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RAPID COMMUNICATIONS

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Qubit-qubit interaction in quantum computers

Julio Gea-Banacloche
University of Arkansas, Fayetteville, Arkansas 72701
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Limitations to the performance of a quantum computer arising from direct interaction between qubits are considered, and the basic scaling laws (with the computation time and the number of qubits) are established for the specific example of the quantum Fourier transform algorithm. These results should be relevant for several of the currently proposed quantum computer systems, where the dominant interaction is of the magnetic dipole-dipole type, in the limit of many qubits and long computation times. [S1050-2947(98)50601-4]

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It is now quite likely that there will be quantum computers with perhaps as many as ten ''quantum bits,'' or ''qubits,'' in operation in the very near future (see recent reviews in [1,2]). To be able to scale them up beyond this point will require, among other things, a careful study of all the possible sources of error and of how these scale up as well. The purpose of this Rapid Communication is to draw attention to one such source, namely, the direct interaction between qubits, and to exhibit how its influence scales with both the size of the computer and the computation time; this is illustrated for the specific task of calculating the quantum version of the fast-Fourier transform, or ''quantum Fourier transform'' (QFT).

Interaction between qubits is different from other sources of ''coherent'' error in a quantum computer in that it is not a single-qubit effect; rather, in the most general case, it leads to phase factors that are configuration dependent; that is, they depend on the state of all the qubits. This might make it particularly difficult to undo the error (even though the process is deterministic and thus, in principle, reversible). In fact, one should expect this particular error to *worsen* when conventional (single-qubit) error correction measures are implemented, since these require an increase in both the number of qubits and the computation time.

As a simple illustration, consider just two qubits with states $|0\rangle$ and $|1\rangle$, and configuration energies E_{ij} $(i,j=0,1)$. An initially factorizable state such as $\frac{1}{2}(|0\rangle+|1\rangle)(|0\rangle+|1\rangle)$ evolves into $\frac{1}{2}(e^{-iE_{00}t/\hbar}|00\rangle+e^{-iE_{01}t/\hbar}|01\rangle+e^{-iE_{10}t/\hbar}|10\rangle+e^{-iE_{11}t/\hbar}|11\rangle)$. The purity of the state of the first qubit decreases as $\mathrm{Tr}(\rho_1^2)=\frac{3}{4}+\frac{1}{4}\cos[(E_{00}+E_{11}-E_{10}-E_{01})t/\hbar]$. The argument of the cosine is zero in the absence of interaction, or if the configuration energies are otherwise additive as in $E_{ij}=E_i+E_j$. Otherwise, the state will almost certainly become entangled. The rate at which purity is destroyed is, for short times, quadratic in t and in a difference of configuration energies. I shall show below that these features seem to be quite general.

In the ion-trap quantum computers originally proposed by Cirac and Zoller [3], and studied elsewhere [4,5], the qubit basis states would have nonvanishing quadrupole moments and the first term in the interaction between qubits that distinguishes between their internal states in a nonadditive way would be the quadrupole-quadrupole term, which decreases as r_{ij}^{-5}. These systems, however, do not appear to be the most promising candidates for quantum computers because of their relatively short radiative lives. Other schemes have been proposed using the hyperfine split of the ground state of trapped ions (as in the quantum logic gate demonstrated in [6]), or simply Zeeman sublevels of the ground state. For these systems there would be a magnetic dipole-dipole interaction between neighboring qubits, as the electron's spin state is different in each of the two states $|0\rangle$ and $|1\rangle$. A magnetic dipole-dipole interaction would also occur naturally in the recently proposed NMR systems [7] (in fact, the NMR systems rely on the spin-spin interaction for their op-

eration and, therefore, have ways around some of the problems discussed here; see below for further comments). This interaction decreases as r_{ij}^{-3} and is governed by the Hamiltonian

$$H_{ij}=\frac{\mu_0}{4\pi}\left(g\,\frac{e}{2m}\right)^2\frac{1}{r_{ij}^3}\left[S_{1z}S_{2z}+S_{1y}S_{2y}-2S_{1x}S_{2x}\right] \quad (1)$$

(assuming that the qubits lie along the x axis, perpendicular to the quantization z axis) where g and m are the appropriate g factors and masses ($m=m_e$ for the ion case, m_p for the NMR case) and S is the spin operator of either the electron or the nucleus, respectively. For an order of magnitude, we find interaction energies $E_{i,i+1}/\hbar\sim 0.1/d^3$ rad/s for the ion trap, where d is the distance between ions in micrometers, and $E_{i,i+1}/\hbar\sim 10^5/d^3$ rad/s for the NMR case, with d in angstroms.

