On the role of entanglement in quantum computational speed-up

Richard Jozsa† and Noah Linden§

†Department of Computer Science, University of Bristol, Merchant Venturers Building, Bristol BS8 1UB U.K.
§Department of Mathematics, University of Bristol, University Walk, Bristol BS8 1TW U.K.

Abstract

For any quantum algorithm operating on pure states we prove that the presence of multi-partite entanglement, with a number of parties that increases unboundedly with input size, is necessary if the quantum algorithm is to offer an exponential speed-up over classical computation. Furthermore we prove that the algorithm can be classically efficiently simulated to within a prescribed tolerance $\eta$ even if a suitably small amount of global entanglement (depending on $\eta$) is present. We explicitly identify the occurrence of increasing multi-partite entanglement in Shor’s algorithm. Our results do not apply to quantum algorithms operating on mixed states in general and we discuss the suggestion that an exponential computational speed-up might be possible with mixed states in the total absence of entanglement. Finally, despite the essential role of entanglement for pure state algorithms, we argue that it is nevertheless misleading to view entanglement as a key resource for quantum computational power.

1 Introduction

Quantum computation is generally regarded as being more powerful than classical computation. The evidence for this viewpoint begins with Feynman’s pioneering observation [1] that the simulation of a general quantum evolution on a classical computer appears to require an exponential overhead in computational resources compared to the physical resources needed for a direct physical implementation of the quantum process itself. Subsequent work by Deutsch [2], Bernstein and Vazirani [3], Simon [4], Grover [5], Shor [6] and others showed how quantum evolution can be harnessed to carry out some useful computational tasks more rapidly than by any known classical means. Perhaps the most dramatic such result is Shor’s quantum algorithm for integer factorisation which succeeds in factoring an integer of $n$ digits in a running time that grows less rapidly than $O(n^3)$ whereas the best known classical algorithm is exponentially slower (with running time $O(\exp(n^{\frac{1}{3} \log n^2}))$). Thus for some computational tasks (such as factoring) quantum physics appears to provide an exponential benefit but for other tasks (such as satisfiability or other NP complete problems[7]) the quantum benefits appear to be inherently more restricted[8] (giving perhaps at most a polynomial speedup).

The concept of computational power provides a fundamentally new language and set of tools for studying the relationship between classical and quantum physics. Indeed it is of great interest to try to characterise from this point of view, the essential non-classical ingredients that give rise to the enhanced quantum computational power. Also an understanding
of the limitations of quantum computational power (such as the apparent lack of an efficient solution of an NP complete problem) may provide insights into the strange architecture of the quantum formalism, perhaps even leading to physical principles, formulated in terms of the concept of computational complexity, that may guide the development of new physical theories by severely restricting acceptable forms of proposed new formalisms. Indeed arbitrarily created “toy” physical theories (including most proposed non-linear generalisations of quantum theory[9]) tend to engender immense computing power. The apparently limited nature of quantum computational power makes quantum theory rather atypical so this observation is probably significant.

One fundamental non-classical feature of the quantum formalism is the rule for how the state space \( S_{AB} \) of a composite system \( AB \) is constructed from the state spaces \( S_A \) and \( S_B \) of the parts \( A \) and \( B \)[11]. In classical theory, \( S_{AB} \) is the cartesian product of \( S_A \) and \( S_B \) whereas in quantum theory it is the tensor product (and the state spaces are linear spaces). This essential distinction between cartesian and tensor products is precisely the phenomenon of quantum entanglement viz. the existence of pure states of a composite system that are not product states of the parts.

In quantum theory, state spaces always admit the superposition principle whereas in classical theory, state spaces generally do not have a linear structure. But there do exist classical state spaces with a natural linear structure (e.g. the space of states of an elastic vibrating string with fixed endpoints) so the possibility of superposition in itself, is not a uniquely quantum feature.

In [11, 13] it was argued that there is a relationship between entanglement and the apparent ability of a quantum process to perform a computational task with exponentially reduced resources (compared to any classical process). We briefly recall the two main points made in [11, 13]. The first point concerns the physical resources needed to represent superpositions in quantum versus classical theory. To represent a superposition of \( 2^n \) levels classically, the levels must all correspond to a physical property of a single system (with no subsystems) as classical states of separate systems can never be superposed. Hence we will need an exponentially high tower of levels and the amount of the physical resource needed will grow exponentially with \( n \). In contrast, in quantum theory because of entanglement, a general superposition of \( 2^n \) levels may be represented in \( n \) 2-level systems. Thus the amount of the physical resource (that defines the levels) will grow only linearly with \( n \) (i.e. the number of 2-level systems). In the classical case one may attempt to circumvent the need for an exponential tower by considering a linear system with infinitely many levels that accumulate below a finite upper bound. In this way we could represent exponentially growing superpositions with only a constant cost in the physical resource. But now the levels must crowd exponentially closely together and we will need to build our instruments with exponentially finer precision. This again will presumably require exponentially increasing physical resources.

This first point may be expressed in more computational terms as follows. Any positive integer \( N \) may be represented in unary or binary. The unary representation (being a string of 1’s of length \( N \)) is exponentially longer than the binary representation (having length \( \log N \)). We may equivalently take the unary representation as a string of \((N - 1) 0's\)
followed by a single 1, which we view as a single mark at height $N$. Now consider physical implementations of these representations of numbers. The unary representation corresponds to the $N^{th}$ level of a single system and hence we can superpose unary representations of numbers in either classical or quantum physics. For binary numbers we can exploit the compactness of the representation by using $\log N$ 2-level systems. In that case we can superpose these representations in quantum theory but not in classical theory. In summary, physical representations of binary numbers exist in both classical and quantum systems but only in the quantum case can these representations be superposed. This is precisely the phenomenon of quantum entanglement. If we wish to perform computations on superpositions of numbers in a classical setting then this is possible but we must use the exponentially more costly unary representation i.e. the quantum formalism offers a far greater potential power for computations in superposition.

The second point made in [11] concerns the classical computational cost of mimicking a typical step in a quantum computation, which we epitomise as follows. Suppose that at some stage of a quantum computation the state is an $n$-qubit (generally entangled) state $|\alpha\rangle = \sum a_{i_1...i_n} |i_1\rangle \ldots |i_n\rangle$ and suppose that the next step is the application of a 1-qubit gate $U$ to the first qubit. The updated state is then $|\alpha'\rangle = \sum a'_{i_1i_2...i_n} |i_1\rangle \ldots |i_n\rangle$ where

$$a'_{i_1i_2...i_n} = \sum_{j_1} U_{i_1j_1} a_{j_1i_2...i_n}$$

and $U_{ij}$ are the matrix elements of $U$. This is only one step of quantum computation, on only $n$ qubits, but to classically compute the updated state description via eq. (1) we would require exponentially many arithmetic operations and also the classical description of the state itself is exponentially large (compared to the compact $n$ qubit quantum physical representation). Now the point is that these exponential gaps between classical and quantum resources can be connected to the concept of entanglement as follows. If the state $|\alpha\rangle$ were unentangled i.e. if $a_{i_1...i_n}$ is given as a product $a_{i_1}b_{i_2} \ldots d_{i_n}$ then for the classical representation, both the state description and the computation of its update become polynomially sized, with $O(n)$ resources for the state description and a constant amount of computation for the update, and these are now equivalent to the corresponding quantum resources. This suggests that if entanglement is absent in a quantum algorithm then the algorithm can be classically simulated with an equivalent amount of classical resources. Stated otherwise, if a quantum algorithm (on pure states) is to offer an exponential speedup over classical algorithms, then entanglement must appear in the states used by the quantum algorithm.

Our discussion above has been qualitative and we have glossed over various significant issues. Firstly, the terms in eq. (1) are complex numbers and from a computational point of view they have potentially infinite sized descriptions. Hence they will need to be restricted to, or replaced by, suitably finitely describable numbers (such as rationals) if we are to avoid a potentially prohibitively large cost for the classical computation of individual arithmetic operations. The second issue concerns how much entanglement and what type of entanglement is required if a quantum algorithm is to offer exponential speedup over classical algorithms. This is a main concern of the present paper. Let $p$ be any fixed positive integer. A state of $n$ qubits will be called $p$-blocked if no subset of $p + 1$ qubits are entangled together. Thus a $p$-blocked state may involve a large amount of entanglement.
but this entanglement is restricted, in its multi-partiteness, to sets of a most \( p \) qubits. Now suppose that a quantum algorithm has the property that the state at each step is pure and \( p \)-blocked. We note that the qubits in each block can vary from step to step in the algorithm; indeed each qubit can be entangled with every other qubit at some stage of the computation. Then we will show that again the algorithm can be classically simulated with an amount of classical resources that is equivalent to the quantum resources of the original algorithm (i.e. the classical resources needed are polynomially, but not exponentially, larger than the quantum resources).

