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Energy and efficiency of adiabatic quantum search algorithms

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Abstract
We present the results of a detailed analysis of a general, unstructured adiabatic quantum search of a database of N items. In particular, we examine the effects on the computation time of adding energy to the system. We find that by increasing the lowest eigenvalue of the time-dependent Hamiltonian *temporarily* to a maximum of $\propto\sqrt{N}$, it is possible to do the calculation in constant time. This leads us to derive the general theorem which provides the adiabatic analogue of the $\sqrt{N}$ bound of conventional quantum searches. The result suggests that the action associated with the oracle term in the time-dependent Hamiltonian is a direct measure of the resources required by the adiabatic quantum search.

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1. Introduction

The subject of quantum computation and quantum information theory has attracted a great deal of attention in the recent past (for reviews, see [1–3]). This is mainly due to the existence of many algorithms showing that the principles of quantum mechanics can be used to greatly enhance the efficiency of solving specific computational problems. Notable among them are the factorization algorithm due to Shor [4], the algorithms of Deutsch and Jozsa [5, 6] and the data search algorithm due to Grover [7], which is the subject of the present paper.

Assume that there are a total of N items in a completely unstructured database, out of which exactly one is marked (item m say). The task is to find that marked element in as few steps as possible. Classically, on average $N/2$ steps are required, but Grover was able to devise a quantum search algorithm which finds the marked element in $\mathcal{O}(\sqrt{N})$ steps [7]. Moreover, this is the best that one can do since Grover's algorithm saturates the lower bound found by

Bennett *et al* [8] (henceforth referred to as the BBBV bound; see also [9–11]). Recently it was suggested [9, 12] that such gates can be replaced entirely by a continuously time varying Hamiltonian which evolves a chosen initial quantum mechanical state directly to the required marked item/state in an efficient way. The details of this 'adiabatic' approach are as follows: consider $N \equiv 2^n$ items in the database, each associated with one vector in the complete orthonormal vector set $\{|i\rangle, i = 0, \ldots, N-1\}$ in the Hilbert space of n spin-1/2 objects. Assume that the initial state of the quantum computer is the symmetric (normalized) state:

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle. \tag{1}$$

Let $|m\rangle$ denote the eigenstate associated with the marked item. Now define the two Hermitian operators

$$H_0 = I - |\psi_0\rangle\langle\psi_0| \tag{2}$$

$$H_1 = I - |m\rangle\langle m| \tag{3}$$

whose ground states are $|\psi_0\rangle$ and $|m\rangle$, respectively, and the time-dependent Hamiltonian

$$H(t) = (1 - s(t))H_0 + s(t)H_1. \tag{4}$$

In the above, $s(t)$ is some monotonically increasing function of time t, subject to the conditions

$$s(0) = 0 \qquad s(T) = 1 \tag{5}$$

where T is the total computation time. Note that H_1, which projects out the marked state, plays the role of the 'oracle' of the Grover algorithm.

As long as the time evolution is slow enough, the adiabatic theorem guarantees that the state $|\psi_0\rangle$ will evolve into the desired state $|m\rangle$ in time T. In [13] it was shown that the optimal running time for such an adiabatic quantum search goes as $\mathcal{O}(\sqrt{N})$, consistent with the BBBV bound.

The purpose of this paper is to present the results of a detailed and rigorous analysis of the general form of this search algorithm. The corresponding equations reduce exactly to a two-dimensional system which can easily be solved numerically for arbitrary N without making any approximations. In principle, the generalized algorithm can be used to speed up the search, but, as one might expect this comes at a cost: it is necessary to inject a large amount of energy, albeit *temporarily* into the system. We illustrate this mechanism with a specific example, and then derive the adiabatic analogue of the BBBV bound and comment on its implications.

2. A general class of models

We begin by considering a time-dependent Hamiltonian of the following general form:

$$H(t) = f(t)H_0 + g(t)H_1 \tag{6}$$

where H_0 and H_1 are given by (2) and (3), respectively. $f(t)$ and $g(t)$ are arbitrary functions of time, subject to the boundary conditions

$$f(0) = 1 \qquad g(0) = 0 \tag{7}$$

and

$$f(T) = 0 \qquad g(T) = 1. \tag{8}$$

Once again, the system evolves from the initial state $|\psi_0\rangle$ to the marked state $|m\rangle$ in time T. Note, however, that unlike the usual algorithm, f and g are not necessarily monotonic (and

hence bounded above by one), nor do they obey the constraint $f + g = 1$. This will play an important role later on.

