structure of the product $\oplus$ is the same as the compact structure of the product $\bullet$. Here the compact structure of the black-dot is used in the lower picture to recover the plus-dot. The compact structure of both dots produce the same cup as $\Phi^+ = |00\rangle + |11\rangle = |++\rangle + |--\rangle$ that is, Φ^+ is invariant under a Hadamard transform.



III. GATES

Readers would have already had some exposure to quantum gates. In what follows, we will explain a general method to construct controlled two-qubit gates. This is important as it could be presented as 'machine code' to several types of quantum computers — including NMR Quantum Computation (JA Jones in Oxford Physics).

A. From Hamiltonians to the CN-gate

The Controlled NOT-gate is fundamental to many universal quantum processor proposals. The map performs

$$\mathsf{CN} : \mathbb{C}^2 \otimes \mathbb{C}^2 \to \mathbb{C}^2 \otimes \mathbb{C}^2 :: |a\rangle \otimes |b\rangle \mapsto |a\rangle \otimes |a \oplus b\rangle \tag{21}$$

with $a, b \in \{0, 1\}$. The CN gate is self inverse, Hermitian and hence has a spectrum in ± 1. It is possible to realize the unitary CN gate by exponentiating the Hamiltonian

$$H_{\mathsf{CN}} = |1\rangle\langle 1| \otimes \sigma^x + |0\rangle\langle 0| \otimes \mathbf{1} \tag{22}$$

as $H_{\mathsf{CN}}^2 = \mathbf{1}$ using

$$\exp[-itH_{\mathsf{CN}}] = \mathbf{1}\cos(t) - iH_{\mathsf{CN}}\sin(t) \tag{23}$$

for $t = \pi/2$. The phase factor $-i\mathbf{1}$ commutes with all elements of the group and can safely be ignored when considering a two-qubit system. However, the phase factor becomes relevant when the CN-gate acts on a component of a larger composite system.

It is typically the case that one must realise CN as a sequence of Unitaries, generated by timing a Hamiltonian (such as (1)) to sequence gates, as quantum processors will not have a Hamiltonian with all controllable couplings (particularly $\sigma^z\sigma^x$) and hence won't be capable of realising H_{CN} as the evolution of a single Hamiltonian. By using the standard factorisation of Unitary maps via the Schur decomposition, we will describe a general method to realise any controlled two-qubit gate, of which the CN-gate becomes a special case.

Let CU be a controlled unitary and then $U = PDP^\dagger$ where P is a unitary change of basis, and D is diagonal as U is normal. We then write

$$CU = |1\rangle\langle 1| \otimes PDP^\dagger + |0\rangle\langle 0| \otimes \mathbf{1} \tag{24}$$

P acts on the single qubit state space $\mathbb{C}^2$ and so can be realized by an evolution $P = \exp[-it\underline{\sigma}.\underline{A}]$. By finding the logarithm a suitable polarisation vector $\underline{A}$ can be found, and P can be realised up to a global phase factor.

Alternatively, it is well known in the theory of Lie groups that any element in the group $\mathbf{U}(2)$ can be written as a product

$$\forall U \in \mathbf{U}(2),\ \exists \alpha, \beta, \gamma \in \mathbb{R}, \quad \text{such that} \quad U = \exp[-i\alpha\sigma^i]\exp[-i\beta\sigma^j]\exp[-i\gamma\sigma^i] \tag{25}$$

where $i \neq j \in \{x, y, z\}$, and where we have neglected the global phase term $\exp[-i\kappa]$.