We note that, in contrast, in communication tasks, entanglement restricted to merely bi-partite entanglement suffices for exponential benefits (for example an exponential reduction of communication complexity [19]) but for “standard” computational tasks our results show that the availability of (even increasing amounts of) only bi-partite entanglement cannot give an exponential speed-up (despite the fact that 2-qubit gates suffice for universal computation). Also our results show that a distributed quantum computer, which has any number of quantum processors but each with bounded size and only classical communication between them, cannot offer an exponential speed up over classical computation - if the local processors have size up to \( p \) qubits each then the state will be \( p \)-blocked at every stage.

In section 3 we will prove our main result, that for any quantum algorithm operating on pure states, the presence of multi-partite entanglement, with a number of parties that increases unboundedly with input size, is necessary if the quantum algorithm is to offer an exponential speed-up over classical computation (theorem 1). Furthermore we will prove that the algorithm can be classically efficiently simulated to within a prescribed tolerance \( \eta \) even if a suitably small amount of entanglement (depending on \( \eta \)) is present (theorem 2). The presence or absence of increasingly widespread multi-partite entanglement is not an obvious feature of a given family of quantum states and in section 4 we will explicitly identify the presence of this resource in Shor’s algorithm.

The theorems of section 3 apply to quantum algorithms that operate on pure states which are required to be \( p \)-blocked (for some fixed \( p \)) at every stage. As such, the theorems actually also apply to quantum algorithms on mixed states, where the state is again required to be \( p \)-blocked at each stage (i.e. any such algorithm can be classically efficiently simulated). Now, for pure states, the \( p \)-blocked condition corresponds exactly to the absence of entanglement (of more than \( p \) qubits) but this is no longer true for mixed states: a mixed state \( \rho \) is \( p \)-blocked if it is a product of mixtures (cf definition 4) whereas \( \rho \) is unentangled if it is separable i.e. a mixture of products (of \( p \)-qubit states) and such \( \rho \)'s are not necessarily \( p \)-blocked. Thus for mixed states, the \( p \)-blocked condition is considerably stronger than the condition of absence of entanglement. This leads to the following question: suppose that a quantum algorithm operates on general mixed states and at every stage the state is unentangled (in the sense of being separable). Can the algorithm be classically simulated with an amount of classical resources that is (polynomially) equivalent to the quantum resources of the original algorithm? This fundamental question remains unresolved. In section 5 we will discuss some essential differences between pure and mixed unentangled states which suggest a negative answer (in contrast to the case of pure states) i.e. that an exponential computational speed-up might plausibly be achievable in quantum algorithms on mixed quantum states that have no entanglement.
According to our main results above we can say that entanglement is necessary in a quantum algorithm (on pure states) if the algorithm is to offer an exponential speed-up over classical computation. Does this mean that entanglement can be identified as an essential resource for quantum computational power? In section 6 we will suggest (perhaps somewhat surprisingly) that this is not a good conclusion to draw from our results! Indeed our theorems are based entirely on the idea of mathematically representing quantum states as amplitudes and then classically computing the quantum evolution with respect to this mathematical description. From our computational point of view entanglement emerges as a significant property because absence of entanglement implies a polynomially sized description of the quantum process, when the process is mathematically expressed in the amplitude description. But suppose that instead of the amplitude description we choose some other mathematical description $D$ of quantum states (and gates). Indeed there is a rich variety of possible alternative descriptions. Then there will be an associated property $\text{prop}(D)$ of states which guarantees that the $D$-description of the quantum computational process grows only polynomially with the number of qubits if $\text{prop}(D)$ is absent (e.g. if $D$ is the amplitude description then $\text{prop}(D)$ is just the notion of entanglement). Thus, just as for entanglement, we can equally well claim that $\text{prop}(D)$ for any $D$, is an essential resource for quantum computational speed-up! Entanglement itself appears to have no special status here. In summary, the point is that we can have different mathematical formalisms for expressing quantum theory, and although they are fully mathematically equivalent, they will lead to quite different families of states (of increasingly many qubits) that have a polynomially sized description with respect to the chosen formalism. Hence we also get different notions of a physical quality that guarantees a state will not be of the latter form. Then every one of these qualities must be present in a quantum algorithm if it is to offer an exponential speed-up over classical algorithms.

2 Preliminary definitions

We will need a precise definition of the notion of a quantum computational process and a definition of what it means to classically efficiently simulate such a process.

The term ‘state’ will be used to mean a general (mixed) state. The term $\text{poly}(n)$ will refer to a function $f(n)$ whose growth is bounded by a polynomial function in $n$ i.e. there exists a polynomial $p(n)$ such that $f(n) \leq p(n)$ for all sufficiently large $n$.

We adopt the gate array model of quantum computation as our working definition. Let $G$ be a fixed finite set of 2-qubit gates.

**Definition 1** A quantum computational process (or quantum algorithm) with running time $T(n)$ comprises the following description. For each fixed positive integer $n$ (input size) we have a sequence of triples $A_n = \{(U_{i_0}, a_0, b_0), (U_{i_1}, a_1, b_1), \ldots, (U_{i_T(n)}, a_T(n), b_T(n))\}$

where the $U_{i_k}$’s are chosen from $G$ and $a_k$ and $b_k$ are positive integers. More precisely, there is a classical algorithm running in $\text{poly}(T(n))$ time, which given $n$, will output the list $A_n.$
The quantum algorithm corresponding to the sequence \( \{A_n: n = 1, 2, \ldots\} \) runs as follows. For each input \( i_1 \ldots i_n \) of size \( n \) we start with a row of qubits \( |i_1\rangle |i_2\rangle \ldots |i_n\rangle |0\rangle |0\rangle \ldots \) giving the input extended by zeroes. We apply the sequence of \( T(n) \) computational steps given in \( A_n \), where the \( k^{\text{th}} \) step is the application of the 2-qubit gate \( U_{i_k} \) to qubits \((a_k, b_k)\) in the row. After \( T(n) \) steps we measure the leftmost qubit in the computational basis and output the result (0 or 1) i.e. we give a sample from the probability distribution \( P = \{p_0, p_1\} \) defined by the quantum measurement on the final state.

Remark Later we will also discuss quantum computational processes on mixed states. For such a process of \( T(n) \) steps we will require that the input state is a mixed state of \( n \) qubits with a poly(\( n \)) sized description (rather than just a computational basis state of \( n \) qubits as above). Also the computational steps could be unitary or more generally, trace preserving completely positive maps on two qubits. Equivalently we could require the computational steps to be unitary transforms of six qubits (i.e. having a 4-qubit ancilla space) whose locations are all specified similar to the pairs of qubits in the above definition.

We will also need a notion of distance between states and between probability distributions. For this purpose we will use the trace norm \( |\!|\!\!| \cdot |\!\!\!| \). For any operator \( A \) (on a finite dimensional state space), the trace norm \( |\!|A|\!\!\!| \) is defined by
\[
|\!|A|\!\!\!| = \text{tr} \sqrt{A^\dagger A} = \sum_i \mu_i
\]
where \( \mu_i \) are the singular values of \( A \). If \( A \) is hermitian then \( \mu_i \) are the absolute values of the eigenvalues. If \( \rho \) is a density matrix then \( |\!|\rho|\!\!\!| = 1 \).

The trace norm distance \( |\!|\rho - \sigma|\!\!\!| \) between states has an especially useful property of being contractive under any trace preserving quantum operation \([18]\). In particular if \( \rho_{AB} \) and \( \sigma_{AB} \) are bipartite states and \( \rho_A, \sigma_A \) denote the corresponding reduced states of \( A \) then
\[
|\!|\rho_A - \sigma_A|\!\!\!| \leq |\!|\rho_{AB} - \sigma_{AB}|\!\!\!|.
\]
Also if \( P \) and \( Q \) are the probability distributions for the outcomes of any quantum measurement on two states \( \rho \) and \( \sigma \) respectively then
\[
|\!|P - Q|\!\!\!| \leq |\!|\rho - \sigma|\!\!\!| \tag{3}
\]
where \( |\!|P - Q|\!\!\!| = \sum |p_i - q_i| \) is the trace norm distance between the distributions viewed as diagonal states.

Finally we give our definition of the notion of classical efficient simulation.

