Exponential vanishing of the ground-state gap of the QREM via adiabatic quantum computing

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In this note we compile and slightly generalise ideas of Farhi, Goldstone, Gosset, Gutmann, Nagaj and Shor by discussing a lower bound on the run time of their quantum adiabatic search algorithm and its use for an upper bound on the energy gap above the ground-state of the generators of this algorithm. We illustrate these ideas by applying them to the quantum random energy model (QREM). Our main result is a simple proof of the conjectured exponential vanishing of the energy gap of the QREM.

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I. QUANTUM SEARCH ALGORITHMS

Finding the minimum value in an unstructured energy landscape $u : \{1, \ldots, M\} \to \mathbb{R}$ is a task which by any classical algorithm generally amounts to order $M$ trials to succeed. Ever since Grover proposed his algorithm, it is known that this search can be sped up by a factor of $\sqrt{M}$ through quantum computations\textsuperscript{12,13}. Shortly after, Farhi and collaborators\textsuperscript{8,9} proposed another quantum search algorithm which has the advantage of being based on the continuous time-evolution without using quantum gates. Their idea was to encode the energy landscape $u$ in a diagonal matrix

$$U = \text{diag}(u(1), \ldots, u(M)),$$

which is sometimes referred to as the ‘Problem-Hamiltonian’ and acts on $\mathbb{C}^M$. The task of finding a minimum is now equivalent to the search for a ground-state of $U$. To accomplish this the authors suggested to proceed through the quantum evolution

$$i \frac{d}{dt} \psi(t) = H(t) \psi(t), \quad \psi(0) \in \mathbb{C}^M, \quad (I.1)$$

generated by time-dependent Hamiltonians of the form

$$H(t) = H_D(t) + c(t) U$$
on $\mathbb{C}^M$, where

\begin{itemize}
  \item[A1] $c : \mathbb{R} \to [0, 1]$ is continuous and bounded, and
  \item[A2] $H_D : \mathbb{R} \to \text{Herm}(\mathbb{C}^{M \times M})$ is a continuous map into the Hermitian matrices, which is referred to as the ‘Driving-Hamiltonian’.
\end{itemize}

Since one aims for an algorithm which can perform the search for any unstructured $u$ equally well, it is reasonable to assume permutation invariance of the initial-state as well as of the Driving-Hamiltonian:

\begin{itemize}
  \item[A3] No preferred initial direction:

$$\psi(0) = \frac{1}{\sqrt{M}} (1, \ldots, 1)^T.$$

  \item[A4] Permutation-invariance of the ‘Driving-Hamiltonian’:

$$\Pi_{jk} H_D(t) \Pi_{jk} = H_D(t) \quad (I.2)$$

for all $j, k \in \{1, \ldots, M\}$ and $t \in \mathbb{R}$.
\end{itemize}

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The unitary and hermitian permutation matrices \( \Pi_{jk} \) on \( \mathbb{C}^M \) are defined on the canonical orthonormal basis \( (e_1, \ldots, e_M) \) through

\[
\Pi_{jk}e_m := \begin{cases} 
  e_k & m = j \\
  e_j & m = k \\
  e_m & \text{else}
\end{cases}
\]

for any \( j, k, m \in \{1, \ldots, M\} \).

A. Lower bound on the run time

Initially, the aim was to outperform the Grover algorithm in this set-up. In particular, in case of search problems which belong to the NP-complete class the hope was to have identified a quantum search algorithm which has polynomial run time. That this is not the case was realised shortly after. From a computational complexity point of view the above quantum search algorithm is equivalent to all other models for universal quantum computation.

Farhi, Goldstone, Gutmann, and Nagaj later quantified this fact through the following lower bound on the run time of the algorithm.

**Theorem 1** (cf. Ref. 10). Consider the quantum-time evolution (1.1) with initial state and generator satisfying A1-4. If the state \( \psi(T) \in \mathbb{C}^M \) at some later time \( T > 0 \) satisfies \(|\langle e_{j_0}, \psi(T) \rangle|^2 \geq b \) for some \( j_0 \in \{1, \ldots, M\} \) and \( b > 0 \), then

\[
T \geq \frac{bM - 2\sqrt{M}}{4\sigma_M(u)},
\]

where \( \sigma_M(u) := \sqrt{\sum_{k=1}^M (u(k) - u(j_0))^2} \).

The proof of this theorem is essentially contained in Ref. 10. However, since the formulation is slightly more general, we included a proof in Appendix A.

