On the Power of One Bit of Quantum Information

E. Knill¹, R. Laflamme²

¹ MS B265, ² MS B288, Los Alamos National Laboratory, Los Alamos, NM 87455
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In standard quantum computation, the initial state is pure and the answer is determined by making a measurement of some of the bits in the computational basis. What can be accomplished if the initial state is a highly mixed state and the answer is determined by measuring the expectation of σ_z on the first bit with bounded sensitivity? This is the situation in high temperature ensemble quantum computation. We show that in this model it is possible to perform interesting physics simulations which have no known efficient classical algorithms, even though the model is less powerful then standard quantum computing in the presence of oracles.

Recent discoveries show that quantum computers can solve problems of practical interest much faster than known algorithms for classical computers [1,2]. This has lead to widespread recognition of the potential benefits of quantum computation. Where does the apparent power of quantum computers come from? This power is frequently attributed to "quantum parallelism", interference phenomena derived from the superposition principle, and the ability to prepare and control pure states according to the Schrödinger equation. Real quantum computers are rarely in pure states and interact with their environments, which leads to non-unitary evolution. Furthermore, recent proposals and experiments using NMR at high temperature to study quantum computation involve manipulations of extremely mixed states. Recent research in error-correction and fault-tolerant computation has shown that non-unitary evolution due to weak interactions with the environment results in no loss of computational power, if sufficiently pure states can be prepared [3–6]. Here we consider the situation where there are no errors or interactions with the environment, but the initial state is highly mixed. We investigate the power of one bit of quantum information available for computing, by which we mean that the input state is equivalent to having one bit in a pure state and arbitrarily many additional bits in a completely random state. The model of computation which consists of a classical computer with access to a state of this form is called deterministic quantum computation with one quantum bit (DQC1). We demonstrate that in the presence of oracles, such a computer is less powerful than one with access to pure state bits. However, it can solve problems related to physics simulations for which no efficient classical algorithms are known. DQC1 is the first non-trivial entry in the class of models of computations which are between classical computation and standard quantum computation. Investigations of such models are expected to lead to a better understanding of the reasons for the power of quantum computation.

There are many kinds of problems that one might like to solve using a computational device. The three main problems not involving communication are function evaluation, non-deterministic function evaluation and distribution sampling. Let S be the set of all binary strings and S_n the set of binary strings of length n. The k'th letter in a binary string b is denoted by b_k . In function evaluation, we are given a function $f: S \to S$ and a binary string b. The goal is to determine f(b). In non-deterministic function evaluation, we are given a relation $R \subseteq S \times S$ and a binary string b. The goal is to determine a string c such that R(b,c). In distribution sampling, we are given a probability distribution P on S and a length n. The goal is return a string b of length n sampled according to P(b|n).

In this paper we focus on deterministic function evaluation. A one-bit function is a function whose values are single bits. Any deterministic function evaluation problem reduces to that of evaluating a number of one-bit functions, one for each bit of the output string (a bound on the length of the output needs to be known).

Any computation requires a certain amount of resources to obtain the desired answer. The most important resources are time and space. How much of either is required can depend on the computational power of the device, which determines the applicable model of computation. For a given problem, one usually tries to determine the resources required as a function of the *problem* size, which for one-bit functions is simply the number of bits in the input string. (For general functions, one can take it to be the sum of the sizes of the input and the output string.) The computational power of two models of computation is considered to be the same if for any algorithm in one model, there is a corresponding algorithm in the other one using at most a constant multiple of the resources of the first algorithm. An algorithm is considered to be efficient if the resource requirements are polynomial in the problem size. For the purpose of discussing efficient computation, the power of two models is considered to be the same if for any algorithm in one model, there is an equivalent algorithm in the other model which uses at most a polynomial multiple of the resources. We adopt this definition for the remainder of the paper. In most cases below, the polynomial multiple is linear or constant. For a comprehensive treatment of classical computational complexity theory, see [7].