Definition 2 A quantum computation \( \{A_n: n = 1, 2, \ldots\} \) with output probability distribution \( P \) can be efficiently classically simulated if the following condition is satisfied:
Given only classical means (i.e. a universal classical computer which is also able to make probabilistic choices) and the description \( A_n \) (i.e. the classical poly-time algorithm for generating \( A_n \) from \( n \)), then for any \( \eta > 0 \), we are able to sample once a distribution \( P' \) with \( |\!|P - P'|\!\!\!| \leq \eta \), using a classical computational effort that grows polynomially with \( n \) and \( \log(\frac{1}{\eta}) \).
In the above definition we should be more precise about the computer’s ability to make probabilistic choices. Just as computational steps cannot be arbitrary, but must be chosen from a fixed finite set of gates (giving a measure of computational effort for any desired transformation) we need to have a measure of how much computational effort is required to sample a given probability distribution \( \{p_0, p_1\} \). We assume that the computer can only toss a fair coin i.e. sample the probability distribution \( \{\text{prob}(0) = \frac{1}{2}, \text{prob}(1) = \frac{1}{2}\} \) and this counts as a single computational step. Let \( 0 \leq x \leq 1 \) be any number whose binary expression has at most \( n \) binary digits: \( x = 0.i_1i_2\ldots i_n \). Then the computer can sample the distribution \( P_x = \{x, 1-x\} \) in \( n \) steps as follows: toss the fair coin \( n \) times giving a sequence of results \( j_1 \ldots j_n \). View \( j_1 \ldots j_n \) as an \( n \) digit binary number (and similarly \( i_1 \ldots i_n = 2^n x \)). Then \( \text{prob}(j_1 \ldots j_n < i_1 \ldots i_n) = x \) so we get a sampling of \( P_x \) by comparing the random output \( j_1 \ldots j_n \) to the given \( i_1 \ldots i_n \). If \( x \) has an infinite binary expansion we can sample an \( n \) digit approximation to \( P_x \) by the above method using \( \text{poly}(n) \) steps i.e. we can sample \( P' \) having \( ||P' - P|| \leq \eta \), with \( \text{poly}(\log 1/\eta) \) computational effort and we adopt the latter simulation rate as the definition of efficient simulability for a general probability distribution.

In many applications we do not need to consider arbitrarily small \( \eta \) as in definition \( \ref{7} \) and a weaker simulation requirement suffices. Suppose that the quantum computation is a BQP algorithm for a decision problem. Thus for any input, the output distribution \( P = \{p_0, p_1\} \) has the property that the probability of obtaining a correct answer is \( > \frac{2}{3} \). In that case the decision problem will have a classical efficient (BPP) algorithm if we can efficiently classically simulate a distribution \( P' = \{p'_0, p'_1\} \) with \( ||P - P'|| \leq \eta_0 \) where \( \eta_0 < \frac{1}{6} \) is a constant, so that the probability of a correct answer with \( P' \) is still bounded away from \( \frac{1}{2} \). Indeed we will see (theorem \( \ref{7} \) below) that for such a finite tolerance classical simulation to be ruled out, not only must the quantum algorithm exhibit multi-partite entanglement in its states but furthermore the amount of this entanglement must be suitably large (with a lower bound depending on \( \eta_0 \) and the running time of the algorithm).

### 3 Simulation by classical computation

One method for classically simulating a quantum computation is to directly compute the state at each step from the sequence of unitary operations prescribed in the quantum algorithm. We will investigate the implications of this simulation for the power of quantum computing compared to classical computing, especially noting conditions which guarantee that this simulation is efficient.

Let \( |\alpha_j\rangle \) be the state after \( j \) steps of computation, which we may assume is a general state of at most \( 2j \) qubits (by neglecting unused qubits from the initial row). In the computational basis we have:

\[
|\alpha_j\rangle = \sum a_{i_1i_2\ldots i_{2j}} |i_1\rangle |i_2\rangle \ldots |i_{2j}\rangle.
\]

Then \( |\alpha_{j+1}\rangle \) is obtained by applying the 2-qubit gate \( U_{i_j} \) to qubits \( a_j \) and \( b_j \). For clarity let us assume that these are the first two qubits i.e. \( a_j = 1 \) and \( b_j = 2 \) (all other possible cases are similar). The amplitudes \( \tilde{a} \) of the updated state are calculated as:

\[
\tilde{a}_{i_1i_2i_3\ldots i_{2j}} = \sum_{j_1, j_2 = 0, 1} M_{i_1i_2}^{j_1j_2} a_{j_1j_2i_3\ldots i_{2j}}
\]
where $M_{i_1j_1i_2j_2}$ is the 4 by 4 matrix of $U_{ij}$.

This classical computation may fail to be efficient for two reasons. Firstly there are exponentially many amplitudes that need to be computed and the matrix multiplication of $M$ in eq. (3) needs to be carried out exponentially many times. This inefficiency is intimately related to the fact that the states $|\alpha_j\rangle$ are generally entangled and the implications of this obstacle to efficient simulation will be elaborated below.

The second possible difficulty with the computation in eq. (5) arises from the fact that the matrix entries of $M$ are generally continuous parameters (real or complex numbers) so that even the individual arithmetic operations (additions and multiplications) involved might be prohibitively costly. This second issue will be circumvented by considering rational approximations to gates.

**Definition 3** A quantum gate is **rational** if its matrix elements (in the computational basis) have rational numbers as real and imaginary parts.

The main property of rational numbers that we will need is the following.

**Lemma 1** Let $D = \{r_1, \ldots, r_L\}$ be a finite set of rational numbers whose numerators and denominators have at most $m$ digits. For any $j$ let $x$ be an arithmetic expression constructed from the elements of $D$ using at most $j$ additions and multiplications. Then $x$ can be computed exactly (as a rational number) using a number of steps of computation that grows polynomially with $j$ and $m$.

**Proof** This is an easy consequence of the polynomial (in the number of digits) computability of integer arithmetic and of the fact that the number of digits of the numerator and denominator of an arithmetic expression in the rationals in $D$ grows at most linearly with the number of operations. **QED**.

Apart from rational gates, many other possible classes of gates, having the essential polynomial property of lemma [4], would suffice for our purposes. For example we could allow the matrix elements to be members of a finite algebraic extension of the rationals. This would allow numbers such as $\frac{1}{\sqrt{2}}$ and $\cos \frac{\pi}{8}$ which appear as matrix elements of commonly used universal sets of gates [18].

Let us now return to the relation of entanglement to the efficiency of the classical computation in eq. (5).

**Definition 4** Let $\rho$ be a state of $m$ qubits where the qubits are labelled by $B = \{1, 2, \ldots, m\}$. $\rho$ is $p$-blocked if $B$ can be partitioned into subsets of size at most $p$:

$$B = B_1 \cup B_2 \cup \ldots \cup B_K \quad |B_i| \leq p$$

and $\rho$ is a product state for this partition:

$$\rho = \rho_1 \otimes \rho_2 \otimes \ldots \otimes \rho_K$$

where $\rho_i$ is a state of the qubits in $B_i$ only.

Note that a pure state is $p$-blocked if and only if no $p + 1$ qubits are all entangled together. But a mixed state $\rho$ can be unentangled in the sense of being separable, without
being \( p \)-blocked i.e. the \( p \)-blocked condition (“product of mixtures”) is stronger than the separability condition (“mixture of products”).

Our next result transparently shows the necessity of multi-partite entanglement for exponential quantum computational speed-up in a restricted situation where there are no additional complications arising from the description of the gates (as they are assumed to be rational).

**Lemma 2** Let \( \mathcal{G} \) be a finite set of rational 2-qubit gates and \( p \) a fixed positive integer. Suppose that \( \{ A_n : n = 1, 2, \ldots \} \) using gates from \( \mathcal{G} \), is a polynomial time quantum computation with the property that at each stage \( j = 1, \ldots, \text{poly}(n) \) the state \( |\alpha_j\rangle \) is \( p \)-blocked. Then the final probability distribution \( \mathcal{P} \) can be classically exactly computed with \( \text{poly}(n) \) computational steps so the quantum computation can be classically efficiently simulated.

**Proof of lemma 2**

Any \( p \)-blocked pure state \( |\psi\rangle \) of \( m \) qubits may be fully described with the following data:

(a) (Block locations) A list of \( m \) integers \( (b_1, \ldots, b_m) \) where \( 1 \leq b_i \leq m \). \( b_i \) gives the number of the block to which the \( i \)-th qubit belongs. For example the list \( (3, 5, 4, 3, 3, \ldots) \) denotes that qubit 1 is in block 3, qubit 2 is in block 5 and so on. Note that the number of blocks can grow at most linearly with \( m \).

(b) (Block states) For each block we give its state by listing the amplitudes in the computational basis. This requires at most \( 2^{p+1} \) real numbers since each block has size at most \( p \) qubits.

Note that for fixed \( p \) and increasing \( m \) the total size of the description grows only polynomially with \( m \) assuming that the real numbers in (b) can each be described with \( \text{poly}(m) \) bits of memory. This is in contrast to the exponentially growing number of amplitudes needed to describe a general entangled state.

Now to classically simulate the \( p \)-blocked algorithm we simply update the ((a),(b)) description of the state at each step. Note that the location of the blocks (i.e. (a)) will generally change as well as the states of the blocks themselves (i.e. (b)). The \( j \)-th computational step is given by the action of a 2-qubit gate \( U_{ij} \) on a \( p \)-blocked state and we distinguish two cases:

Case 1: the gate acts on two qubits which are already in the same block. Thus (a) remains unchanged and the state of the chosen block is updated in (b) by applying the unitary matrix of size at most \( 2^p \times 2^p \), requiring a constant number of arithmetic operations (which does not grow with \( j \), the counter describing the step of the quantum algorithm that is being simulated).

