Are all reversible computations tidy?

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Abstract

It has long been known that to minimise the heat emitted by a deterministic computer during its operation it is necessary to make the computation act in a logically reversible manner [Lan61]. Such logically reversible operations require a number of auxiliary bits to be stored, maintaining a history of the computation, and which allows the initial state to be reconstructed by running the computation in reverse. These auxiliary bits are wasteful of resources and may require a dissipation of energy for them to be reused. A simple procedure due to Bennett [Ben73] allows these auxiliary bits to be "tidied", without dissipating energy, on a classical computer. All reversible classical computations can be made tidy in this way. However, this procedure depends upon a classical operation ("cloning") that cannot be generalised to quantum computers [WZ82]. Quantum computations must be logically reversible, and therefore produce auxiliary qubits during their operation. We show that there are classes of quantum computation for which Bennett's procedure cannot be implemented. For some of these computations there may exist another method for which the computation may be "tidied". However, we also show there are quantum computations for which there is no possible method for tidying the auxiliary qubits. Not all reversible quantum computations can be made "tidy". This represents a fundamental additional energy burden to quantum computations. This paper extends results in [Mar01].

1 Reversible Classical Computation

A reversible calculation may be defined as one which operates, upon an input state \( i \) and an auxiliary system, prepared in an initial 'known' state \( \text{Aux}0 \), to produce an output from the calculation \( O(i) \), and some additional information \( \text{Aux}(i) \):

\[
F : (i, \text{Aux}0) \rightarrow (O(i), \text{Aux}(i))
\]

in such a manner that there exists a complementary calculation:
Given that the mapping \( i \rightarrow O(i) \) will, for deterministic computation, be many-to-one, the existence of the auxiliary output bits is necessary to uniquely specify the input state from the output state, so that the computation can be reversed. They may be considered to be a ‘history’ of the computation that retains the information that an irreversible computation would have discarded.

A general procedure for discovering the complementary calculation \( F' \) can be given like this:

- Take all the logical operations performed in \( F \), and reverse their operation and order.

As long as all the logical operations in \( F \) are reversible logic gates, this is possible. It is known that the reversible Fredkin-Toffoli gates are capable of performing all classical logical operations, so it is always possible to make a computation logically reversible.

However, they also represent wasted resources which we would like to recover, to be used in further calculations. One way to do this would be to reset the bits using Landauer Erasure\[^{[Lan61]}\]. However, this would require work to be performed upon the system which would be dissipated as heat. Another way to recover the bits would be to reverse the computation, using \( F' \), but this would lose us all record of the output of the computation, so is of little use.

Bennett\[^{[Ben73]}\] showed that a solution was to find a different reverse calculation \( F'' \)

\[
F'': (O(i), Aux(i)) \rightarrow (i, Aux0)
\]

The reconstruction of the original input states \( i \) is sufficient to secure reversibility. A general procedure for \( F'' \), is:

- Copy \( O(i) \) into a further auxiliary system \( AuxO \) by means of a Controlled-NOT gate;
- Run \( F' \) on the original system.

This has also been shown to be the optimal procedure\[^{[LTV98, LV96]}\] for \( F'' \). We call such a calculation TIDY. All classical reversible computations can be made TIDY.

The great strength of Bennett’s procedure is that it does not require any calculation of what are the specific, determinate but ‘unknown’, states of the auxiliary bits or the output states. Although they will be some determinate function of the input states, (eg. of the form \( (A \ XOR \ B) \ AND \ (C \ OR \ D) \) ) we cannot use this directly to reset the auxiliary states non-dissipatively (eg. by calculating whether the state is zero or one and performing a NOT operation upon it if it is one). To construct such an augmented computation, we would first have to calculate what the outputs would be for each input state and this is just to run the calculation \( F \) itself!
2 Reversible Quantum Computation

When we attempt to apply Bennett’s procedure to quantum computations, we find it can fail. The cause is well known. The problem is that the Controlled-NOT gate does not act as a universal copying gate for quantum computers. In fact, the universal copying gate does not exist, as a result of the ‘no-cloning theorem’ [WZ82].