What remains is to realize the Hermitian term

$$|1\rangle\langle 1| \otimes D + |0\rangle\langle 0| \otimes \mathbf{1} \tag{26}$$

which is diagonal is the computational basis and hence can be generated by a controllable Hamiltonian with an Ising type interaction

$$H_I = \sum_i h_i\sigma_i^z + \frac{1}{2}\sum_{i,j} J_{ij}\sigma_i^z\sigma_j^z \tag{27}$$

For instance, a term such as $|0\rangle\langle 0|_1 \otimes \mathbf{1}$ can be generated by exponentiating $\frac{1}{2}(1 + \sigma_1^z)$ and for $D = \mathrm{diag}(\lambda_0, \lambda_1)$, straightforward calculation yields

$$\frac{\lambda_0 + \lambda_1}{4}(\mathbf{1} - \sigma_1^z) + \frac{\lambda_1 - \lambda_0}{4}\sigma_2^z + \frac{\lambda_1 - \lambda_0}{4}\sigma_1^z\sigma_2^z \tag{28}$$

and hence we can read of the values for the coupling matrix $(J_{ij})_{ij}$ and the coupling vector $(h_i)_i$. Since the terms in (III A) all commute, any sequence of the gates realising each term will realise the operator.

Example III.1. *(Preparing Bell states) In the present Section (III A), we have described a general method to construct any general controlled gate acting on the two-qubit Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$. Realisation of the symmetric Bell state $|00\rangle + |11\rangle$ can be done by preparing*

a state into the product eigenstate $|0\rangle \otimes |0\rangle$ *of observable* $\sigma^z\sigma^z$ *and then acting on it by a Hamiltonian* $\sigma^x\sigma^x$*. Since* $\sigma^x\sigma^x|00\rangle = |11\rangle$ *we can guess that the Bell state will be in the single parameter subgroup generated by this Hamiltonian. In other words,*

$$\exp[-it\sigma_1^x\sigma_2^x]|00\rangle \approx [1 - it\sigma_1^x\sigma_2^x + o(t^2)]|00\rangle \tag{29}$$

has overlap with the target state of interest (similarly, $\exp[-it\sigma^z\sigma^z]|+\rangle|+\rangle = |00\rangle + |11\rangle + o(t^2)$*). Clearly, this Hamiltonian squares to identity and hence from* (I A) *we find*

$$\exp[-it\sigma_1^x\sigma_2^x] = \mathbf{1}\cos(t) - i\sigma_1^x\sigma_2^x\sin(t) \tag{30}$$

and on choosing $t = \pi/2$ *one recovers the desired Bell state, up to a phase factor which can be removed, or safely ignored, depending on application.*

Exercise III.2. *Construct a single qubit unitary map and corresponding Hamiltonian to map 30 into* $|00\rangle + |11\rangle$*.*

B. Transforming atemporal graphs into casually connected quantum processes

As we have mentioned, quantum circuits are acyclic directed diagrams, where by convention time passage is typically considered as moving from left to right on the page. In such diagrams, the wires from left to right on the page are the qubits, whereas the wires going up and down on the page are logical connections (see Figure III B). These logical connections can be replaced with qubits, and we call such wires, *virtual qubits*. In the categorical model, the three networks are considered equivalent in terms of string diagrams. They can be realised as a casually connected set of operations on a quantum computer. This is illustrated in Figure III B.

Placing cups at the start of a quantum circuit (on the left) can be accomplished by preparing Bell states. The caps at the ends (on the right) of a circuit appear to be diagrams that are directed backwards in time — see Figure III B. As the figure shows, they can be constructed sequentially in time by preforming a Bell basis measurements with correction (dependent on outcome) or by post-selection.

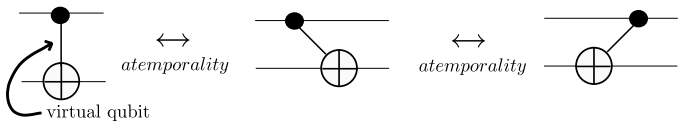


FIG. 3. The atemporality circuit rewrite rule allows one to transform quantum circuits in non-standard ways. Using bra-ket duality, temporality can always be restored and hence, the quantum state corresponding to any of the networks we consider in this work can always be realised by a quantum process.