It is a straightforward exercise to find all N eigenvalues $\{E_j(t)\}$ of the Hamiltonian $H(t)$ and their corresponding eigenvectors $|E_j, t\rangle$. The two lowest eigenvalues are

$$E_\pm(t) = \frac{1}{2}\left[(f+g) \pm \sqrt{(f-g)^2 + \frac{4}{N}fg}\right]. \tag{9}$$

The higher energy eigenvalue is $(N-2)$-fold degenerate:

$$E_i(t) = f + g \qquad i \neq \pm. \tag{10}$$

From expression (9) it follows that the eigenvalues $E_\pm$ are non-degenerate as long as f and g are non-negative and do not vanish simultaneously.

Without loss of generality we now write the solutions $|\psi(t)\rangle$ to the time-dependent Schrödinger equation in terms of the complete basis of energy eigenstates:

$$|\psi(t)\rangle = \sum_{j=\pm,i} a_j(t) \exp\left(-\frac{i}{\hbar}\int_0^t E_j(t')\,\mathrm{d}t'\right)|E_j, t\rangle. \tag{11}$$

The probability amplitudes $a_\pm(t)$ for the two lowest energy eigenstates decouple from those of the higher excitations. They obey the simple equations:

$$\dot{a}_\pm = F_\pm a_\mp. \tag{12}$$

In the above $\dot{} \equiv \mathrm{d}/\mathrm{d}t$ and

$$F_+ = -F_-^* = \frac{\sqrt{N-1}}{N}\frac{\dot{g}f - g\dot{f}}{\omega^2}\exp\left(\mathrm{i}\int_0^t \omega\,\mathrm{d}t'\right) \tag{13}$$

and we have defined

$$\omega(t) := E_+(t) - E_-(t) = \sqrt{(f-g)^2 + \frac{4}{N}fg}. \tag{14}$$

We have also used the following matrix elements:

$$\langle E_+, t|\frac{\mathrm{d}H}{\mathrm{d}t}|E_-, t\rangle = \frac{\sqrt{N-1}}{N}\frac{\dot{f}g - \dot{g}f}{\omega} \tag{15}$$

$$\langle E_\pm, t|\frac{\mathrm{d}H}{\mathrm{d}t}|E_i, t\rangle = 0 \qquad i \neq \pm. \tag{16}$$

According to the adiabatic theorem [14], as used in [12], if there is a small number $\epsilon \ll 1$, such that for all t,

$$\langle E_+, t|\frac{\mathrm{d}H}{\mathrm{d}t}|E_-, t\rangle\frac{1}{\omega^2} \leqslant \epsilon \tag{17}$$

and if the system starts in the ground state $|\psi_0\rangle$ of $H(t)$ at $t = 0$, then the probability of transition to the excited state, $|a_+(t)|^2$, will not exceed a number of order ϵ^2. Note that for the theorem to hold, the eigenvalues $E_\pm(t)$ must never cross. For a given desired computational accuracy ϵ, equation (17) limits the rate at which the Hamiltonian can evolve, and therefore puts a lower bound on the total running time T. In order to calculate the bound, one needs more information about the form of functions $f(t)$ and $g(t)$. For example, if $f(t) = 1 - s(t)$ and $g(t) = s(t)$, as in equation (4), the total running time T can be minimized by choosing $\mathrm{d}s/\mathrm{d}t$ to saturate the bound (17) at each instant in time. This results in a running time of order $\sqrt{N}$ [13], consistent with the BBBV bound [8].

3. A specific example

We now illustrate with a specific example that more general choices for the functions $f(t)$ and $g(t)$ allow the computation to be performed considerably more rapidly. Consider $f(t)$ and $g(t)$ to be quadratic functions of $s(t)$:

$$f(s) = 1 - s + As(1-s) \qquad g(s) = s + As(1-s) \qquad (0 \leqslant s \leqslant 1) \tag{18}$$

where A is a constant and $s(t)$ is again a function of time that varies monotonically between 0 and 1, so that the required boundary conditions (7) and (8) are satisfied. Note that f and g are not monotonic in this case. Their peak values are $A/4 + 1/2 \mp 1/4A$, respectively (occurring at $s = 1/2(1 \mp 1/A)$, respectively). The 'adiabaticity condition' (17) in this case becomes (we use $\mathrm{d}/\mathrm{d}t = (\mathrm{d}s/\mathrm{d}t)\,\mathrm{d}/\mathrm{d}s$)

$$\frac{\mathrm{d}s}{\mathrm{d}t}\frac{\sqrt{N-1}}{N}\frac{1 + A(1 - 2s + 2s^2)}{\left[(1-2s) + \frac{4}{N}s(1-s)\left[1 + A - s(1-s)A^2\right]\right]^{3/2}} \leqslant \epsilon. \tag{19}$$