Clearly, in the case where the output states from a quantum computer are in a known orthogonal set, then the quantum computation can be made tidy. This is suggestive not of a general quantum computation, but of limited quantum algorithmic boxes: each connected by classical communication. Distributed quantum information may be desirable - in particular, a more general conception of quantum computation may be required which takes inputs from different sources, and/or at different times. In Figure 1 we see an example of this - Alice performs some quantum computation, and stores the result of it in a ‘quantum data warehouse’. At some later time, Bob takes part of these results as an input into his own computation.

We are going to take our definition of a quantum computation\(^1\) as the operation:

\[
U_C : |i\rangle |Aux0\rangle \rightarrow |O(i)\rangle |Aux(i)\rangle
\]

so that the output is always in a separable state.

In other words, we regard the ‘output’ of the computation as the subsection of the Hilbert space that is interesting, and the ‘auxiliary’ as everything that is uninteresting. If the ‘output’ were entangled with the ‘auxiliary’ space, then there would be additional information relevant to the ‘output’, contained in the super-correlations.

\(^1\)There is further complication when entanglement enters the problem. When the output part of an entangled state is non-recoverably transmitted, the loss of free energy in the remainder is always at least equal to \(kT\) times the entropy of the reduced density matrix of the output. However, this minimum loss of free energy requires knowledge of an accurate representation of the resulting density matrix - which may not be possible without explicitly calculating the output states.
between 'output' and 'auxiliary' spaces. In any event, such entanglement can only increase the energy lost.

As any quantum computation must be performed by a unitary operation, all quantum computers must be reversible. But are they TIDY?

If this model of computation is classical, then each time data is sent to the central database, the local user can copy the data before sending it, and tidy up their computer as they go along. At end of all processing - if it happens - reconstruction of computation from stored input would allow tidying of any stored data no longer needed. The difference between computation using distributed classical algorithmic boxes and a single classical computation is a trivial distinction, as the computation may be tidied up along the way. However, this distinction depends upon the classical nature of the information transferred between the algorithmic boxes.

In our generalised quantum computation network, we can no longer guarantee that the operations performed at separate locations are connected by classical signals only. We now need to generalise the definition of tidiness to quantum computers.

Considering a general operation, unitarity requires that the inner products between different input states and between the corresponding output states is unchanged by the computation. Reversibility must always hold. This leads to the conditions:

Reversible

\[ \langle i | j \rangle \langle Aux0 | Aux0 \rangle = \langle O(i) | O(j) \rangle \langle Aux(i) | Aux(j) \rangle \]

Tidy

\[ \langle i | j \rangle \langle Aux0 | Aux0 \rangle \langle AuxO | AuxO \rangle = \langle i | j \rangle \langle O(i) | O(j) \rangle \langle Aux0 | Aux0 \rangle \]

We can eliminate \( \langle Aux0 | Aux0 \rangle = 1 \) and \( \langle AuxO | AuxO \rangle = 1 \), leaving only three cases.

### 2.1 Orthogonal Outputs

The output states are orthogonal set:

\[ \langle O(i) | O(j) \rangle = \delta_{ij} \]

Reversibility requires the input states to be an orthogonal set \( \langle i | j \rangle = 0 \), and the TIDY condition will hold. This is not too surprising, as an orthogonal set of outputs can be cloned, and so can be tidied using Bennett’s procedure.

### 2.2 Orthogonal Inputs

The input states are an orthogonal set \( \langle i | j \rangle = \delta_{ij} \), but the output states are not. To satisfy reversibility, this requires the auxiliary output states are orthogonal.

\[ \langle Aux(i) | Aux(j) \rangle = \delta_{ij} \]
Now, when we examine the TIDY condition, we find there does exist a unitary operator (and therefore a computable procedure) for tidying the computation, without losing the output. However, this tidying computation is not Bennett’s procedure. If we were to clone the auxiliary output, and run the reverse operation, we would lose the output, and be left with the ’junk’!

It is possible\(^2\) to construct a modified version of Bennett’s procedure for this case:

- Copy the joint states \(|O(i)\rangle |Aux(i)\rangle\) to a second system. As these states are mutually orthogonal, due to the orthogonality of the \(|Aux(i)\rangle\) states, a controlled-NOT gate can be constructed working in this basis.