The models of computation considered here subsume classical computation. The available computational de-

vices are assumed to include a classical probabilistic computer conforming (for example) to the model of an abstract random access machine with access to random bits, and a quantum system consisting of as many (quantum) bits as needed. Without loss of generality, we can assume that the procedure used to evaluate the function f on input b consists of repetitions of two parts. The first uses the classical computer to generate a sequence of unitary operations. The second applies these operations to the quantum system in a specified initial state. A measurement of the quantum system then yields the answer. Answers from one repetition may be used to make decisions in the next ones. The models differ in what are the permitted initial states and measurements, and sometimes in the allowed unitary operations (a.k.a. quantum gates). In these models, function evaluation is performed probabilistically and we are satisfied with an answer which is correct with high probability, provided that we can make the probability of success high enough.

The state space of the quantum system of n bits is the complex hilbert space Q^n generated by the computational basis. This basis is labeled by the strings in S_n ; the basis element corresponding to string b is denoted by $|b\rangle$. Q^n is the n-fold tensor product of Q^1 . To describe unitary operators and states, it is convenient to use the operator basis consisting of tensor products of the Pauli operators [8]

$$I \doteq \sigma_{00} \doteq \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{1}$$

$$\sigma_x \doteq \sigma_{01} \doteq \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{2}$$

$$\sigma_y \doteq \sigma_{10} \doteq \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{3}$$

$$\sigma_z \doteq \sigma_{11} \doteq \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{4}$$

The binary form of the indices consists of two-bit strings. A Pauli operator acting on the k'th bit is denoted by $\sigma_b^{(k)}$. A general tensor product of Pauli operators is denoted by σ_b , where $b_{2k-1}b_{2k}$ is the index of the operator acting on the k'th bit.

A pure state of the quantum system consisting of n bits is a unit vector in \mathcal{Q}^n . In general, the quantum system can be correlated with other systems that we do not have access to. As a result, the general state of the system can be described as a distribution of pure states. However, this description is overdetermined and a better one is based on the density operator formalism. A state is a positive definite trace one hermitian operator on \mathcal{Q}^n . Pure states are of the form $|\psi\rangle\langle\psi|$ (think of $|\psi\rangle$ as a column vector, and $\langle\psi|$ as its hermitian transpose). All other states are obtained as convex combinations of pure states.

When using highly mixed states, that is those with all eigenvalues small, it is convenient to describe the state by means of deviations from the identity expressed as sums of Pauli operators. In general, a state ρ can be written in the form

$$\rho = \frac{1}{2^n} (I + \sum_{b \neq \mathbf{0}} a_b \sigma_b), \tag{5}$$

where the a_b are real and $\mathbf{0}$ is the bit string of all 0's. The deviation of ρ is the non-identity component of the sum given by $\sum_{b\neq\mathbf{0}}a_b\sigma_b$. For example, the deviation of the state where the first bit is 0 and the other bits are completely random is given by $\sigma_z^{(1)}$.

The effect of an operation on the quantum system can be described by a unitary operator U which maps an input state $|\psi\rangle$ to the output state $U|\psi\rangle$. In terms of operators, U takes the state ρ to $U\rho U^{\dagger}$.

In both of the models of quantum computation to be discussed in this letter, the elementary operations (quantum gates) that can be applied to the quantum system are a complete set of one and two bit unitary operators [9,10]. Since global phase factors in operations have no effect on the computation, it suffices to have a complete set of determinant one operators. A simple such set consists of $e^{-i\sigma_a^k\pi/8}$ for $a \neq 0$ (the $\pi/8$ rotation) and the controlled π rotation $e^{-i\sigma_z^{k_1}\otimes\sigma_z^{k_2}\pi/4}$ [3]. This is a variant of the more familiar conditional sign-flip operation. For $k_1 = 1, k_2 = 2$, it takes $|0b\rangle \rightarrow i\sigma_z^2 \pi/4 |0b\rangle$ and $|1b\rangle \rightarrow^{i\sigma_z^2\pi/4} |1b\rangle$. The difference in the effect on the second bit depending on the state of the first is a π rotation. More generally, one can use any $U(b,t) \doteq e^{-i\sigma_b t}$. The U(b,t) can be implemented with fidelity $1-\epsilon$ using $\operatorname{polylog}(1/\epsilon)n$ of the previously mentioned set of operations (this is a consequence of the results in [11]). A network implementation of a unitary operator U is a decomposition of U as a product of elementary gates. $U = \prod_i G_i$.