In case \( j_0 \) is the slot we are searching for, the square of the scalar-product \(|\langle e_{j_0}, \psi(T) \rangle|^2 \) is the probability of the search algorithm to succeed at time \( T \).

If the energy gaps of \( u \) are of order one, the quantity \( \sigma_M(u) \) will be of order \( \sqrt{M} \). The above theorem, then implies that the quantum search algorithm is not faster than order \( \sqrt{M} \) – the timescale of the Grover algorithm. This is a well-known fact which has been discussed early on in various special cases.

B. Adiabatic quantum evolution and a gap estimate

In the above set-up and in particular in Theorem 1 it is neither relevant that \( u(j_0) \) is the minimum configuration of the energy landscape, nor that the quantum dynamics is performed adiabatically. However, the usual application of the search algorithm is in the realm of adiabatic evolution where one considers the initial-value problem

\[
i \frac{d}{dt} \psi(t) = h(t/T) \psi(t), \quad \psi(0) = \phi(0),
\]

with an adiabatic time-scale \( T > 0 \). One is mostly interested in the special case that the initial state \( \phi(0) \in \mathbb{C}^M \) is the unique ground-state of \( h(0) \). The probability \(|\langle \phi(1), \psi(T) \rangle|^2 \) that the time-evolution (1.3) ends up in the unique ground-state \( \phi(1) \) of \( h(1) \) is then estimated with the help of the adiabatic theorem of Kato. The following is an explicit version taken from Ref. 14.

**Theorem 2** (cf. Ref. 14). Let \( h : [0, 1] \rightarrow \text{Herm}(\mathbb{C}^M \times M) \) be a family of twice continuous differentiable hermitian matrices with

1. a non-degenerate ground-state \( \phi(s) \in \mathbb{C}^M \), and
2. an energy-gap \( \gamma(s) > 0 \) above the ground-state.

Then the unique solution of the initial-value problem (1.3) satisfies:

\[
\sqrt{1 - |\langle \psi(T), \phi(1) \rangle|^2} \leq \frac{1}{T} \left[ \frac{1}{\gamma(0)^2} \|h'(0)\| + \frac{1}{\gamma(1)^2} \|h'(1)\| + \int_0^1 \frac{7}{\gamma(s)^2} \|h'(s)\| ds + \frac{1}{\gamma(s)^2} \|h''(s)\| ds \right].
\]
where we assume:

a1 \( c : [0, 1] \rightarrow [0, 1] \) is twice-continuously differentiable with \( c(0) = 0 \) and \( c(1) = 1 \),

a2 \( h_D : [0, 1] \rightarrow \text{Herm}(\mathbb{C}^M \times M) \) is twice-continuously differentiable and permutation invariant in the sense of (I.2). Moreover:

1. \( \phi(0) = \frac{1}{\sqrt{M}} (1, \ldots, 1)^T \) is the unique ground-state of \( h_D(0) \).
2. \( h_D(1) = 0 \),

a3 \( h(s) \) has a non-degenerate ground-state \( \phi(s) \in \mathbb{C}^M \) for any \( s \in [0, 1] \).

Since \( h(1) = U \), this in particular requires \( u \) to have a unique minimum. In this set-up, we can apply Theorem 1 to obtain a lower bound on the run time of the quantum adiabatic search for the unique minimum \( u(j_0) = \min_k u(k) \).

Fahri, Goldstone, Gosset, Gutmann, and Shor now combined this lower bound on the run time with the adiabatic theorem to obtain an upper bound on the smallest gap, \( \min_{s \in [0, 1]} \gamma(s) \), above the ground-state energy of the family (I.5). The ideas for the proof of the following explicit lower bound are taken from Ref. [11].

**Corollary 3.** For a family of Hamiltonians of the form (I.5) satisfying Assumptions a1-3, the energy-gap \( \gamma(s) > 0 \) above the unique ground-state satisfies:

\[
\gamma_{\#} := \min_{s \in [0,1]} \{ \gamma(s)^3, \gamma(s)^2 \} \leq \frac{8\sqrt{2} \sigma_M(u)}{M - 4\sqrt{M}} \left( 9 \max_{s \in [0,1]} \| h'(s) \| + \max_{s \in [0,1]} \| h''(s) \| \right)
\]

for all \( M > 16 \).