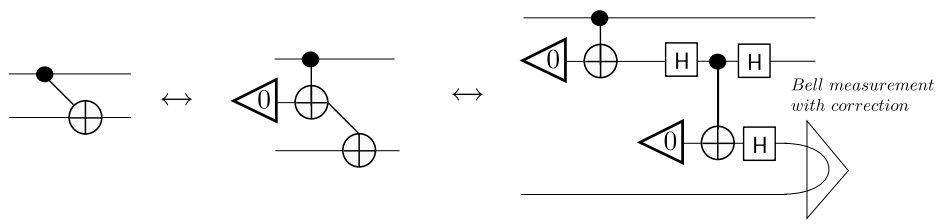


FIG. 4. Atemporality can result in several equivalent physical realisations of the same network. Because there are maps from two qubits into a single qubit state space, the circuit on the left must be transformed for realisation on a quantum processor. The equivalent circuit on the right is casually connected, provided all of the operations are preformed from left to right, including the Bell-basis measurement with correction.

Remark III.3. *Typically in quantum circuits, at each time slice (that is vertically divided between gates), one will factor the network into a sequence of gates, each of which is unitary. In the general networks considered here, although each time-slice is a valid quantum process, each slice does not always represent a unitary map.*

IV. GRAPHICAL TRANSPOSE OF A LINEAR MAP

A common theme in this course is duality of states and maps. Here we will present some nice examples of these concepts.

We can consider a map U which can be written as

$$U = \sum_{ij} u_{ij} |i\rangle\langle j| \tag{31}$$

we recall the linear maps

$$\eta = \sum_i |i\rangle \otimes |i\rangle \tag{32}$$

$$\epsilon = \sum_i \langle i| \otimes \langle i| \tag{33}$$

and consider the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$. Consider the map U acting on $\mathcal{H}_2$. We can then act with η and ϵ to bend the wires of U and hence construct a map from $\mathcal{C} \to \mathcal{H}_1 \otimes \mathcal{H}_2$ or $\mathcal{C} \to \mathcal{H}_2 \otimes \mathcal{H}_3$ depending on which wire of U we wish to bend and which Hilbert space we let η or ϵ act. Consider

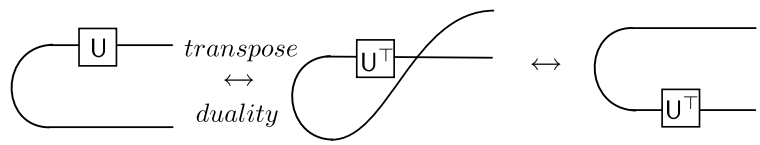
$$\epsilon_{12} \circ U = \sum_{ijk} u_{jk} \langle i|\langle i|j\rangle\langle k| = \sum_{ijk} u_{jk} \langle i|\delta_{ij}\langle k| = \sum_{jk} u_{jk} \langle j|\langle k| \tag{34}$$

which is simply a costate representation of the map U, whereas the following amount to

taking a transpose before performing the costate representation:

$$\epsilon_{23} \circ U = \sum_{ijk} u_{jk} \langle i|j\rangle \langle k|\langle i| = \sum_{jk} u_{jk} \langle k|\langle j| = \epsilon_{12} \circ U^{\top} \tag{35}$$

We have delt above with costates, the graphical calculus version of these properties on states are as follows



A. Example: Duality of the CV-gate

This example was not in the lectures. Let U_n be a unitary operator meant to act on a register of n-qubits, depending on the state of some other register. This general setup is a straightforward extension of the controlling register being a single qubit.

$$\mathrm{CU}_{it} = |1\rangle\langle 1|_i \otimes U_t + |0\rangle\langle 0|_i \otimes \mathbf{1}_t, \tag{36}$$

where index i designates the controlling qubit and index t the target.

Consider the gate $\mathsf{V} = \frac{1}{2}\left((1+i)\sigma_x + (1-i)\mathbf{1}\right)$ such that $\mathsf{V}^2 = \mathsf{NOT}$. The controlled V gate has received a lot of interest as it provided one of the first factorisations of universal quantum circuits. Consider the logical XOR operation expressed over the reals, $x \oplus y = x + y - 2xy$. Now raise unitary U to the power of this expression as $U^{x\oplus y} = U^{x+y-2xy}$, rearranging yields $U^{2xy} = U^{-x\oplus y}U^{x+y}$, hence $\mathsf{NOT}^{xy} = (\mathsf{V}^{\dagger})^{x\oplus y}\mathsf{V}^x\mathsf{V}^y$ provides a factorisation of the Toffoli gate, where x, y become logical qubit states and the gate realises the function $|x, y, z\rangle \mapsto |x, y, x \wedge y \oplus z\rangle$.