Deterministic quantum computation with pure states (DQCp): The initial state of the quantum system is $|\mathbf{0}\rangle$ (where bold face means that all bits are in the state $|0\rangle$). In the standard model of quantum computation, the final (one-bit) answer is obtained by a measurement of the first bit. In DQCp, this measurement is replaced by a process which yields the noisy expectation of $\sigma_z^{(1)}$ for the final state. For function evaluation (but not necessarily the other types of problems), there is no loss of power by making this restriction on the final measurement. To be specific, if the state of the quantum system is ρ , the measurement process returns a number which is sampled from a distribution with mean $\langle \sigma_z^{(1)} \rangle = \operatorname{tr}(\sigma_z^{(1)} \rho)$ and bounded variance s, where s is independent of the number of bits used. We call such a measurement an *estimate* of the quantity measured. Repeating the computation and measurement are assumed to yield independent instances of this distribution. Thus, the mean can be estimated to within ϵ with probability of error at most p using $O(\log(1/p)/\epsilon^2)$ repetitions of the computation [12]. DQCp is realized by an idealized bulk NMR quantum computer, where all molecules are initially perfectly polarized, there is no decoherence and there is no operational error.

If U is a unitary operator with a network implementation, then DQCp yields an estimate of $\operatorname{tr}(\sigma_z^{(1)}U|\mathbf{0}\rangle\langle\mathbf{0}|U^\dagger)$. By preprocessing the input state with operators of the form $G=e^{-i\sigma_a\pi/2}$, any quantity of the form $\operatorname{tr}(\sigma_z^{(1)}U|\mathbf{b}\rangle\langle\mathbf{b}|U^\dagger)$ can be estimated. By further post-processing the state with one or two operators of the form $G=e^{-i\sigma_a\pi/4}$, quantities like $\operatorname{tr}(\sigma_c U|\mathbf{b}\rangle\langle\mathbf{b}|U^\dagger)$ can be obtained. Since the resources required for pre- and postprocessing are linear in the number of bits, we can identify (the power of) DQCp with the ability to estimate these quantities.

Deterministic quantum computation with one qubit (DQC1): The deviation of the initial state of the quantum system is $\sigma_z^{(1)}$. The final answer is obtained as in DQCp by a bounded variance process yielding $\langle \sigma_z^{(1)} \rangle$. The initial state corresponds to having one bit in a pure state and the rest completely random.

DQC1 is realized by an idealized high temperature NMR quantum computer where there is no decoherence and no operational error. This is the regime where the initial deviation state can be approximated by $e^{-\beta H}/Z \sim$ $\frac{1}{2^n}(I-\beta\sum_i e_i\sigma_z^{(i)})$ (noninteracting bits). The one-bit initial state can be obtained by eliminating polarization in bits other than the first. Exploiting the additional polarization can reduce the time resource required by at most a factor of 1/n, so that no additional power can be gained. Constraints on the amount of polarization extractable from the high temperature state have been investigated by Sorensen [13]. Note that DQC1 is not robust against many realistic error-models. For example, the results of Aharonov and Ben-Or [14] show that error-correction cannot be used to successfully compensate against depolarizing independent errors due to the rapid loss of information if fresh ground-state bits cannot be introduced during the computation.

Let U be a unitary operator with a network implementation. Using DQC1 and pre- and postprocessing similar to that introduced with DQCp, we can estimate $\operatorname{tr}(\frac{1}{2^n}\sigma_a U \sigma_b U^{\dagger})$ for any a and b. We can therefore identify DQC1 with the ability to perform these estimates.