Case 2: the 2-qubit gate straddles two existing blocks \( B_1 \) and \( B_2 \) of sizes \( p_1 \leq p \) and \( p_2 \leq p \) respectively. We again update the state of all \( p_1 + p_2 \) qubits by applying a unitary matrix of size at most \( 2^{p_1} \times 2^{p_2} \) (requiring a constant number of operations that does not grow with \( j \)). If \( p_1 + p_2 \leq p \) we also update (a) by amalgamating the two block labels into a single label, to complete the step. If \( p_1 + p_2 > p \) we need to identify a new block structure (with blocks of size \( \leq p \)) within the qubits of \( B_1 \) and \( B_2 \). One method is to compute the reduced state \( \rho_X \) of every subset \( X \subseteq B_1 \cup B_2 \) having size \( \leq p \), and compare the global state of \( B_1 \cup B_2 \) with \( \rho_{X_1} \otimes \ldots \otimes \rho_{X_K} \) for each partition \( X_1, \ldots, X_K \) of \( B_1 \cup B_2 \) (looking for an equality of states). This calculation again clearly needs a bounded number of arithmetic...
operations (independent of $j$). Finally we update (a) and (b) with the newly found blocks and their corresponding states.

This gives a classical simulation of the quantum algorithm using a number of rational arithmetic operations that grows linearly with $j$. Finally lemma 2 guarantees that the calculation can be done with poly($j$) elementary computational steps, giving an efficient classical computation of the final state of the quantum algorithm. Finally we identify the block containing the leftmost qubit, compute the probability distribution $P$ and sample it once with a corresponding classical probabilistic choice, completing the efficient classical simulation of the quantum algorithm. QED.

Remark Although lemma 2 has been stated for quantum algorithms with pure states it is readily generalised to the case of mixed states: suppose that a quantum algorithm (with rational gates) has a $p$-blocked mixed state at each stage. Then it can be classically efficiently simulated. Indeed the above proof does not require the block states to be pure. In a similar way, the theorems below also easily generalise to $p$-blocked mixed state processes (although for clarity we give the statements and proofs only for the case of pure states).

Lemma 2 depends on two essential ingredients: (a) $p$-blockedness implying a polynomial number of parameters for state descriptions and (b) rationality of gates, guaranteeing that the classical arithmetic operations can be efficiently carried out. Our next result shows that the condition (b) can be lifted.

**Theorem 1** Let $G$ be a finite set of 2-qubit gates and $p$ a fixed positive integer. Suppose that $\{A_n : n = 1, 2, \ldots\}$, using gates from $G$, is a polynomial time quantum computation with the property that at each stage $j = 1, \ldots, \text{poly}(n)$ the state $|\alpha_j\rangle$ is $p$-blocked. Then the quantum computation can be classically efficiently simulated.

Before going on to consider the proof of theorem 1 we make some remarks on the significance of this result. Theorem 1 shows that multi-partite entanglement with unboundedly many qubits entangled together, is a necessary feature of any quantum algorithm (operating on pure states) if the algorithm is to exhibit an exponential speed-up over classical computation. Indeed absence of increasing numbers of entangled qubits corresponds to a fixed value of $p$. In contrast, in communication tasks, entanglement restricted to merely bi-partite entanglement suffices for exponential benefits (for example an exponential reduction of communication complexity [19]) but for “standard” computational tasks the availability of (even increasing amounts of) only bi-partite entanglement cannot give an exponential speed-up (in contrast to the fact that 2-qubit gates suffice for universal computation) — the number of qubits entangled together must grow as an unbounded function of input size. Indeed even if every pair of qubits become entangled at some stage of the computation and there is no higher order entanglement, the quantum algorithm will still have an efficient classical simulation. This shows that the role of entanglement in computation is essentially different from its role in communication. Theorem 1 also implies that distributed quantum computing (on pure states), which allows any number of local quantum processors, but of bounded size and classical communication between them, cannot offer an exponential speed-up over classical computation — if the local processors have size up to $p$ qubits each then the state will be $p$-blocked at every stage.

Our approach to proving theorem 1 will be to replace general gates by rational approxi-
imations with increasingly high precision. Recall [10] that there exists a finite universal set of rational 2-qubit gates. Hence any quantum computation $QC_1$ with gate set $G_1 = \{ U_i \}$ can be efficiently approximated by a quantum computation $QC_2(\epsilon)$ having rational gates $G_2 = \{ \tilde{U}_i \}$ where $||U_i - \tilde{U}_i|| < \epsilon$ (for any chosen $\epsilon > 0$). As far as a quantum physical implementation is concerned, $QC_2$ behaves very similarly to $QC_1$ in its action on states $|\alpha\rangle$. But for our classical computational simulations there can be a dramatic difference: if $QC_1$ is a $p$-blocked computation (and hence efficiently simulable by the theorem) then the approximation $QC_2$ will generally not be $p$-blocked so we cannot invoke the lemma to claim that $QC_2$ (although near to $QC_1$ and having rational gates) is efficiently simulable. Indeed the fact that $p$-blocked states of $m$ qubits have a poly($m$) sized exact description (which is crucial in the proof of lemma 2) is immediately lost under arbitrarily small perturbations to general states, which require an exponentially large description (of exponentially many independent amplitudes). Hence the theorem is not a straightforward consequence of the lemma via efficient rational approximation of the gates, and as will be seen, its proof will require substantial further ingredients. Our strategy will be to further modify $QC_2$ to a nearby process $QC_2'$ whose states are $p$-blocked transmogrifications of the states of $QC_2$. This leads us to consider the simulation of algorithms whose states remain suitably close to $p$-blocked states, so they may have a small amount of entanglement between the blocks. Consequently we will develop suitable approximations with polynomially sized descriptions, to states that are not $p$-blocked, but are suitably near to $p$-blocked states. This is the content of theorems 2 and 3 below (and theorem 1 will appear as a special case).

Although we are using the gate array model of quantum computation for our arguments, our results will apply to other models as well. Suppose we have any model of quantum computation with the following properties:

(a) At each stage of the computation we have a pure state of a system comprising subsystems of a bounded size;

(b) The update of the state is effected by a unitary transform or by a measurement, each on a bounded number of subsystems.

In that case our proofs readily generalise to show that if the states are $p$-blocked at every stage then the computational process will have an efficient classical simulation i.e. that multi-partite entanglement of unboundedly many subsystems must be present for an exponential computational speed-up. The above criteria for a computational model are satisfied by the quantum turing machine model [3] as well as some recently proposed models that focus on measurement operations [16, 17].

As mentioned above we will prove theorem 1 in a more general form motivated as follows. Let $|\alpha_j\rangle$ be the pure state at step $j$ in a quantum algorithm. Write $\alpha_j$ as an abbreviation for $|\alpha_j\rangle\langle \alpha_j|$. Theorem 1 requires that $\alpha_j$ be exactly $p$-blocked for each $j$. Suppose that $\alpha_j$ is not $p$-blocked but is made up of blocks of size at most $p$ with a “small” amount of entanglement between the blocks. We formalise this by requiring that for each $j$ there is a $p$-blocked (possibly mixed) state $\beta_j$ close to $\alpha_j$:

$$||\alpha_j - \beta_j|| \leq \epsilon.$$  

(6)

Theorem 1 states that if $\epsilon = 0$ then a classical efficient simulation exists. Our question now is: how large can $\epsilon$ be in eq. (6) so that the quantum algorithm can still be efficiently
classically simulated? i.e. we wish to study the stability of efficient simulability under small perturbations of the $p$-blockedness condition. The following theorem says that if we accept an error tolerance $\eta$ in the output probability distribution, then the quantum algorithm will have an efficient classical simulation (to within the tolerance) for nonzero $\epsilon$ exponentially small in the running time ($\epsilon \sim \eta c^T$ for $0 < c < 1$).

**Theorem 2** Let $\mathcal{G}$ be a finite set of 2-qubit gates and $p$ a fixed positive integer. Suppose that $\{A_n : n = 1, 2, \ldots\}$ using gates from $\mathcal{G}$, is a polynomial time quantum computation with running time $T = \text{poly}(n)$. Let $P$ be the output probability distribution of the algorithm. For $j = 0, \ldots, T$ let $|\alpha_j\rangle$ denote the state at stage $j$ and write $|\alpha_j\rangle\langle\alpha_j| = \alpha_j$.

Suppose that the states $\alpha_j$ are not exactly $p$-blocked but there exists a sequence of $p$-blocked states $\beta_j$ (generally depending on $n$ too) such that

$$||\alpha_j - \beta_j|| \leq \epsilon.$$  \hfill (7)

(The identities of the states $\beta_j$ are not assumed to be known).