Let us then consider map state duality applied to the CV gate

$$\mathsf{CV} = \frac{1}{2}|1\rangle\langle 1|_i \otimes \left((1+i)\sigma_x + (1-i)\mathbf{1}\right) + |0\rangle\langle 0|_i \otimes \mathbf{1} \tag{37}$$

We want to express this as a state in Hilbert space. First, the unit for the control is $|+\rangle$. Letting this gate act on $|+\rangle \otimes \mathbf{1}$ where we use compactness results in the map

$$\mapsto \frac{1}{2}|1\rangle \otimes \left((1+i)(|0\rangle\langle 1| + |1\rangle\langle 0|) + (1-i)(|0\rangle\langle 0| + |1\rangle\langle 1|)\right) + |0\rangle \otimes (|0\rangle\langle 0| + |1\rangle\langle 1|). \tag{38}$$

We then want to flip the direction of the bra $\langle\ |$, in the bracket $|\ \rangle\langle\ |$. This can be done by using a cup $\supset$, which is represented by the Bell state $|00\rangle + |11\rangle$ acting on the second qubit state space.

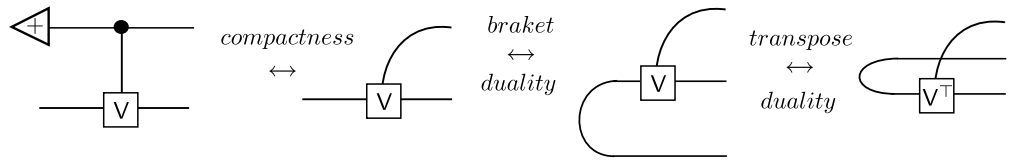


FIG. 5. A figure showing several rewrite rules applied to the controlled V-gate, starting with compactness of the black-dot. The duality rewrite rule one from the rightmost (e.g. bending a wire) is equivalent to preparing a Bell state and is justified by considering the action of the linear map $\epsilon := \sum_i \langle i| \otimes \langle i|$. The rightmost duality is justified in Section IV.

V. VIOLATION OF BELL'S INEQUALITY

In the lectures we presented a violation of Bell's inequality. The calculation was made trivial uses some of the mathematical tricks we presented during the first half of the class. We considered the singlet state

$$\Phi^- = |01\rangle - |10\rangle \tag{39}$$

We showed that with $\mathbf{A}^2 = \mathbf{B}^2 = \mathbf{1}$ and if

$$\langle\Phi^-|(\mathbf{A}\otimes\mathbf{B})\Phi^-\rangle = \langle\Phi^-|(\mathbf{A}\otimes\mathbf{1})\Phi^-\rangle\langle\Phi^-|(\mathbf{1}\otimes\mathbf{B})\Phi^-\rangle \tag{40}$$

then this implies that

$$\langle\Phi^-|(\mathbf{A}_1\otimes\mathbf{B}_1)\Phi^-\rangle + \langle\Phi^-|(\mathbf{A}_1\otimes\mathbf{B}_2)\Phi^-\rangle + \langle\Phi^-|(\mathbf{A}_2\otimes\mathbf{B}_1)\Phi^-\rangle - \langle\Phi^-|(\mathbf{A}_2\otimes\mathbf{B}_2)\Phi^-\rangle \leq 2 \tag{41}$$

where we will express these observables as polarisation vectors

$$\mathbf{A}_1 = (A_1, A_2, A_3).(\sigma^x, \sigma^y, \sigma^z) \tag{42}$$

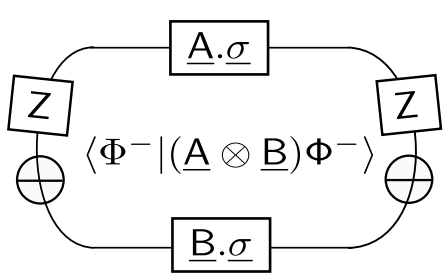
$$\mathbf{B}_1 = (B_1, B_2, B_3).(\sigma^x, \sigma^y, \sigma^z) \tag{43}$$

are observables representing spin projections along two vectors.