DQCp and DQC1 can be used to estimate any coefficient of certain operator expansions of U. For DQC1, write $U = \sum_b \alpha_b \sigma_b$, with $\alpha_b = \frac{1}{2^n} \mathrm{tr}(\sigma_b U)$. This is the Pauli operator expansion of U. To determine α_b , use the network for U to construct a network for the operator V which maps $|0\rangle|b\rangle \rightarrow |0\rangle U|b\rangle$ and $|1\rangle|b\rangle \rightarrow |1\rangle|b\rangle$. This is a "conditional" U operator and can be implemented with a linear amount of additional resources [10]. Then

$$\frac{1}{2^{n+1}}\operatorname{tr}(\sigma_x^{(1)}V\sigma_x^{(1)}\sigma_bV^{\dagger}) = \frac{1}{2}(\operatorname{tr}(U\sigma_b) + \operatorname{tr}(\sigma_bU^{\dagger})) \tag{6}$$

$$= \operatorname{Re}(\alpha_b),$$

$$\frac{1}{2^{n+1}}\operatorname{tr}(\sigma_y^{(1)}V\sigma_x^{(1)}\sigma_bV^{\dagger}) = \frac{1}{2}(i\operatorname{tr}(U\sigma_b) - i\operatorname{tr}(\sigma_bU^{\dagger})) \quad (7)$$

$$= -\operatorname{Im}(\alpha_b).$$

Thus the coefficients α_b can be estimated with two computations. Since $U\sigma_bU^{\dagger}$ is a unitary operator easily implemented given networks for U, the ability to estimate the coefficients of the Pauli operator expansion is equal in power to DQC1.

If the trick of the previous paragraph is used with DQCp, we can obtain any $\operatorname{tr}(U|b\rangle\langle b|)$. Since $\operatorname{tr}(U|a\rangle\langle b|)$ can be written as a sum of expressions of the form $\operatorname{tr}(U\frac{1}{2}(|a\rangle+e^{i\phi}|b\rangle)(\langle a|+e^{-i\phi}\langle b|),$ and the states in the second operator can be generated from $|0\rangle$ with O(n) gates, any of the transition amplitudes of U can be determined to get coefficients of the $matrix\ U$ in the computational basis. To see that the ability to estimate $\langle a|U|b\rangle$ is as powerful as DQCp, observe that $\operatorname{tr}(\sigma_z^{(1)}U|0\rangle\langle 0|U^\dagger)=\operatorname{tr}(\langle 0|U^\dagger\sigma_z^{(1)}U|0\rangle).$

Let the evolution of a quantum mechanical system be described by a (possibly time varying) hamiltonian H on a hilbert space \mathcal{H} . To efficiently simulate this evolution using a quantum computer with n bits, it is sufficient to have a unitary embedding of \mathcal{H} in \mathcal{Q}^n and an extension H' of the embedded hamiltonian for which there are efficient quantum networks approximating $e^{-iH'(t)\delta}$ (taking $\hbar = 1$) for small δ to within $O(\delta^2)$. (To define efficiency properly requires problem instances for each n, in which case a resource bound polynomial in n and $1/\delta$ can be imposed.) A class of such hamiltonians consists of those which are a polynomially bounded sum of two bit hamiltonians [15]. Whether it is useful to implement this simulation depends on what information one wants to obtain. If one simply wants to predict the outcome of a measurement in an experiment involving this system, it is possible to do that by simulation, provided that the initial state can be computed, and the final measurement can be represented as a measurement in the computational basis. DQCp and DQC1 are further restricted to measurements of expectations of operators which can be approximated as a sum of a reasonable number of computable conjugates of $\sigma_z^{(1)}$.

Even if the initial state is restricted to the deviation $\sigma_z^{(1)}$, there are no known classical algorithms for simulating an arbitrary sum of two bit hamiltonians as described above. Since many real-world situations involve highly mixed initial states (e.g. most NMR experiments), such an algorithm is very interesting. In fact there are ongoing experiments exploiting the fact that many $\frac{1}{r^3}$ interactions can be simulated in solid state systems such as calciumfluoride by modifying the dipolar interaction, but are difficult to simulate using classical computation [16]. The observation that it it appears to be difficult to efficiently implement such simulations in DQC1 makes this model

useful and the question of the relationship between the powers of DQC1 and DQCp or classical computation non-trivial.