Then for any $\eta > 0$, if $\epsilon \leq \frac{\eta}{(2p+4)T}$, we can classically sample a distribution $P'$ with $||P - P'|| \leq \eta$ using $\text{poly}(T, \log 1/\eta)$ classical computational steps.

**Proof of theorem 2** We have a computational process

$$|\alpha_0\rangle = |i_1\rangle \ldots |i_n\rangle |0\rangle |0\rangle \ldots |\alpha_j+1\rangle = U_j |\alpha_j\rangle \quad j = 0, \ldots, T$$

where each $U_j$ is a rational 2-qubit gate. Using the existence of the sequence $\beta_j$ we will show that there is a sequence of states $\rho_j$ and numbers $e_j$ with the following properties:

**Theorem 3** Suppose that $\{A_n : n = 1, 2, \ldots\}$ is a polynomial time quantum computation with running time $T = \text{poly}(n)$ and using only rational gates. Let $m$ (which may grow with $n$) be the largest number of digits of the denominators and numerators of the rational gates used in $\{A_k : 1 \leq k \leq n\}$. Let $P$ be the output probability distribution of the algorithm. For $j = 0, \ldots, T$ let $|\alpha_j\rangle$ denote the state at stage $j$ and write $|\alpha_j\rangle\langle\alpha_j| = \alpha_j$.

Suppose that the states $\alpha_j$ are not exactly $p$-blocked but there exists a sequence of $p$-blocked states $\beta_j$ (generally depending on $n$ too) such that

$$||\alpha_j - \beta_j|| \leq \epsilon.$$  \hfill (8)

(The identities of the states $\beta_j$ are not assumed to be known).

Then for any $\eta > 0$, if $\epsilon \leq \frac{\eta}{(2p+4)T}$, we can classically sample a distribution $P'$ with $||P - P'|| = \eta$ using $\text{poly}(T, m)$ classical computational steps.

**Proof of theorem 3** We have a computational process

$$|\alpha_0\rangle = |i_1\rangle \ldots |i_n\rangle |0\rangle |0\rangle \ldots |\alpha_j+1\rangle = U_j |\alpha_j\rangle \quad j = 0, \ldots, T$$

where each $U_j$ is a rational 2-qubit gate. Using the existence of the sequence $\beta_j$ we will show that there is a sequence of states $\rho_j$ and numbers $e_j$ with the following properties:
(a) $\|\rho_j - \alpha_j\| \leq e_j$.
(b) $\rho_j$ is $p$-blocked.
(c) $\rho_j$ can be classically computed in $\text{poly}(j, m)$ steps.
(d) $e_0 = 0$ and $e_{j+1} \leq (2p+3)(e_j + \epsilon)$.
(Note that the $p$-blocked states $\beta_j$ are not assumed to be known and they will not generally satisfy the crucial condition (c)).

Assuming all the above is given, we see from (d) that $e_1 \leq (2p+3)\epsilon$ and $e_{j+1} \leq (2p+4)e_j$ so
$$e_j \leq \epsilon(2p + 4)^j.$$
Hence, given $\eta$, if we choose any $\epsilon \leq \eta(2p + 4)^{-T}$ we will have
$$\|\rho_T - \alpha_T\| \leq e_T \leq \eta.$$
Consequently by eq. (3):
$$\|P - P'| \leq \eta$$
where $P'$ is the probability distribution arising from a quantum measurement on $\rho_T$. Hence by (c), $P'$ can be efficiently classically sampled, as required.

The states $\rho_j$ are calculated sequentially as follows. Set $\rho_0 = \alpha_0$ so $\|\rho_0 - \alpha_0\| \leq e_0 = 0$. Suppose we have generated a $p$-blocked state $\rho_j$ for the $j$th step with
$$\|\rho_j - \alpha_j\| \leq e_j.$$ 
We construct $\rho_{j+1}$ as follows. Let $\tau = U_j \rho_j U_j^\dagger$, with the 2-qubit rational gate $U_j$ acting on qubits from $C = C_1 \cup C_2$ where $C_1$ and $C_2$ are blocks in $\rho_j$ (so $|C| \leq 2p$). $\tau$ might not be a $p$-blocked state if $|C| > p$ but outside of $C$ $\tau$ remains $p$-blocked because $\rho_j$ was $p$-blocked (and $\tau$ and $\rho_j$ agree outside $C$). Since $\alpha_{j+1} = U_j \alpha_j U_j^\dagger$ too, we have $\|\alpha_{j+1} - \tau\| = \|\alpha_j - \rho_j\| \leq e_j$ so
$$\|\tau - \beta_{j+1}\| \leq e_j + \epsilon. \quad (9)$$
For any subset $X$ of qubit positions let $\tau_X$ (respectively $\rho_X$ and $\beta_X(j+1)$) denote the reduced state of $X$ in $\tau$ (respectively $\rho_j$ and $\beta_{j+1}$). We aim to decompose $C$ into $K \leq 2p$ blocks $E_i$ of size at most $p$ so that $\|\tau_C - \tau_{E_1} \otimes \ldots \otimes \tau_{E_K}\|$ remains suitably small.

Now $\beta_{j+1}$ is $p$-blocked so the reduced state $\beta_{C(j+1)}$ is $p$-blocked too. Hence $\beta_{C(j+1)} = \beta_{D_1(j+1)} \otimes \ldots \otimes \beta_{D_K(j+1)}$ where $C = D_1 \cup \ldots \cup D_K$, $|D_i| \leq p$ and $K \leq 2p$. From eq. (8) we have $\|\beta_{C(j+1)} - \tau_{E_i}\| \leq e_j + \epsilon$ and
$$\|\beta_{D_i(j+1)} - \tau_{D_i}\| \leq e_j + \epsilon \quad \text{for } i = 1, \ldots, K.$$ 
Thus (cf the hybrid argument of [13])
$$\|\beta_{D_1(j+1)} \otimes \ldots \otimes \beta_{D_K(j+1)} - \tau_{D_i} \otimes \ldots \otimes \tau_{D_K}\| \leq K(e_j + \epsilon) \leq 2p(e_j + \epsilon)$$
and using the triangle inequality
$$\|\tau_C - \tau_{D_1} \otimes \ldots \otimes \tau_{D_K}\| \leq \|\tau_C - \beta_{C(j+1)}\| + \|\beta_{C(j+1)} - \beta_{D_1(j+1)} \otimes \ldots \otimes \beta_{D_K(j+1)}\| + \|\beta_{D_1(j+1)} \otimes \ldots \otimes \beta_{D_K(j+1)} - \tau_{D_i} \otimes \ldots \otimes \tau_{D_K}\| \leq (e_j + \epsilon) + 0 + 2p(e_j + \epsilon) = (2p + 1)(e_j + \epsilon). \quad (10)$$
Hence there exists a partition of $C$ such that the corresponding product of reduced states of $\tau$ approximates $\tau_C$ to within $(2p+1)(e_j + \epsilon)$. Thus we compute $\|\tau_C - \tau_{E_1} \otimes \ldots \otimes \tau_{E_L}\|$ for all partitions $C = E_1 \cup \ldots \cup E_L$ of $C$ and choose one satisfying eq. (14). Finally to get $\rho_{j+1}$ we update $\tau_C$ by the chosen $\tau_{E_1} \otimes \ldots \otimes \tau_{E_L}$, giving a $p$-blocked state with

$$\|\rho_{j+1} - \alpha_{j+1}\| \leq \|\rho_{j+1} - \tau\| + \|\tau - \beta_{j+1}\| + \|\beta_{j+1} - \alpha_{j+1}\|$$

$$\leq (2p+1)(e_j + \epsilon) + (e_j + \epsilon) + \epsilon$$

i.e. $e_{j+1} \leq (2p+3)(e_j + \epsilon)$ as required. The entire calculation in updating $\rho_j$ to $\rho_{j+1}$ is carried out within a block $C$ of size at most $2p$ using only rational arithmetic operations and the number of operations does not grow with $j$. Hence by lemma 1, $\rho_T$ is calculated using a number of computational steps that grows polynomially with $T$ and $m$. QED.

**Proof of theorem** 2 Let $\tilde{U}_j$ be rational gates with

$$\|\tilde{U}_j - U_j\| \leq \xi \quad (11)$$

(with $\xi$ to be chosen later to match $\eta$ and $T$) and the rational matrix elements of $\tilde{U}_j$ have numerators and denominators with $O(\log \frac{1}{\xi})$ digits, which is always possible by eq. (11) (and the use of a universal rational 2-qubit gate [10]). Consider the process

$$\tilde{\alpha}_0 = \alpha_0 \quad \tilde{\alpha}_{j+1} = \tilde{U}_j \tilde{\alpha}_j \tilde{U}_j^\dagger \quad j = 0, 1, \ldots, T - 1 \quad (12)$$

which we will compare to the process with $\alpha_{j+1} = U_j \alpha_j U_j^\dagger$.