We will then consider

$$\sigma_1^z\sigma_1^x(|00\rangle + |11\rangle) = |01\rangle - |10\rangle \tag{44}$$

The general expectation value $\langle\Phi^-|(\mathbf{A}\otimes\mathbf{B})\Phi^-\rangle$ is given diagramatically as



The operators σ^z and σ^x are self adjoint and so slide on boxes unchanged. They then

evalulate their action on the basis of $(A_1, A_2, A_3).(\sigma^x, \sigma^y, \sigma^z)$ as

$$\sigma^z \sigma^x (\sigma^x, \sigma^y, \sigma^z) \sigma^x \sigma^z \tag{45}$$

Now recalling that

$$\sigma_i \overline{\sigma_j} \sigma_i = -\sigma_j \tag{46}$$

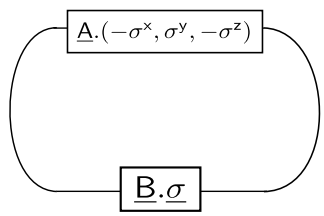
whenever $i \neq j$ (if $i = j$ this map acts trivially). With this definition, we see that σ^x takes the basis to

$$\sigma^z (\sigma^x, -\sigma^y, -\sigma^z) \sigma^z \tag{47}$$

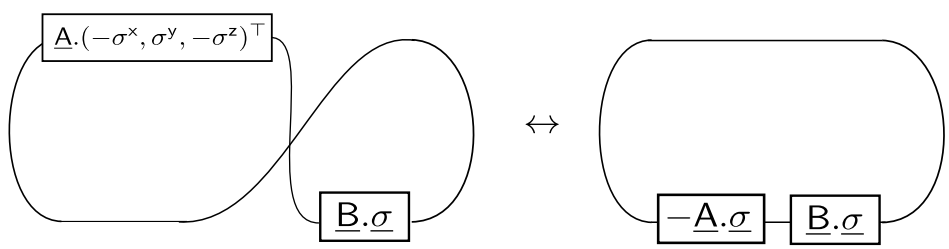
and finally, σ^z takes this basis to

$$(-\sigma^x, \sigma^y, -\sigma^z) \tag{48}$$

which diagramatically becomes



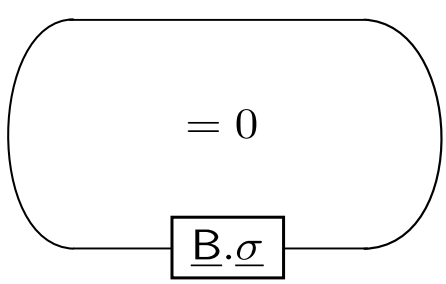
and to evalulate the product, we will need to 'slide' one of the operators around the wires to interact with the other. This is done by considering transpose duality. Sliding a box around a wire takes a transpose in this case, which is given diagrammatically as



The crux of the matter is that the product (using the results from Section I A) then becomes

$$\underline{A}.\underline{B} = \cos\theta \tag{49}$$

Exercise V.1. *Using the definitions of η and ϵ or otherwise, show that the following diagram gives zero for any polarisation vector $\underline{B}$*



VI. REMARKS

That concluded the first lecture.

- Course homepage: http://www.comlab.ox.ac.uk/activities/quantum/course/
- See also the tablet PC generated notes from the lecture!
- If you see any typos please let me know. Thanks to **Shane Mansfield** for doing just that!

VII. REFERENCES

- S Abramsky and B Coecke, A categorical semantics of quantum protocols, Logic in Computer Science, 2004. http://arxiv.org/pdf/quant-ph/0402130
- Bob Coecke and Ross Duncan, Interacting Quantum Observables: Categorical Algebra and Diagrammatics, 2009. http://arxiv.org/abs/0906.4725
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