For a system satisfying the constraint (19), the minimum computation time can again be found by adjusting $s(t)$ so that the inequality is saturated at all times. This yields a minimum running time of

$$T_{\min} = \frac{1}{\epsilon}\frac{\sqrt{N-1}}{N}\int_0^1 \mathrm{d}s \frac{|1 + A(1 - 2s + 2s^2)|}{\left[(1-2s) + \frac{4}{N}s(1-s)[1 + A - s(1-s)A^2]\right]^{3/2}}. \tag{20}$$

If $A = 0$, the result of [12] is reproduced. However, by choosing A appropriately, considerably lower running times can be achieved. For example, if $A = \sqrt{N} \gg 1$, we get

$$T_{\min} = \frac{1}{\epsilon}\left(1 + \frac{\pi}{2}\right) + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right). \tag{21}$$

The limit (21) can be obtained by Taylor expanding the integrand in (20) about $N = \infty$. This is possible for the choice $A = \sqrt{N}$ because the denominator does not vanish anywhere when $N = \infty$. One has to be considerably more careful in deriving the limit for other values of A. We have also verified (21) numerically.

Thus, we see that the data search can be completed in a constant time, independent of N. The cost of this improvement is that the energy of the system gets very large for a finite time before returning to zero at the end of the computation. In particular, for the choices of f and g in (18), $E_-(s)$ reaches a maximum of $(A+1)/4$ (for $N \gg 1$) at $s = 1/2$, so that if $A = \sqrt{N}$, the maximum energy grows with $\sqrt{N}$ as well.

By numerically solving (12), it can be confirmed that the quantum computer indeed remains in the ground state at all times. One can explicitly calculate the transition probability $P_-(t) = |a_-(t)|^2$ as a function of time (by the equations of motion (12), the corresponding $P_+(t) = |a_+(t)|^2$ is guaranteed to be $1 - P_-(t)$). Figure 1 illustrates a sample solution with $A = \sqrt{N}$ and $s(t)$ chosen to saturate the inequality (19) at all times t. The transition probability $|a_-|^2$ remains above $\sim(1 - \epsilon^2)$ and the graph is plotted till the end of running time $\epsilon t = 1 + \pi/2 \approx 2.57$.

We have explored numerically other choices of A. For $A \sim N^\alpha$, where $\alpha \geqslant 0.5$, the calculational running time approaches a constant for large N, with the constant of proportionality decreasing as α increases. A systematic analysis of this problem is in progress [15], but in light of this and the discussion below, it is interesting to speculate what happens to the running time for a non-polynomial choice such as $A \sim \mathrm{e}^N$.

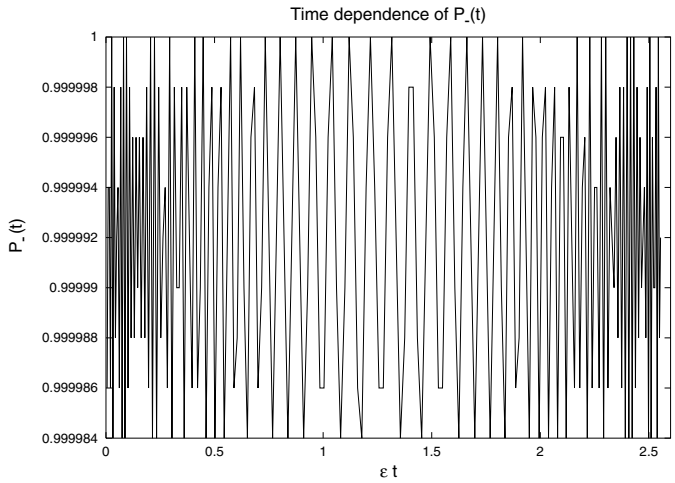

Figure 1. Numerical solution for $P_-(t) \equiv |a_-(t)|^2$ for $N = 100\,000$ and $\epsilon = 0.002$ with $A = \sqrt{N}$.

4. Adiabatic version of the BBBV bound

At this stage it is natural to ask what are the most general conditions that allow a speed up of the search algorithm. This question is answered in the following theorem, which generalizes the results of [8–11, 13].

Theorem. *Suppose there exists an unstructured adiabatic quantum search algorithm that can successfully evolve the initial state (1) to any one of a complete set of orthogonal states* $\{|m\rangle\}$ *via a Hamiltonian containing an oracle term of the form* $g(t)|m\rangle\langle m|$. *Then, the time T for the computation is bounded below by the relationship*

$$\frac{1}{\hbar}\int_0^T g(t)\,\mathrm{d}t \geqslant \frac{k\sqrt{N}}{4} \tag{22}$$

in the limit that N is large (k is a constant of order unity).