For two qubits, the difference between configuration energies are of the same order of magnitude as the energies themselves, but for L qubits they will typically scale as $L^{1/2}$, as the following very simplified model shows. Consider only nearest-neighbor interactions so that $H=\Sigma_{i=1}^{L-1}H_{i,i+1}$. For L qubits with states $|0\rangle$ and $|1\rangle$, each basis state can be labeled by a sequence of zeros and ones, or, alternatively, by the integer n between 0 and 2^L-1 of which such a sequence is the binary representation. In the spirit of perturbation theory, we take $E_n=\langle n|H|n\rangle$ [9]. Then we define δ so that $\langle n|H_{i,i+1}|n\rangle=\hbar\delta/2$ if the contiguous spins i and $i+1$ are in the same state (0 or 1) and $=-\hbar\delta/2$ if they are in different states. If the energy E_0 of the state $|0\rangle=|0\ldots0\rangle$ is set to 0 for reference, then the energy E_n of an arbitrary configuration $|n\rangle=|011\ldots010\rangle$ is equal to $-\hbar\delta$ times the number of ''steps'' (from 0 down to 1 or from 1 up to 0) in the binary representation of n with L ''digits.'' It is straightforward to see that the energies thus obtained are binomially distributed, with mean $-\frac{1}{2}\hbar\delta(L-1)$ and standard deviation $\frac{1}{2}\hbar\delta(L-1)^{1/2}$.

From the foregoing, one expects that the interaction between qubits will degrade the performance of the quantum computer whenever the product of $\delta t\sqrt{L}\sim 1$ (where $\hbar\delta$ is the two-qubit interaction energy and t is the total computation time). The following model explores this in detail for the case of a quantum computer performing a discrete Fourier transform to determine the period of a certain function (the last step in Shor's quantum factorization algorithm).

To calculate a discrete Fourier transform with a quantum computer one begins by preparing the computer in a superposition of basis states whose coefficients are the values of the function at the discrete points $\{n\}$, so that the initial state is $|\psi\rangle=\Sigma_{n=0}^{2^L-1}f(n)|n\rangle$. Then a sequence of unitary transformations are applied to $|\psi\rangle$. These are of two kinds: L one-bit operations A_j and $L(L-1)/2$ two-bit operations B_{ij}. At the end (after bit reversal, a relatively trivial complication), one has a state $|\tilde{\psi}\rangle=\Sigma_{m=0}^{2^L-1}\tilde{f}(m)|m\rangle$ in which the coefficients are the discrete Fourier transform of f: $\tilde{f}(m)=2^{-L/2}\Sigma_{n=0}^{2^L-1}\exp(2\pi imn/2^L)f(n)$ [10].

To simulate the impact of qubit-qubit interaction on this quantum Fourier transform (QFT) algorithm, I have used the following prescription. After every unitary operation, of either the A or the B type, simply multiply each basis state $|n\rangle$ by $\exp(-iE_n\tau/\hbar)$, with E_n calculated as in the model above. This is intended to take into account the fact that each unitary operation takes a certain time (τ in this model) during which the system evolves more or less freely (except, of course, for the one or two qubits that are being acted upon, but this is a complication that should not alter the results substantially in the limit of many qubits L). The overall result is still a unitary transformation: a basis vector such as $|n\rangle$ is transformed into the superposition

$$|n\rangle\rightarrow\frac{1}{\sqrt{2^L}}\sum_{m=0}^{2^L-1}e^{i\theta(n,m)}e^{2\pi imn/2^L}|m\rangle. \quad (2)$$