If $\|\tilde{\alpha}_j - \alpha_j\| = e_j$, writing $A_j = \tilde{U}_j - U_j$ we have $\|A_j\| \leq \xi$ and

$$\|\tilde{\alpha}_{j+1} - \alpha_{j+1}\| = \|(U_j + A_j)\tilde{\alpha}_j(U_j^\dagger + A_j^\dagger) - U_j \alpha_j U_j^\dagger\|$$

$$= \|U_j(\tilde{\alpha}_j - \alpha_j)U_j^\dagger + A_j \tilde{\alpha}_j U_j^\dagger + U_j \alpha_j A_j^\dagger + A_j \tilde{\alpha}_j A_j^\dagger\|$$

$$\leq e_j + \xi + \xi + \xi^2$$

where we have used the properties $\|UAV\| = \|A\|$ and $\|AB\| \leq \|A\| \|B\|$ for any unitary $U, V$ and arbitrary $A, B$. Thus $e_{j+1} = \|\tilde{\alpha}_{j+1} - \alpha_{j+1}\| \leq e_j + 3\xi$. Hence

$$\|\tilde{\alpha}_j - \alpha_j\| \leq 3j\xi \quad j = 0, \ldots, T - 1. \quad (13)$$

If $\tilde{\mathcal{P}}$ (respectively $\mathcal{P}$) is the output distribution of the final measurement of the quantum algorithm performed on $\tilde{\alpha}_T$ (respectively $\alpha_T$) we get

$$\|\tilde{\mathcal{P}} - \mathcal{P}\| \leq 3T\xi. \quad (14)$$

Now $\tilde{\alpha}_j$ are generated with rational gates but they are not necessarily $p$-blocked. However they lie close to the $p$-blocked states $\beta_j$. From $\|\alpha_j - \beta_j\| \leq \epsilon$ and eq. (13) we get

$$\|\tilde{\alpha}_j - \beta_j\| \leq 3j\xi + \epsilon \leq 3T\xi + \epsilon$$

and we can apply theorem 3 to claim the following: given any $\eta > 0$ (and writing $c = \frac{1}{(2p+4)}$), if $\xi$ and $\epsilon$ are chosen so that

$$3T\xi + \epsilon \leq \eta c^T \quad (15)$$

14
then we can sample a distribution $\mathcal{P}'$ with $||\tilde{\mathcal{P}} - \mathcal{P}'|| \leq \eta$ using $\text{poly}(T, \log \frac{1}{\xi})$ classical computational steps. From eq. (14) we have

$$||\mathcal{P} - \mathcal{P}'|| \leq 3T\xi + \eta \leq \eta e^T + \eta \leq 2\eta.$$ 

Now we can satisfy eq. (15) by fixing $\xi = \frac{1}{6T\eta e^T}$ and letting $\epsilon < \frac{1}{2}\eta e^T$ so $\log \frac{1}{\xi} = \log \frac{1}{\eta} + \text{poly}(T)$ and $\text{poly}(T, \log \frac{1}{\xi}) = \text{poly}(T, \log \frac{1}{\eta})$. Finally replacing $\eta$ by $\eta/2$ in the above, we see that for any $\eta > 0$, if $\epsilon < \frac{1}{4}\eta e^T$ then we can sample $\mathcal{P}'$ with $||\mathcal{P} - \mathcal{P}'|| \leq \eta$ using $\text{poly}(T, \log \frac{1}{\eta})$ classical computational steps, as required. QED.

4 Multi-partite entanglement in Shor’s algorithm

Shor’s algorithm [6] is generally believed to exhibit an exponential speed-up over any classical factoring algorithm. Thus, in the light of the arguments given above, one would expect that there is entanglement of an unbounded number of particles in Shor’s algorithm. This is indeed the case as we now show. Of course, this does not show that there is no classical polynomial algorithm for factoring; however if it had been the case that only a bounded number of particles had been entangled for any value of the input size, then the results in the previous sections would have furnished a classical polynomial-time algorithm for factoring.

To see that an unbounded number of particles becomes entangled in Shor’s algorithm, it suffices to show that this happens at some point in the algorithm. The key construction of the algorithm is a method for determining the period $r$ of the function $f(x) = a^x \mod N$ (16)

where $N$ is the input number to be factorised and $a < N$ has been chosen at random. Following a standard description of the algorithm (e.g. as given in [8]) we see that at an appropriate stage we will have a periodic state of about $2\log N$ qubits, of the form

$$\sum_k |x_0 + kr\rangle,$$

(17)

where $0 < x_0 < r$ is unknown and has been chosen at random (and we have omitted the normalisation factor).

We will now show that, with high probability, these “arithmetic progression” states have unbounded numbers of particles entangled as $N$ increases. In order to see how the argument proceeds, consider first a case in which an arithmetic progression state is blocked. This case is the state (with $r = 3$)

$$|\text{AP}_1\rangle = \sum_{k=0}^{3} |3 + 3kr\rangle = |3\rangle + |6\rangle + |9\rangle + |12\rangle.$$ 

(18)

Expressing each state in binary we have

$$|\text{AP}_1\rangle = |0_30_21_10_0\rangle + |0_31_21_10_0\rangle + |1_30_20_11_0\rangle + |1_31_20_10_0\rangle.$$ 

(19)
We have labelled the qubits with a subscript indicating the power of two to which it refers. We now re-order the qubits to make it easy to see that \(|AP_1\rangle\) is blocked (into two blocks each containing two qubits):

\[
|AP_1\rangle = |0_31_10_21_0\rangle + |0_31_11_20_0\rangle + |1_30_10_21_0\rangle + |1_30_11_20_0\rangle
= ((|0_31_1\rangle + |1_30_1\rangle) \otimes (|0_21_0\rangle + |1_20_0\rangle)).
\] (20)

The demonstration that this state is blocked proceeded by identifying which qubits are in which block. Let us now consider a general arithmetic progression. Imagine that it can be \(p\)-blocked. Thus we can rearrange the ordering of the qubits so that the state may be written

\[
(|a_1\rangle + |a_2\rangle + \ldots |a_{p!}\rangle) \otimes (|b_1\rangle + |a_2\rangle + \ldots |b_{p^2}\rangle) \otimes \ldots \otimes (|z_1\rangle + |z_2\rangle + \ldots |z_{p^k}\rangle);
\] (21)

For example if \(|a_2\rangle = |1_30_1\rangle\) then \(a_2 = 8\). Each term \(a_i\) in the first bracket will have a binary expression where non-zero digits all lie in a given subset of positions (of size at most \(p\)) i.e. the block corresponding to the first bracket. Different round brackets correspond to disjoint such blocks of digit positions.

We will arrange the terms in each round bracket in increasing order of the binary string labelling the state. The full state in the progression with lowest binary string is \(|a_1\rangle|b_1\rangle \ldots |z_1\rangle\); i.e. the binary string is \(a_1 + b_1 \ldots + z_1\). The next lowest term in the progression is \(a_1 + b_1 \ldots + z_1 + r\). Thus one of the brackets must have the property that the difference between the two smallest binary strings is \(r\). Let us say that this bracket is the one containing the \(|a_i\rangle\) (i.e. \(a_2 - a_1 = r\)). Remember that all the binary numbers in the superposition in that bracket must be expressible using a given set of up to \(p\) bits (where \(p\) does not increase with \(N\)). Now as \(N\) increases, so will the typical values of \(r\). A typical \(r\) will contain the pair “10” at two adjacent places in its binary representation many times (typically one quarter of the time). For large enough \(r\), this pair “10” will inevitably occur at binary positions not included among the (at most \(p\)) qubits representing the \(a_i\). Thus it is not possible to choose a fixed number \(p\) so that \(a_1\) and \(a_2 = a_1 + r\) are both expressible using only a bounded number of binary digits. Thus the full arithmetic progression state will not be \(p\)-blocked in general.

Therefore for general values of \(N\), the number we wish to factor, the state of the computer at this stage in the calculation is not \(p\)-blocked. Of course, as we have seen, certain carefully chosen truncated arithmetic progression states may be blocked (e.g. it is not difficult to construct 2-blocked arithmetic progressions of length \(2^m\) for any \(m\)), but these are highly atypical.

Actually our argument above shows more generally, that almost all states of the form \(|a\rangle + |a + r\rangle + |b_1\rangle + \ldots + |b_m\rangle\) where \(b_i > a + r\) for all \(i\), will not be \(p\)-blocked. Now Simon’s algorithm \([4, 12]\) involves states of the form \(|x_0\rangle + |x_1\rangle\) where \(x_0\) and \(x_1\) are general \(n\)-qubit strings. Hence this algorithm too utilises multi-partite entanglement of unboundedly many qubits.
Computations with mixed states

The significance of entanglement for pure state computations derives from the fact that unentangled pure states (or more generally $p$-blocked pure states) of $n$ qubits have a description involving only $\text{poly}(n)$ parameters (in contrast to $O(2^n)$ parameters for a general pure state) and consequently if entanglement is absent in a quantum computational process then the process can be efficiently classically simulated.