- Conditionally reset the copy of the \(|Aux(i)\rangle\) states using the originals:

\[
U_R : |Aux(i)\rangle |Aux(i)\rangle \rightarrow |Aux(i)\rangle |Aux0\rangle
\]

This is also possible, by constructing a controlled-NOT gate in the \(|Aux(i)\rangle\) basis.

- Reverse the computation, leaving only the copied output states.

However, this raises an interesting complication: do we know the two basis in question? The strength of Bennett’s procedure for classical computations is that we do not need to know the contents of the output or auxiliary bits. For quantum computations we have no universal copying operation. We can construct copying operations for any given orthogonal set of states, but this means that to implement the tidying procedure we need to know in advance at least the orthogonal basis in which the copying operation needs to take place. Note, we do not need to know which specific output states \(|O(i)\rangle |Aux(i)\rangle\) are associated with the specific input states \(|i\rangle\), but we do need to know what the set of auxiliary output states \(|Aux(i)\rangle\) will be and their correlation to the useful output states \(|O(i)\rangle\).

It is not clear whether the operator can be constructed without explicitly computing each of the auxiliary output states on a second system - which may entail re-running the computation itself, for each input, and measuring the auxiliary output basis\(^3\). This is precisely the problem that Bennett’s procedure avoids for classical computation.

### 2.3 Non-orthogonal Inputs

The input states are a non-orthogonal set. This corresponds to Bob’s position in the quantum distribution network of Figure 1, and should be considered the most general case.

If we look at the requirements for a TIDY computation, this leads to:

\[
\langle O(i) | O(j) \rangle = 1
\]

\(^2\)This section revises results reported in [Mar01, Mar02].

\(^3\)A similar problem, of constructing a Controlled-NOT in a specific basis, exists for the case of orthogonal outputs, but in this case it seems reasonable assume that we do know in advance the set of the output states we are trying to compute, just not their relation to the input states.
The output is always the same, regardless of the input! Obviously for a computation to be meaningful, or non-trivial, at least some of the output states must depend in some way upon the particular input state. So in this case we can say there are NO procedures $F''$ that allow us to tidy our output from $F$. To state this exactly:

There does not exist any non-trivial ($|O(i)\rangle \neq |O(j)\rangle$) computations of the form

$$ G : |i\rangle |Aux0\rangle |AuxO\rangle \rightarrow |i\rangle |Aux0\rangle |O(i)\rangle $$

for which $\langle i | j \rangle \neq \delta_{ij}$.

It should be made clear: this does NOT mean useful quantum computations of the form

$$ F : |i\rangle |Aux0\rangle \rightarrow |Aux(i)\rangle |O(i)\rangle $$

do not exist if $\langle i | j \rangle \neq \delta_{ij}$ - simply that such computations cannot be TIDY. For such computations, not only are the bits used to store the auxiliary output unrecoverable, without dissipating energy, but also the input state cannot be recovered, except through losing the output. For our distributed network, this means that not only can Bob not tidy his computation, but he cannot restore Alice’s data to the database.

### 3 Conclusion

For classical computations, Bennett provides a procedure by which a reversible computation may be made tidy. The great advantage of this procedure is that it does not require one to have advance knowledge of the output of the computation. Instead, simply the knowledge of the successive logical operations comprising the computation is sufficient to implement the tidying procedure.

However, this procedure rests upon the use of the Controlled-NOT operator, to clone the output states. For a general quantum computation this is not possible. Where the output states of a quantum computation form an orthogonal set, then a Controlled-NOT style gate can indeed be constructed. For such computations Bennett’s procedure will work. If the output states of a quantum computation are not orthogonal, then the required generalisation of a Controlled-NOT gate would be a quantum state cloning device, and no such device exists.

When the input states are orthogonal, then for non-orthogonal output states, the auxiliary outputs must be an orthogonal set. In this case we know that a unitary operator must exist for the tidying procedure. However, unlike for Bennett’s procedure, it is unclear that there is a simple prescription for finding the tidying operation. If we are given the output auxiliary states, then we can derive a suitable operation. However, we will not, in general, know these states without having to actually perform the calculation with all the possible input states. Thus this method defeats the purpose of trying to produce the tidy computation.

Finally where input states are not orthogonal, then there is no possible tidying algorithm. To recover the auxiliary bits requires a dissipative resetting. This represents a fundamental energy requirement upon quantum computations that is not present in classical computations.
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