The coefficient in Eq. (2) should be a pure sinusoidal function (Fourier transform of a δ function). The interaction between qubits introduces the additional phase factor represented by the function $\theta(n,m)$. For the very simple model used here, it should be possible to calculate $\theta(n,m)$ explicitly for given values of n and m by just going through the steps of the QFT algorithm; I have not, however, been able to derive a compact general expression for it, but one remarkable result of the numerical simulations is that, for sufficiently large L, it seems to be a good approximation to assume that $\theta(n,m)$ is given by the sum of two functions

$$\theta(n,m)\simeq\theta'(n)+\theta''(m). \quad (3)$$

This means that an arbitrary function $f(n)$ is transformed according to

$$\tilde{f}(m)\simeq\frac{1}{2^{L/2}}e^{i\theta''(m)}\sum_{n=0}^{2^L-1}e^{2\pi imn/2^L}e^{1\theta'(n)}f(n). \quad (4)$$

If, as is the case for Shor's factorization algorithm, one is only interested in the magnitude of $\tilde{f}(m)$, the $\theta''(m)$ part can be ignored. The result is the Fourier transform of the product of the original function and a phase factor $e^{i\theta'(n)}$. Within the framework of the approximation (3), the function $\theta'(n)$ can be calculated as $\theta'(n)\simeq\theta(n,0)-\theta''(0)$ by going through the QFT algorithm step by step and figuring out the phase factors picked by the $|0\rangle$ component of each basis vector $|n\rangle$. The result is, up to an unimportant constant, given by the recursion

$$\theta'(0)=0,$$

$$\theta'(1)=\delta\tau(\tfrac{1}{2}L(L+1)-1),$$

$$\theta'(2^j+k)=\theta'(k)+\delta\tau((L-j)(L-j+1)-2),\qquad 0\leqslant k<2^{j-1},$$

$$=\theta'(k),\quad 2^{j-1}\leqslant k<2^j, \quad (5)$$

where $1\leqslant j<L$. These phases are clearly not random, but for sufficiently large L they are found to fall on an approximately Gaussian distribution (Fig. 1). It is not very hard to calculate explicitly that the average of the phases (5) is $\delta\tau L(L-1)(L+4)/12$; it can also be shown that the variance is

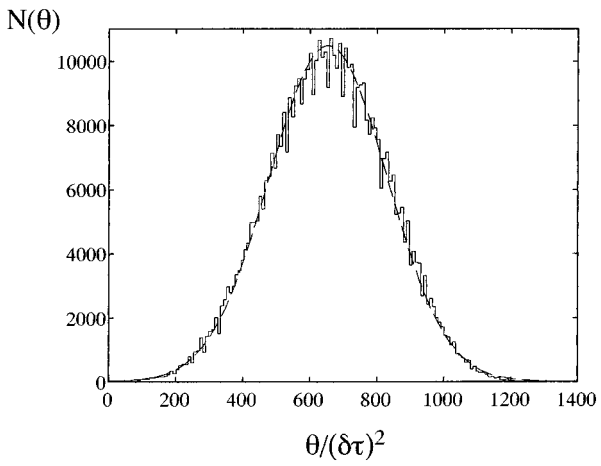

FIG. 1. Distribution of the phases $\theta'(k)$ [Eq. (5)] for $L=19$. The dashed line is a Gaussian distribution with the same mean and standard deviation σ [Eq. (6)]. The size of the bins is $\sigma/20$.

$$\sigma_0^2=(\delta\tau)^2\left[\tfrac{1}{80}L^5-\tfrac{1}{48}L^3+\tfrac{1}{8}L^2+\tfrac{23}{60}L-\tfrac{1}{2}\right]\simeq\frac{(\delta\tau)^2}{80}L^5. \tag{6}$$

In Shor's factorization algorithm, the QFT is used to find the period r of a function $f(n)$ which is zero everywhere except when $n=l+kr$, where k is an integer and $l<r$ is a random offset. If $k_{\max}$ equals the largest integer not greater than $(2^L-1-l)/r$, a properly normalized form of $f(n)$ is

$$f(n)=\frac{1}{\sqrt{k_{\max}+1}}\sum_{k=0}^{k_{\max}}\delta_{n,l+kr}. \tag{7}$$

Further, it is expected that the period r will be much smaller than the number of basis vectors 2^L; indeed, one expects that $r<2^{L/2}$ by construction. This means that, for large L, $k_{\max}$ is a very large number; the ''comb'' of δ functions $f(n)$ will sample the phases $\theta'(n)$ in Eq. (4) at many points n and presumably generate a pseudorandom sequence of phases in the process.