The corresponding situation for mixed states is dramatically different: we define a mixed state $\rho$ to be unentangled if it is separable i.e. among all the possible ways of representing $\rho$ as a mixture of pure states, there is a mixture involving only product states. Then it may be shown [20, 21, 22] that unentangled mixed states have a non-zero volume in the space of all mixed states. As an explicit example [22] the $n$ qubit state

$$\rho = (1 - \epsilon) \frac{1}{2^n} I + \epsilon \xi$$

is unentangled for all mixed states $\xi$ if $\epsilon < \frac{1}{16^n}$. Hence unentangled mixed states require the same number of parameters for their description as do general mixed states. Consequently if a quantum algorithm has unentangled (mixed) states at each stage then the classical simulation by direct computation of the updated state, fails to be efficient. From this parameter counting point of view an unentangled mixed state has the same capacity for coding information as a general mixed state so it is plausible that the computational power of general mixed (or pure) quantum states is already fully present in the restricted case of unentangled mixed states. Stated otherwise, we have the following fundamental (unresolved) question. Suppose that a quantum computation of $N$ steps on mixed states has a separable state $\alpha_j$ at each stage $j$. Suppose also that the starting state $\alpha_0$ has a $\text{poly}(N)$ sized description. Then, can the algorithm be classically efficiently simulated?

At first sight one might expect that the direct computational simulation method used in the previous section could be adapted to become efficient. Indeed a separable state is just a classical probabilistic mixture of unentangled pure states and we can efficiently simulate unentangled pure state processes so maybe we could just supplement the latter with some extra classical probabilistic choices. Indeed such a modification works in the restricted case of classical probabilistic processes i.e. processes in which the state at any stage is a probabilistic mixture of computational basis states. As a simple example consider a process involving $n$ coins and the $j$th step is to toss the $j$th coin. Then the complete state description grows exponentially with $j$ (being a probability distribution over $2^j$ outcomes at state $j$). But to simulate the process (i.e. sample the final distribution once) we do not need to carry along the entire distribution – we just make probabilistic choices along the way (i.e. follow one path through the exponentially large branching tree of possibilities, rather than computing the whole tree and then sampling the final total distribution at the end).

Unfortunately this idea appears not to work in the quantum case. Suppose that $\rho_1$ is an unentangled state, being a mixture of product states $|\xi_i\rangle$ with probabilities $p_i$ i.e. $\rho_1 = \sum p_i |\xi_i\rangle \langle \xi_i|$. Suppose that $\rho_2 = U \rho_1 U^\dagger$ is also unentangled for a unitary operation $U$ (the computational step). Let $|\eta_i\rangle = U |\xi\rangle$. Then $\rho_2$ is a mixture of state $|\eta_i\rangle$ with
probabilities $p_i$ but there is no guarantee that $|\eta_i\rangle$ are product states! As a simple example with 2 qubits let $\rho_1$ be an equal mixture of the product states $|\xi_1\rangle = (|0\rangle + |1\rangle)|1\rangle$ and $|\xi_2\rangle = (|0\rangle - |1\rangle)|1\rangle$ (where we omit normalisation factors) and let $U$ be the controlled NOT gate. Then by updating these pure state we get $\rho_2$ as an equal mixture of two maximally entangled states $|\eta_1\rangle = |0\rangle |1\rangle + |1\rangle |0\rangle$ and $|\eta_2\rangle = |0\rangle |1\rangle - |1\rangle |0\rangle$. Although these component states are entangled, the overall mixture is unentangled, being equivalent to an equal mixture of the product states $|0\rangle |1\rangle$ and $|1\rangle |0\rangle$. The existence of a separable mixture is not a property of individual component states $|\eta_i\rangle$ but a global property of the whole ensemble $\{|\eta_i\rangle : p_i\}$. Hence we cannot follow a single probabilistic path of pure states through a branching tree of possibilities since these pure states become entangled (and so the simulation becomes inefficient). At each stage we need to re-compute a new separable decomposition of the state. This computation generally requires knowledge of the whole ensemble and hence cannot be efficient in the required sense.

Quantum computation with mixed states has attracted much attention in recent years because of the experimental implementation of quantum computation using liquid state NMR techniques \[18\] which utilises an interesting class of mixed states. The basic idea is to consider so-called pseudo-pure states of the form

$$\rho = (1 - \epsilon) \frac{1}{2} I + \epsilon |\psi\rangle \langle \psi|$$

(23)

(which occur in NMR experiments for suitably small $\epsilon$). Then for any unitary transformation $U$ the state $U \rho U^\dagger$ is also pseudo-pure with $|\psi\rangle$ replaced by $U |\psi\rangle$. Hence given any pure state quantum algorithm, if we implement it on the pseudo-pure analogue of its starting state, the entire pure state algorithm will unfold as usual on the pure state perturbation $\epsilon |\psi\rangle \langle \psi|$ of eq. (23). Furthermore if $A$ is any traceless observable then from eq. (23) we get the expectation value

$$\langle A \rangle = \text{tr} A \rho = \epsilon \langle \psi | A |\psi\rangle$$

(24)

i.e. we obtain the average value of $A$ in the pure state $|\psi\rangle$ but the signal is attenuated by $\epsilon$.

We have seen in eq.(22) that for sufficiently small $\epsilon$ all pseudo-pure states are separable so we have the intriguing possibility of implementing any quantum pure state algorithm with its original running time, in a setting with no entanglement at all! Can this provide a computational benefit (over classical computations) in the total absence of entanglement? Although this not not known for general algorithms, it has been shown for Shor's algorithm (and structurally related algorithms) \[23\] and for Grover's algorithm \[24\] that the answer is negative: if the pseudo-pure states are required to remain separable at each stage in these algorithms then it can be proven \[23, 24\] that the value of $\epsilon$ must decrease exponentially with input size. Consequently to obtain the output result reliably via an expectation value as in eq. (24) we either need to repeat the algorithm exponentially many times or else, use an exponentially increasing bulk of fluid in the liquid state NMR implementation. In either case the implementation becomes inefficient. Indeed equivalent possibilities are available in a purely classical setting. For example a classical algorithm for factoring $N$ that test divides by all numbers up to $\sqrt{N}$ can be run in polynomial time if we have an exponential bulk of parallel computers available, or else in exponential time on a single computer if we run the trial divisions sequentially.
Is entanglement a key resource for computational power?

Recall that the significance of entanglement for pure state computations derives from the fact that unentangled pure states (or more generally \( p \)-blocked pure states) of \( n \) qubits have a description involving only \( \text{poly}(n) \) parameters (in contrast to \( \mathcal{O}(2^n) \) parameters for a general pure state). But this special property of unentangled states (of having a “small” description) is contingent on a particular mathematical description, as amplitudes in the computational basis. If we were to adopt some other choice of mathematical description for quantum states (and their evolution) then although it will be mathematically equivalent to the amplitude description, there will be a different class of states which now have a polynomially sized description i.e. two formulations of a theory which are mathematically equivalent (and hence equally logically valid) need not have their corresponding mathematical descriptions of elements of the theory being interconvertible by a polynomially bounded computation. With this in mind we see that the significance of entanglement as a resource for quantum computation is not an \textit{intrinsic} property of quantum physics itself but is tied to a particular additional (arbitrary) choice of mathematical formalism for the theory.

Thus suppose that instead of the amplitude description we choose some other mathematical description \( \mathcal{D} \) of quantum states (and gates). Indeed there is a rich variety of possible alternative descriptions. Then there will be an associated property \( \text{prop}(\mathcal{D}) \) of states which guarantees that the \( \mathcal{D} \)-description of the quantum computational process grows only polynomially with the number of qubits if \( \text{prop}(\mathcal{D}) \) is absent (e.g. if \( \mathcal{D} \) is the amplitude description then \( \text{prop}(\mathcal{D}) \) is just the notion of entanglement). Thus, just as for entanglement, we can equally well claim that \( \text{prop}(\mathcal{D}) \) for any \( \mathcal{D} \), is an essential resource for quantum computational speed-up! Entanglement itself appears to have no special status here.