**Proof.** Abbreviating \( n_M(h) := 9 \max_{s \in [0,1]} \| h'(s) \| + \max_{s \in [0,1]} \| h''(s) \| \), the adiabatic theorem (Theorem 2) yields:

\[
\sqrt{1 - |\langle \psi(T), \phi(1) \rangle|^2} \leq \frac{n_M(h)}{T \gamma_{\#}}.
\]

Since this bound holds for all \( T > 0 \), it may be applied with \( T = \sqrt{2} n_M(h) / \gamma_{\#} \) in which case we conclude that \( |\langle \psi(T), \phi(1) \rangle|^2 \geq 1/2 \). Consequently, Theorem 1 with \( b = 1/2 \) yields

\[
\sqrt{2} \frac{n_M(h)}{\gamma_{\#}} \geq \frac{M - 4\sqrt{M}}{8 \sigma_M(u)}.
\]

Solving for \( \gamma_{\#} \) yields the claim. \( \square \)

**II. ILLUSTRATION: QREM**

Among the physically relevant examples of unstructured energy landscapes are spin glasses. The simplest (mean-field version) is the random energy model (REM) by Derrida in which one considers the configuration space \( Q_N = \{0, 1\}^N \) of \( N \) Ising spins. To each of these \( M = 2^N \) spin configurations, one assigns a random energy

\[
u(\sigma) = \sqrt{N} g(\sigma), \quad \sigma \in Q_N,
\]

where \( \{ g(\sigma) \}_{\sigma \in Q_N} \) are independent and identically standard normally distributed random variables. The scaling factor in (II.1) ensures that the values of \( u \) are found on in the range

\[
-\frac{N}{\kappa_c} \leq u(\sigma) \leq \frac{N}{\kappa_c} \quad \text{with} \quad \kappa_c = \frac{1}{\sqrt{2 \ln 2}}.
\]

This can be seen and stated more precisely through the Gaussian extremal value statistics (II.4) below.
One may render $\mathcal{Q}_N$, a graph by declaring vertices $\sigma, \sigma' \in \mathcal{Q}_N$ as neighbours, i.e. $\sigma' \sim \sigma$, if they differ by one spin flip. The graph Laplacian on this so-called Hamming-cube is then given by

$$(\Delta \psi)(\sigma) = \sum_{\sigma' \sim \sigma} \psi(\sigma') - N\psi(\sigma), \quad \psi \in L^2(\mathcal{Q}_N) \cong \mathbb{C}^{2^N}.$$  

By identifying the canonical basis in $\mathbb{C}^{2^N}$ with the joint eigenbasis of the third-components $\sigma_j^z$, $j = 1, \ldots, N$, of the spin-operators of $N$ spin-1/2 particles, the Laplacian may be interpreted as a transversal constant magnetic field on those spins, $-\Delta = N - \sum_{j=1}^N \sigma_j^z$. Adding the REM energies in form of a diagonal matrix $U$ gives rise to the quantum random energy model (QREM):

$$\mathcal{H}(\kappa) = -\Delta + \kappa U, \quad \kappa > 0.$$  

(II.2)

Among the interesting properties of this model is a first-order phase transition of the ground-state of $\mathcal{H}(\kappa)$ at $\kappa = \kappa_c$. Numerical findings of Jörg, Krzakala, Kurchan and Maggs\cite{Jorg2015} suggest that:

**Case** $\kappa < \kappa_c$: the ground-state is delocalised with energy $E_0(\kappa) = -\kappa^2 + o(1)$ whose fluctuations are suppressed exponentially in $N$.

**Case** $\kappa > \kappa_c$: the ground-state is localised approximately in the eigenvector corresponding to the unique minimum of $u$ with energy $E_0(\kappa) = N + \kappa \min_{\sigma} u(\sigma) + O(1)$.

**Case** $\kappa = \kappa_c$: The energy gap $\gamma_{\min}(\kappa) = E_1(\kappa) - E_0(\kappa)$ above the unique ground-state closes exponentially in $N$.

In this context, it is useful to recall that the spectrum of the Laplacian $\mathcal{H}(0)$ can be easily computed (as a sum of $N$ commuting operators). It coincides with the even integers $\{0, 2, \ldots, 2N\}$ and the unique ground-state is the maximally delocalised state $\phi(0) = \frac{1}{\sqrt{2^N}} (1, \ldots, 1)^T \in \mathbb{C}^{2^N}$.

The full justification of the above sketched low-energy properties of the QREM will be the topic of another paper\cite{Jorg2015}. Our main aim here is to point out that the conjectured vanishing of the gap $\gamma_{\min}(\kappa)$ at some $\kappa > 0$ is a straightforward corollary of the general considerations in the first section.