In Ref. [11], Barenco *et al.* introduced the concept of a ''Q factor'' to quantify how well one could reconstruct the period of a function from a noisy QFT. This factor would equal the total probability of obtaining a value of m as close as possible to a multiple of $2^L/r$, when the final state of the system is measured in the $\{|n\rangle\}$ basis. That is, Q equals a sum of terms $|\langle m|\tilde{\psi}\rangle|^2=|\tilde{f}(m)|^2$, where the m's in the sum are the integers closest to whole multiples of $2^L/r$.

When the function (7) is used in Eq. (4), one obtains

$$|\tilde{f}(m)|^2=\frac{1}{2^L}+\frac{1}{2^L(k_{\max}+1)}\sum_{k\neq k'=0}^{k_{\max}}\times e^{2\pi i m(k-k')r/2^L}e^{i\theta'(l+kr)-i\theta'(l+k'r)}. \tag{8}$$

Now, in Eq. (8) it turns out to be a good approximation to replace the last phase factor, involving the phases θ', by its average over a Gaussian distribution with variance σ^2 [treating also $\theta'(l+kr)$ and $\theta'(l+k'r)$ as essentially independent random variables]. This is because there are many terms

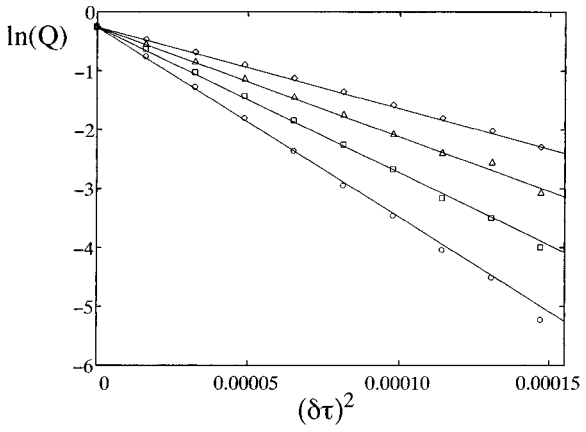

FIG. 2. How the Q factor degrades with increasing interaction energy (δ) or computation time (τ) for $L=19$. Each point is the result of a calculation for a periodic function of the form (7) with period and offset chosen randomly, except that the periods are made to be multiples of 16 (diamonds), 8 but not 16 (triangles), 4 but not 8 (squares), and 2 but not 4 (circles). The straight lines are plots of the last term of Eq. (10) with the appropriate variances given by Eq. (11).

in the sum for which the first phase factor will have the same value (all those with the same value of $k-k'$), and these appear to be enough to sample a representative set of values for θ' in every case. The average is $\exp(-\sigma^2)$, so we have, resuming the geometric series,

$$|\tilde{f}(m)|^2\simeq\frac{1}{2^L}(1-e^{-\sigma^2})+\frac{e^{-\sigma^2}}{2^L(k_{\max}+1)}\frac{\sin^2[\pi m(k_{\max}+1)r/2^L]}{\sin^2[\pi mr/2^L]}. \tag{9}$$

When calculating Q, one must sum Eq. (9) over all the values of m that are closest to an integer multiple of $2^L/r$. This means that m above is a number of the form $m=\lambda 2^L/r+x$, where λ is an integer and x a number between $-\frac{1}{2}$ and $\frac{1}{2}$ [12]. Substituting in Eq. (9) and recalling that $r/2^L\simeq 1k_{\max}\ll 1$, we find that the last factor becomes $k_{\max}^2\sin^2[\pi x]/(\pi x)^2$. Summing over m has the effect of averaging this term over the range $-\frac{1}{2}<x<\frac{1}{2}$, as well as adding an overall factor r to the whole expression, since there are r integer multiples of $2^L/r$ between 0 and 2^L. The end result is

$$Q\simeq\frac{1}{k_{\max}}(1-e^{-\sigma^2})+0.774e^{-\sigma^2}, \tag{10}$$

where the first term will typically be negligible, except for very large σ.