This inequality is virtually identical to the one obtained by [13]. The one important difference is that we do not restrict $g(t)$ to be less than one, nor do we impose the constraint $f(t)+g(t) = 1$. Details of the proof can be found in [13] so we will not repeat the details, merely outline the important ingredients. The key is to decompose the Hamiltonian into two parts,

$$H(t) = H_{2m}(t) + H_1(t) \tag{23}$$

where

$$H_{2m}(t) = -g(t)|m\rangle\langle m| \tag{24}$$

contains all the dependence on the needle state $|m\rangle$ and $H_1(t)$ is an arbitrary term independent of the state $|m\rangle$ (in particular, for the Hamiltonian (6), $H_1(t) = f(t) + g(t) - f(t)|\psi_0\rangle\langle\psi_0|$). Note, however, that $H_1(t)$ is completely general, apart from the restriction that it does not depend explicitly on the state $|m\rangle$.

Consider two computers at time t, evolving to states $|m\rangle$ and $|m'\rangle$, respectively, represented by the wavefunctions $|\psi_m, t\rangle$ and $|\psi_{m'}, t\rangle$, respectively subject to the boundary conditions

$$|\psi_m, 0\rangle = |\psi_{m'}, 0\rangle = |\psi_0\rangle \tag{25}$$

$$|\psi_m, T\rangle = |m\rangle \qquad |\psi_{m'}, T\rangle = |m'\rangle. \tag{26}$$

In terms of the specific model we considered earlier, this requires $f(T) = 0$ and $g(T) = 1$. Following the steps in [13], it is straightforward to obtain the inequality

$$\sum_{m,m'}[1 - |\langle\psi_m, T|\psi_{m'}, T\rangle|^2] \leqslant \frac{4N^{3/2}}{\hbar}\int_0^T g(t)\,\mathrm{d}t. \tag{27}$$

The assumed orthogonality of the final states at time T implies that

$$1 - |\langle\psi_m, T|\psi_{m'}, T\rangle|^2 \geqslant k \qquad \forall m \neq m' \tag{28}$$

where k is a number of order 1. Summing over m and m' in equation (27) for $N \gg 1$ yields equation (22) as desired. Again we stress that equation (22) is virtually identical to the result obtained in [13]. The key difference concerns our relaxed assumptions about the functions f and g in the Hamiltonian.

Equation (22) shows that the BBBV bound can only be beaten if the mean value of $g(t)$ over the time T grows as some power of N. If this power is $1/2$ then the above theorem states that the running time T may be bounded by a constant independent of N, as in the example quoted in this paper. Note that this result is a generalization of a similar bound obtained in [13] for the special case given by (4), in which $g(t)$ never exceeds order unity. It also is a natural extension of the result presented by Farhi and Gutmann in [9] for constant g.

5. Conclusions

In summary, we have presented the results of an analysis of a generalized adiabatic quantum search algorithm. The corresponding Schrödinger equation was shown to reduce exactly to a two-dimensional system for arbitrary N. We derived the adiabatic analogue of the BBBV bound. Our theorem shows that the optimal speed normally associated with Grover's search algorithm can be improved in this framework by a suitable choice of the time-dependent Hamiltonian. As one might expect from dimensional grounds, this speed up requires an increase in energy, at least temporarily. However, it should be emphasized that it is not the total Hamiltonian that needs to be increased, rather only the coefficient in front of the oracle term. In principle, this leaves open the possibility of speeding up the search while keeping the ground state energy of the system small. Another way to keep the ground state energy zero would be to use a new Hamiltonian obtained from (6) by subtracting the term $E_-(t)I$ from the latter. Note that although the resultant Hamiltonian cannot be written in the form $fH_0 + gH_1$, since $E_-(0) = 0 = E_-(T)$, it would still evolve the initial state to $|m\rangle$. Moreover, the 'gap' $\omega(t)$, as well as the matrix element (15) will remain intact, implying that the running time will still be a constant, given by (21). In any case, our analysis suggests that the physical quantity $\frac{1}{\hbar}\int_0^T g(t)\,\mathrm{d}t$ provides an adiabatic analogue of resources required for the unstructured search, just as the number of operations does for the conventional quantum search.

It must be emphasized that the system considered here is highly idealized. The Hamiltonian is non-local in the sense that H_0 and H_1 require all qubits to be coupled simultaneously. It is therefore not clear how to implement such a Hamiltonian in a realistic physical system. One should therefore investigate the circumstances under which one can find simpler, more local, Hamiltonians that have the same ground states and hence can be used as the basis of a realistic adiabatic quantum search algorithm. This issue will be the subject of a separate publication [16].

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