**Theorem 4.** There is $\kappa > 0$ and a numerical constant $C < \infty$ such that the energy gap above the unique ground-state of the QREM is bounded from above by

$$0 < E_1(\kappa) - E_0(\kappa) \leq C (1 + \kappa) N^2 \frac{1}{2^N}$$  

(II.3)

for all $N > 4$ and all realisations of the REM aside from a fraction whose probability vanishes exponentially as $N \to \infty$.

**Proof.** We aim to apply Corollary\cite{Jorg2015} with $M = 2^N$ and

$$h(s) = -(1 - s)\Delta + sU, \quad s \in [0, 1].$$

To do so, we note that Assumption a1 as well as the first requirements in a2 are evidently satisfied. The Laplacian is permutation invariant by construction and indeed has $\phi(0)$ as its unique ground-state. It remains to check a3. Since $h(s)$ generates for each $s \in [0, 1)$ a positivity improving semigroup, the ground-state of $h(s)$ is unique by the Perron-Frobenius theorem. In case $h(1) = U$ the almost-sure uniqueness of the ground-state follows from the almost-sure non-degeneracy of the $2^N$ Gaussian random variables.

Moreover, we may estimate

$$\sigma_M(u) \leq \sqrt{M} 2\|u\|_\infty,$$

$$\|h'(s)\| \leq \|\Delta\| + \|U\| \leq 2N + \|u\|_\infty,$$

and $h''(s) = 0$. For all realisations of the REM aside from a fraction whose probability vanishes exponentially as $N \to \infty$, we also have

$$\|u\|_\infty = \max_\sigma |u(\sigma)| \leq \frac{2N}{\kappa_c}.$$  

This follows from the extremal value statistics of the REM, i.e. for any $x > -\frac{\ln N}{10^2}$:

$$\mathbb{P}\left( \min u \geq -N v_N(x) \right) = \left( 1 - 2^{-N} e^{-x} \right)^{2^N} \to e^{-e^{-x}}.$$  

(II.4)
with $v_N(x) := \frac{1}{\kappa_c} + \frac{2\kappa_c}{N} x - \frac{\ln(4\pi \ln 2N)}{2} + o\left(N^{-\frac{3}{2}}\right)$, cf. Ref. [5]. Summarizing the above estimates and using $\min_{s \in [0,1]} \gamma(s) \leq \gamma(0) = 2$, we may conclude that from (I.6) that

$$\min_{s \in [0,1]} \gamma(s)^3 \leq 2 - \frac{8\sqrt{2}}{\sqrt{M}} - 4 \frac{4N}{\kappa_c} 18N (1 + \kappa_c^{-1}) \leq C^3 \frac{N^2}{\sqrt{M}}$$

provided $N > 4$.

In order to relate the QREM to $h(s)$, we write

$$\mathcal{H}(\kappa) = (1 + \kappa) h\left(\frac{\kappa}{1 + \kappa}\right).$$

This completes the proof.

As a by-product of the above proof, we also get the lower bound

$$T \geq \frac{2^{N/2} - 4}{32N} \kappa_c$$

for the quantum search algorithm to succeed with quantum probability $b = 1/2$ for all realisations of the REM aside from a fraction whose probability is exponentially small in $N$. The lower bound is smaller than any classical search algorithm and on the timescale of the Grover algorithm.

The fact that first-order phase transitions of the ground-state are the stumbling block to speeding up polynomially the search in various problems in spin-glass theory is well-known - the REM landscape is just one example. Other interesting examples are random optimisation problems from the SAT class, see Refs. [2] [3] [16] and [18] and the recent review Ref. [4] and references therein. The above technique for an estimate on the run time and the gap estimate of their generators applies more generally to these other problems.

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Appendix A: Proof of Theorem [1]

The proof essentially follows the scrambling-strategy of Ref. [10]. We fix $j_0$ and consider for any $k \in \{1, \ldots, M\}$ the family of permuted Hamiltonians

$$H_k(t) = \Pi_{j_0 k} H(t) \Pi_{j_0 k} = H_D(t) + c(t) \Pi_{j_0 k} U \Pi_{j_0 k} =: H_D(t) + c(t) U_k.$$  

The (unique) solution $\psi_k(t)$ of the initial-value problem

$$i \frac{d}{dt} \psi_k(t) = H_k(t) \psi_k(t), \quad \psi_k(0) = \psi(0)$$

coincides with the permuted solution of (I.1): $\psi_k(t) = \Pi_{j_0 k} \psi(t)$.

The proof of Theorem [1] is now based on the following two lemmata. The first is called ‘scrambling’ and essentially taken from Ref. [10].