An explicit example of an alternative formalism and its implications for the power of quantum computation is provided by the so-called stabiliser formalism and the Gottesman–Knill theorem [18, 25]. The essential ingredients are as follows. (See the previous references for details and proofs). The Pauli group \( \mathcal{P}_n \) on \( n \) qubits is the group generated by all \( n \)-fold tensor products of of the Pauli matrices \( \sigma_x, \sigma_y, \sigma_z \), the 1-qubit identity operator \( I \) and multiplicative factors of -1 and \( i \). Any subgroup \( \mathcal{K} \) of \( \mathcal{P}_n \) may be described by a list of at most \( n \) elements which generate the subgroup, so any subgroup has a \( \text{poly}(n) \) sized description. We write \( \mathcal{K} = [g_1, \ldots, g_k] \) if \( g_1, \ldots, g_k \) is a set of generators for \( \mathcal{K} \). For each \( n \) some states \( |\alpha\rangle \) of \( n \) qubits have a special property that they are stabilised by a subgroup \( \mathcal{K}_\alpha = [g_1, \ldots, g_k] \) \( (k \leq n) \) of \( \mathcal{P}_n \) i.e. \( |\alpha\rangle \) is the unique state such that \( g_i |\alpha\rangle = |\alpha\rangle \) for \( i = 1, \ldots, k \). For example \( |0\rangle |0\rangle + |1\rangle |1\rangle \) is the unique state stabilised by \([\sigma_x \otimes \sigma_x, \sigma_z \otimes \sigma_z]\).

Let \( \mathcal{S} \) be the class of all such states (for all \( n \)). States in \( \mathcal{S} \) can be mathematically specified by giving a list of generators of the corresponding stabiliser subgroup i.e. states in \( \mathcal{S} \) have a \( \text{poly}(n) \) sized stabiliser description. Then we have the following facts:

(a) All computational basis states are in \( \mathcal{S} \);
(b) The following gates all preserve \( \mathcal{S} \) and have simple (i.e. efficient) update rules for their effect on the stabiliser description of the states:

the 1-qubit gates (on any qubit): \[
\begin{pmatrix}
1 & 0 \\
0 & i
\end{pmatrix}, \quad
H = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 1 \\
1 & -1
\end{pmatrix}, \quad \sigma_x, \sigma_y, \sigma_z
\]
and the 2-qubit controlled-NOT gate (on any two qubits);
(c) Outcome probabilities for a measurement in the computational basis are efficiently
computable from the stabiliser description of the state;
(d) Application of other gates (such as the Toffoli gate or $\pi/8$ phase gate $[18]$ which would
provide universal computation with the gates in (b)) will generally transform states $|\alpha\rangle$ in
$S$ to states $|\psi\rangle$ outside of $S$. Recall that any unitary transformation may be expressed as a
linear combination of $I, \sigma_x, \sigma_y$ and $\sigma_z$ so we could introduce a stabiliser description of $|\psi\rangle$
as a suitable subalgebra of the group algebra of $P_n$. But this description of $n$-qubit states
$|\psi\rangle$ would not generally remain poly($n$) sized if a computational process involves such more
general gates.

From (a), (b) and (c) we immediately get:

*Gottesman–Knill theorem:* Any quantum computational process that starts with a com-
putational basis state and uses only the gates in (b) above (so that the states remains in
$S$ at each stage) can be efficiently classically simulated (by computation in the stabiliser
description).

Note that such computations can generate large amounts of multi-partite entanglement
of unboundedly many parties (e.g. by repeated use of $H$ and controlled-NOT) so that in
contrast to the stabiliser formalism, if we use the amplitude formalism then the computation
will have an exponentially growing description.

Thus if $prop(S)$ denotes the property of a state that it does not have a polynomially sized
stabiliser description, then we can claim that $prop(S)$ is an essential resource for quantum
computational power (since absence of $prop(S)$ implies efficient classical simulability).

The concept of the stabiliser description of a state (compared to the amplitude description)
provides a hint of how conceptually diverse alternative formulations of quantum theory
can be. Some recent work by Valiant $[26]$ and Terhal and DiVincenzo $[27]$ identifying an-
other interesting class of quantum computations that can be efficiently simulated, appears
to also fit into this framework, utilising a fermionic operator formalism as a mathematical
description of quantum computational processes.

Thus in a fundamental sense, the power of quantum computation over classical computa-
tion ought to derive simultaneously from *all* possible classical mathematical formalisms for
representing quantum theory, not any single such formalism and associated quality (such as
entanglement) i.e. we have arrived at the enigmatic prospect of needing a representation of
quantum physics that does not single out any particular choice of mathematical formalism.

**Acknowledgements**

RJ is supported by the U.K. Engineering and Physical Sciences Research Council. This
work was initiated in 1999 in collaborative opportunities provided by the Workshop on
Quantum Information, Computation and Decoherence, at the Isaac Newton Institute for
Mathematical Sciences, Cambridge, UK. RJ and NL also acknowledge the support of the
European 5th framework networks QAIP (Contract IST-1999-11234) and EQUIP (Contract
IST-1999-11063).
References

[1] Feynman, R. (1982) *Int. J. Th. Phys.* **21**, 467-488.

[2] Deutsch, D. (1985) *Proc. Roy. Soc. London Ser A* **400**, 96-117; Deutsch, D. and Jozsa, R. (1992) *Proc. Roy. Soc. London Ser A* **439**, 553-558.

[3] Bernstein, E. and Vazirani, U. *S. I. A. M. Journal on Computing* (1997) **26**, 1411-1473.

[4] Simon, D. (1994) *Proc. of 35th Annual Symposium on the Foundations of Computer Science*, (IEEE Computer Society, Los Alamitos), p. 116 (Extended Abstract). Full version of this paper appears in *S. I. A. M. Journal on Computing* (1997) **26**, 1474-1483.

[5] Grover, L. (1996) *Proc. 28th Annual ACM Symposium on the Theory of Computing*, (ACM Press, New York), 212-219. See also Grover, L. (1997) *Phys. Rev. Lett.* **78**, 325-328.

[6] Shor, P. (1994) *Proc. of 35th Annual Symposium on the Foundations of Computer Science*, (IEEE Computer Society, Los Alamitos), p. 124 (Extended Abstract). Full version of this paper appears in *S. I. A. M. Journal on Computing* **26** (1997), 1484-1510.

[7] Garey, M. and Johnson, D. *Computers and Intractability: a Guide to the Theory of NP Completeness*, W. H. Freeman and Co. 1979.

[8] Bennett, C. H., Bernstein, E., Brassard, G. and Vazirani, U. (1997) *S. I. A. M. Journal on Computing* **26** (1997), 1510-1523.

[9] Abrams, D. and Lloyd, S. (1998) *Phys.Rev.Lett.* **81** 3992-3995.

[10] Barenco, A. (1995) *Proc. Roy. Soc. London Ser A*, **449**, 679-683.

[11] Jozsa, R. (1998) Pages 369-379 in *The Geometric Universe* edited by S. Huggett, L. Mason, K. P. Tod, S. T. Tsou and N. Woodhouse, Oxford University Press.

[12] Jozsa, R. (1998) *Proc. Roy. Soc. London Ser A*, **454**, 323-337.

[13] Ekert, A. and Jozsa, R. (1998) *Phil. Trans. Roy. Soc. London Ser A* **356**, 1769-1782.

[14] Bhatia, R. *Matrix Analysis*, Graduate Texts in Mathematics vol 169 (Springer verlag 1997).

[15] Vazirani, U. (1998) *Phil. Trans. Roy. Soc. London Ser A* **356**, 1759-1768.

[16] Nielsen, M. (2001) Preprint available at [http://xxx.arXiv.org/abs/quant-ph/0108020](http://xxx.arXiv.org/abs/quant-ph/0108020)

[17] Raussendorf, R. and Briegel, H. (2000) Preprint available at [http://xxx.arXiv.org/abs/quant-ph/0010033](http://xxx.arXiv.org/abs/quant-ph/0010033)
[18] Nielsen, M. and Chuang, I. *Quantum Computation and Quantum Information*, Cambridge University Press 2000.

[19] Raz, R. (1999) *Proc. 31th Annual ACM Symposium on the Theory of Computing*, (ACM Press, New York), 358-367.

[20] Zyczkowski, K., Horodecki, P., Sanpera, A. and Lewenstein, M. (1999) *Phys. Rev. A* **58**, 883.

[21] Vidal, G. and Tarrach, R. (1999) *Phys. Rev. A* **59**, 141.

[22] Braunstein, S., Caves, C., Jozsa, R., Linden, N., Popescu, S. and Schack, R. (1999) *Phys. Rev. Lett.* **83**, 1054-1057.

[23] Linden, N. and Popescu, S. (2001) *Phys. Rev. Lett.* **87**, 047901.

[24] Braunstein, S. and Pati, A. (2000) Preprint available at [http://xxx.arXiv.org/abs/quant-ph/0008018](http://xxx.arXiv.org/abs/quant-ph/0008018)

[25] Gottesman, D. (1997) *Stabiliser codes and quantum error correction*, Ph.D. thesis, California Institute of Technology, Pasadena, CA.

[26] Valiant, L. (2001) *Proc. 33th Annual ACM Symposium on the Theory of Computing*, (ACM Press, New York)

[27] Terhal, B. and DiVincenzo, D. (2001) Preprint available at [http://xxx.arXiv.org/abs/quant-ph/0108010](http://xxx.arXiv.org/abs/quant-ph/0108010)