For any hamiltonian, one of its physical properties of interest is the energy spectrum. This problem of determining the spectral density function is not in the class of one-bit deterministic functions. However, any decision problem based on the spectrum can be thought of as a non-deterministic one-bit function. The non-determinism is needed to permit the possibility that either decision is acceptable. Without this possibility there can be situations where we cannot gain arbitrarily high confidence in the correctness of the decision.

In DQC1 it is possible to directly observe the spectrum with a resolution inversely related to the effort used. Methods to accomplish this type of observation are well known in the NMR literature, where the natural hamiltonians are routinely modified using effective hamiltonian techniques [17]. Decoupling methods used to effectively remove interactions with some nuclei are an application [18]. Here we give a simple method for observing spectra from the point of view of quantum computation.

Let $U(t)=e^{-iHt}$ and assume that an efficient quantum network for applying U(t) with arbitrarily small error is available. Note that the quantum network may increase in complexity if less error is needed. Given the quantum network for U(t), we can derive networks for applying U(t) or $U^{\dagger}(t)$ to bits $2\dots n+1$, conditionally on the state of the first bit. Let V(t) be the unitary operator which maps $|1\rangle|b\rangle \to |1\rangle U^{\dagger}(t/2)|b\rangle$ and $|0\rangle|b\rangle \to |0\rangle U(t/2)|b\rangle$. If we first apply a gate to transform the input state $\sigma_z^{(1)}$ to $\sigma_x^{(1)}$, and apply V(t), then the deviation of the state becomes

$$\rho_f = \sum_{i} (\cos(\lambda_i t) \sigma_x^{(1)} + \sin(\lambda_i t) \sigma_y^{(1)}) |i\rangle \langle i|$$

$$= \frac{1}{2^n} \sum_{i} (\cos(\lambda_i t) \sigma_x^{(1)} + \sin(\lambda_i t) \sigma_y^{(1)}) + \text{rest.}$$
(8)

where the λ_i and $|i\rangle$ are a complete set of eigenvalues and corresponding eigenvectors (with repetition) of H. The second identity gives the expansion of ρ_f in terms of σ_b 's, with terms not of interest suppressed. The coefficients of σ_x and σ_y can be measured and the results combined into a single complex number with value $f(t) = \frac{1}{2^{n+1}} \sum_i e^{-\lambda_i t}$. This can be sampled at as many time points as desired and fourier transformed to obtain a broadened energy spectrum. The same technique can be used to measure the spectrum of a unitary operator by restricting t to integer multiples (corresponding to powers of the operator). If the evolution V(t) is implemented as a power of $V(\Delta t)$, and the measurement in DQC1 is non-destructive, then the spectrum can be observed directly as is done in fourier transform NMR spectroscopy.

DQC1 is strictly less powerful then DQCp in the presence of oracles (a.k.a. black box). Suppose that we

are given a black box implementing a unitary operator U on our quantum system and we wish to determine $\operatorname{tr}\langle \mathbf{0}|U^{\dagger}\sigma_z^{(1)}U|\mathbf{0}\rangle$, whose sign is the one bit answer computed by U on input $|\mathbf{0}\rangle$. One method for obtaining this answer using DQC1 involves preparing a pseudopure state from the deviation $\sigma_z^{(1)}$ [19,20]. Such a state has deviation proportional to that of a pure state. If the deviation is proportional to that of $|\mathbf{0}\rangle\langle\mathbf{0}|$, measurement of $\sigma_z^{(1)}$ after applying U is proportional to the desired answer.

It turns out to be quite simple to prepare a kind of pseudo-pure state from $\sigma_z^{(1)}$ using an ancilla bit, here labeled 0. Let T_n be the unitary operator mapping $|b_0\mathbf{0}\rangle \to |(b_0+1)\mathbf{0}\rangle$ and for $b \neq 0$, $|b_0b\rangle \to |b_0b\rangle$ (addition of bits is modulo two). If we first swap bits 0 and 1, then apply T_n , and finally flip bit 0, the deviation is given by $\sigma_z^{(0)}(2|\mathbf{0}\rangle\langle\mathbf{0}|-I)$. If we apply U to bits 1 through n, then the coefficient α of $\sigma_z^{(0)}\sigma_z^{(1)}$ in the state's deviation is the answer we want. As discussed above, this coefficient can be obtained using DQC1, with an intensity of $\alpha/2^{n+1}$. The exponential loss of intensity implies that it is very difficult to detect α above the noise.