Lemma 5. For all $t \geq 0$:

$$\sum_{k=1}^{M} ||\psi_k(t) - \psi(t)||^2 \leq 4t \sigma_M(u).$$
Proof. A simple computation shows:
\[
\frac{d}{dt}\|\psi_k(t) - \psi(t)\|^2 = -2\frac{d}{dt}\text{Re} \left(\psi_k(t), \psi(t)\right) - 2\text{Im} \left(\psi_k(t), [H_k(t) - H(t)] \psi(t)\right) = 4c(t) (u(k) - u(j_0)) \text{Im} \left(\psi(t), e_k \langle e_{j_0}, \psi(t)\rangle\right)
\leq 4c(t) |u(k) - u(j_0)| |\langle e_{j_0}, \psi(t)\rangle| |e_k, \psi(t)\rangle|
\leq 4 |u(k) - u(j_0)| |\langle e_k, \psi(t)\rangle|.
\]

The Cauchy-Schwarz inequality hence yields:
\[
\frac{d}{dt} \sum_{k=1}^{M} \|\psi_k(t) - \psi(t)\|^2 \leq 4 \sqrt{\sum_{k=1}^{M} |u(k) - u(j_0)|^2} \sqrt{\sum_{k=1}^{M} |\langle e_k, \psi(t)\rangle|^2} = 4\sigma_M(u).
\]

Integrating this inequality and using \(\psi_k(0) = \psi(0)\) we arrive at:
\[
\sum_{k=1}^{M} \|\psi_k(T) - \psi(T)\|^2 = \int_0^T \frac{d}{dt} \sum_{k=1}^{M} \|\psi_k(t) - \psi(t)\|^2 dt \leq 4T \sigma_M(u).
\]

The second lemma is a basic orthogonality estimate in Hilbert-space and also taken from Ref. [10].

Lemma 6. Let \(v_1, \ldots, v_L \in \mathbb{C}^M\) orthonormal vectors and \(\psi_1, \ldots, \psi_L \in \mathbb{C}^M\) normalized vectors, which satisfy:
\[
|\langle v_k, \psi_k \rangle|^2 \geq b > 0
\]
for all \(k \in \{1, \ldots, L\}\). Then any normalised \(\varphi \in \mathbb{C}^M\) satisfies:
\[
\sum_{k=1}^{L} \|\psi_k - \varphi\|^2 \geq b L - 2\sqrt{L}.
\]

Proof. We complete \(v_1, \ldots, v_L\) to an ONB of \(\mathbb{C}^M\) and compute:
\[
\sum_{k=1}^{L} \|\psi_k - \varphi\|^2 = \sum_{k=1}^{L} \sum_{j=1}^{M} |\langle v_j, \psi_k \rangle - \langle v_j, \varphi \rangle|^2 \geq \sum_{k=1}^{L} |\langle v_k, \psi_k \rangle - \langle v_k, \varphi \rangle|^2
= \sum_{k=1}^{L} \left[|\langle v_k, \psi_k \rangle|^2 + |\langle v_k, \varphi \rangle|^2 - 2\text{Re} \left(\psi_k, v_k \langle v_k, \varphi \rangle\right)\right]
\geq L b - 2 \sqrt{\sum_{k=1}^{L} |\langle v_k, \psi_k \rangle|^2} \sqrt{\sum_{k=1}^{L} |\langle v_k, \varphi \rangle|^2} \geq L b - 2\sqrt{L}.
\]

The penultimate inequality is Cauchy-Schwarz.

We are now ready to complete the short proof of Theorem [11].

Proof of Theorem [7]. By assumption we have for all \(k \in \{1, \ldots, M\}\):
\[
|\langle e_k, \psi_k(T)\rangle|^2 = |\langle e_{j_0}, \psi(T)\rangle|^2 \geq b.
\]
Applying Lemma [8] with \(L = M\) and \(v_k = e_k, \psi_k = \psi_k(T)\) and \(\varphi = \psi(T)\), we obtain:
\[
\sum_{k=1}^{M} \|\psi_k(T) - \psi(T)\|^2 \geq b M - 2\sqrt{M}
\]
Inserting this statement in Lemma [5], we conclude:
\[
T \geq \frac{\sum_{k=1}^{M} \|\psi_k(T) - \psi(T)\|^2}{4\sigma_M(u)} \geq \frac{b M - 2\sqrt{M}}{4\sigma_M(u)}.
\]
This completes the proof of Theorem [11].
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