Figure 2 shows the results of the numerical calculation of the QFT with the above model for several functions $f(n)$ chosen at random and how they compare with the predictions of Eq. (10) (last term only) with the appropriate variance. It is found that functions whose periods are multiples of 4 are less affected in this model than functions whose periods are multiples of 2 but not 4, and likewise for 8, 16, ... This is because of the obvious patterns in the phases (5) involving powers of 2. If one samples the function (5) at intervals that

are multiples of 4, 8, 16, ..., one finds progressively smaller variances among the phases. If $\sigma_j^2(L)$ is the variance obtained when the phases (5) are sampled at intervals of 2^j, I find that

$$\sigma_1^2(L)=(\delta\tau)^2[\tfrac{1}{80}L^5+\tfrac{11}{48}L^3-\tfrac{5}{8}L^2+\tfrac{2}{15}L-\tfrac{1}{2}]\simeq\frac{(\delta\tau)^2}{80}L^5,$$

$$\sigma_j^2(L)=\sigma_1^2(L-j+1)\simeq(\delta\tau)^2\left[\frac{L^5}{80}-\frac{L^4(j-1)}{16}\right],\quad j\geqslant 2. \tag{11}$$

Thus σ_1 (for functions where r is even but not a multiple of 4) is not very different from σ_0 [Eq. (6)], but the other variances can be substantially smaller for not-too-large L.

Since, in this model, the total computation time $t\simeq\tau L^2/2$ and $\delta^2 L\simeq 4(\Delta E/\hbar)^2$ (where ΔE, the standard deviation of the configuration energies, scales as $L^{1/2}$, as argued above), one can write $\sigma_1^2\simeq(\Delta E t/\hbar)^2/5$. It then follows from Eqs. (10) and (11) that the interaction between qubits degrades the quantum computer performance in a way that is an exponential of the square of the computation time and of ΔE. Numerical calculations with somewhat more sophisticated models (e.g., ''freezing'' the time evolution of the qubit(s) on which the quantum gate acts) lead to the same general scaling laws for sufficiently large L, only with slightly different numerical coefficients.

Assuming that a scaling of this form holds for the entire factorization algorithm, one can immediately see that this is, in general, not a negligible effect. For instance, for L Ba^+ ions separated a distance $d=1.76$ μm (as assumed, for example, in [5]), one has $\Delta E/\hbar=1.5\times10^{-2}\sqrt{L}$ rad/s. From the estimates of Plenio and Knight [8(b)], factorization of a ten-bit number (without error correction) would require 52 qubits and take a time $t=13$ s in this system, which yields $\Delta E t/\hbar=1.4$, already an appreciable number. With error correction, at least five times more qubits are required and a time at least five times longer, leading to $\Delta E t/\hbar\sim 15$. This would be enough to completely ruin the quantum computer's performance. Needless to say, the magnitude of the effect can be reduced by increasing the distance between the ions, but there are reasons to want to have them as close as possible [5]; in any event, this shows that this effect must be taken into account as a design consideration, at least for these kinds of systems.

The NMR schemes [7] rely on a procedure called ''refocusing'' or ''decoupling'' to remove spin interaction effects, although it is not clear to me whether, in principle, all interaction terms can be completely eliminated in all systems. In any case, since the couplings are so strong in the NMR systems, one needs to address the question of how thoroughly the unwanted phase factors can be erased. If the size of the residual phases can be estimated for a particular system, the results in this paper may be used to estimate their impact on overall performance.

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[8] (a) M. B. Plenio and P. L. Knight, Phys. Rev. A **53**, 2986 (1996); (b) e-print quant-ph/9610015.

[9] This assumes that there are no degeneracies, i.e., that the state $|01\rangle$ is distinguishable from $|10\rangle$ even in the absence of interaction. This would hold for the NMR computers because of the chemical shifts. In the degenerate case, the evolution model to be used below would become rather complicated, although I do not expect substantial qualitative differences with the present, simpler one.

[10] See Ref. [1] for details of the algorithm. Note, however, a typographical error in Eq. (20) of [1], which makes it inconsistent with Eq. (22).

[11] A. Barenco , A. Ekert, K.-A. Suominen, and P. Törmä, Phys. Rev. A **54**, 139 (1996).

[12] I am assuming here that r is ''typical,'' in that it does not equal a power of 2. Otherwise, $x=0$ and the factor 0.774 in Eq. (10) below should be equal to 1 instead. My final result (10) may be regarded as a small refinement over the results of [9] regarding the performance of the QFT in the presence of random-phase noise.