Unfortunately, without the ability to analyze a specification of U (for example, an implementation by a quantum network), we cannot do much better, even if we know that the answer of U is deterministic, that is $\alpha \in \{-1,1\}$. The most general form of a DQC1 algorithm for determining the answer can be described by k independent DQC1 computations consisting of quantum networks and calls to U and an inference function which attempts to determine α from the k measurements. Consider the first of these measurements. The expectation of the result of the measurement can be written in the form

$$v(U) = \frac{1}{2^m} \operatorname{tr}(V_r U \dots U V_0 \sigma_z^{(1)} V_0^{\dagger} U^{\dagger} \dots U^{\dagger} V_r^{\dagger} \sigma_z^{(1)}), \quad (9)$$

where r is the number of invocations of U, the V_i are the quantum networks used in the computation using m bits (of which m-n are ancillas). Since U is deterministic, $U|0\rangle|\mathbf{0}\rangle=|b\rangle|\psi\rangle$. If U is composed with the operator T which conditional on the state of bits 2 to n being $|\psi\rangle$ flips the first bit, we get an operator U' which is also deterministic but has the opposite answer. We must be able to distinguish between the two. T can be written in the form T=I-2P, where P is the pure state given by $\frac{1}{2}(I-\sigma_x^1)\otimes|\psi\rangle\langle\psi|$ (the m-n ancillas have been suppressed in this expression). For unitary operators W_1 and W_2 acting on $m\geq n$ bits, we have $|\frac{1}{2^m}\mathrm{tr}(W_1PW_2)|\leq \frac{1}{2^n}$. By expanding U'=U-2PU in the expression for v(U') we can write

$$\psi(U') \qquad (10)$$

$$= \frac{1}{2^m} (\operatorname{tr}(V_r(-2P)UV_{r-1}U'...) + \operatorname{tr}(V_rUV_{r-1}U'...))$$

$$= \frac{1}{2^m} (\operatorname{tr}(V_r(-2P)UV_{r-1}U'...))$$

$$+\operatorname{tr}(V_{r}UV_{r-1}(-2P)UV_{r-2}U'\ldots) +\operatorname{tr}(V_{r}UV_{r-1}UV_{r-2}U'\ldots)) = \frac{1}{2^{m}}(\operatorname{tr}(V_{r}(-2P)UV_{r-1}U'\ldots) +\operatorname{tr}(V_{r}UV_{r-1}(-2P)UV_{r-2}U'\ldots) + \ldots + v(U)).$$

Thus, $v(U') = \frac{1}{2^m}(a_1 + \ldots + a_{2r} + v(U))$, where $|a_i| \le 2^{m-n+1}$. It follows that $|v(U')-v(U)| \le 4r/2^n$. It is clear that there is a sensitivity problem: To confidently distinguish between U' and U requires exponentially many experiments or invocations of the oracle.

The inequality derived in the previous paragraph suggests that it might be possible to obtain the answer of U with $O(2^n)$ invocations of U rather than the $O(2^{2n})$ experiments required to detect a signal of strength $1/2^n$ in the presence of bounded noise. We do not know whether this is possible.

We have introduced a new model of computation (DQC1) with power between classical computation and deterministic quantum computation with pure states (DQCp). DQC1 is not as powerful as DQCp in the presence of unitary oracles but can solve problems in physics simulation for which there are no known efficient classical algorithms. Since DQC1 requires only one quantum bit of information, the possibility that it adds power to classical computation is surprising. If this is the case, the usual reasons given for why quantum computation appears to be so powerful may have to be revised. On the other hand, a proof that DQC1 can be efficiently simulated by classical computation would be extremely interesting, as this could lead to practical algorithms for simulations of many experimentally interesting physical situations.

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