

Simulating quantum circuits by adiabatic computation: improved spectral gap estimates via eigenstate ansatz

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Adiabatic quantum computing is a framework for quantum computing that is superficially very different to the standard circuit model. However, it can be shown that the two models are computationally equivalent. The key to the proof is a mapping of a quantum circuit to an adiabatic evolution, and then showing that the minimum spectral gap of the adiabatic Hamiltonian is at least inverse polynomial in the number of computational steps L . In this paper we provide a simplified proof that the gap is inverse polynomial, showing that for $L \gg 1$ the minimum gap is bounded by $\min_s \Delta \gtrsim \pi^2/[8(L+1)^2]$, an improvement over previous estimates. Our derivation is reminiscent of the Bethe ansatz, and suggests that it may be possible to use those well-developed methods to find bounds for spectral gaps of Hamiltonians in other scenarios.

I. INTRODUCTION

Aharonov and coworkers [1] proved that any quantum circuit can be efficiently simulated by an adiabatic quantum computation. Since the converse was already known [2], this amounted to a proof that the circuit model and the adiabatic model are computationally equivalent. The important ingredient in the proof is Feynman’s circuit-to-Hamiltonian construction, which enables the mapping of a quantum circuit to a time-independent Hamiltonian [3]. This can then be used to construct an adiabatic evolution that encodes the output of the circuit in its final ground state. However, if the minimum gap during the adiabatic evolution is exponentially small in the number of computational steps L , it will take an exponentially long time to reach the final ground state. Hence, to show that the circuit is *efficiently* simulated by the adiabatic evolution it is also necessary to show that the minimum spectral gap is at least inverse polynomial in L . In Ref. [1] this was achieved by deriving a lower bound for the minimum gap, $\min_s \Delta(s) \geq 1/144L^2$. However, the derivation is quite complicated, and involves using Gerschgorin’s Circle Theorem and a conductance bound from the theory of rapidly mixing Markov chains. In subsequent work, Deift, Ruskai and Spitzer [4] gave an improved bound $\min_s \Delta(s) > 1/[2(L+1)^2]$. An alternative proof of the computational equivalence that does not rely on Feynman’s circuit-to-Hamiltonian construction was given in Ref. [5].

In this paper we provide a relatively simple proof that the minimum gap is bounded by:

$$\begin{aligned} \min_s \Delta(s) &\geq 2\sqrt{2[1 + \cos \epsilon]} - 2[1 + \cos \epsilon] \\ &= \frac{\epsilon^2}{2} + \mathcal{O}(\epsilon^4), \end{aligned}$$

where $\epsilon = \pi/(2L+2)$. As a byproduct of our derivation, we also find good approximations to the eigenstates and to the full spectrum of eigenvalues.

The paper is outlined as follows. In section II we provide some background to the circuit model and Feynman’s mapping of the circuit to a Hamiltonian evolution. In section III we give a brief review of adiabatic quantum computing, and the problem of simulating a circuit with an adiabatic evolution. We then introduce an ansatz for the eigenstates of the adiabatic Hamiltonian in section IV. Based on the ansatz, in section V we derive approximations for the eigenstates and eigenvalues, and then give the lower bound to the spectral gap.

II. FEYNMAN’S CLOCK HAMILTONIAN

In the circuit model of quantum computing, a calculation is implemented in several stages. First, a set of N logical qubits are prepared in the computational basis state $|\alpha(0)\rangle = |0_1 0_2 \cdots 0_N\rangle$. Next, a sequence of one- or two-qubit gates are applied so that after a total of L gates U_1, \dots, U_L the system is in the output state $|\alpha(L)\rangle = U_L \cdots U_1 |\alpha(0)\rangle$ (intermediate states are denoted $|\alpha(l)\rangle = U_l \cdots U_1 |\alpha(0)\rangle$, with $l = 1, \dots, L$). Finally, the output state is measured in the computational basis [6, 7].

Although the computation is implemented by a discrete sequence of unitaries, Feynman showed that it is possible to map the circuit to a continuous time evolution with a time-independent Hamiltonian [3]. This can be done by adding to the N logical qubits an $L+1$ dimensional ancillary “clock” system, and constructing the Hamiltonian:

$$\begin{aligned} H_c = \frac{1}{2} \sum_{l=1}^L &\left(I \otimes |l-1\rangle_c \langle l-1|_c + I \otimes |l\rangle_c \langle l|_c \right. \\ &\left. - U_l \otimes |l\rangle_c \langle l-1|_c - U_l^\dagger \otimes |l-1\rangle_c \langle l|_c \right) \end{aligned} \quad (1)$$

where $\{|l\rangle_c\}_{l=0}^L$ are a set of basis states for the clock system. The clock is prepared in the state $|0\rangle_c$ and the

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gives a vector $H\psi$ with the elements:

$$\begin{aligned} [H\psi]_0 &= \frac{s}{2}(\alpha z + \beta z^{-1}) - \frac{s}{2}(\alpha z^2 + \beta z^{-2}), \\ [H\psi]_k &= \lambda[\psi]_k, \quad \lambda = 1 - \frac{s}{2}(z + z^{-1}), \quad 0 < k < L, \\ [H\psi]_L &= -\frac{s}{2}(\alpha z^L + \beta z^{-L}) + \left(1 - \frac{s}{2}\right)(\alpha z^{L+1} + \beta z^{-L-1}). \end{aligned}$$

We see that ψ is ‘‘almost’’ an eigenvector of H with eigenvalue $\lambda = 1 - \frac{s}{2}(z + z^{-1})$, but not quite, since the first and last elements $[H\psi]_0$ and $[H\psi]_L$ do not have the correct form. Enforcing $[H\psi]_0 = \lambda[\psi]_0$ and $[H\psi]_L = \lambda[\psi]_L$ leads to the conditions $s(\alpha + \beta) = (2 - s)(\alpha z + \beta z^{-1})$ and $\beta = \alpha z^{2L+3}$, respectively. Substituting the second equation into the first gives a new condition:

$$\begin{aligned} s &= \frac{2(z^{-L-1/2} + z^{L+1/2})}{z^{L+3/2} + z^{L+1/2} + z^{-L-1/2} + z^{-L-3/2}} \\ &\equiv f(z), \end{aligned} \quad (2)$$

where, for later convenience, we have introduced the function $f(z)$. If z is a solution to Eq. 2, our ansatz ψ is an eigenstate of $H(s)$. We also note that the eigenvalue $\lambda = 1 - \frac{s}{2}(z + z^{-1})$ must be real, since the Hamiltonian H is symmetric. This implies that there are two possibilities for z : either z is real or z is complex with unit modulus.

A. Real z solution

We first consider the case where z is real. Writing $z = e^\theta$ the eigenvalue and (unnormalised) eigenvector elements are:

$$\lambda = 1 - s \cosh \theta, \quad [\psi]_k = \cosh[(L - k + 1/2)\theta],$$

where, substituting $z = e^\theta$ into Eq. 2, we see that θ is a solution to the equation:

$$s = f(e^\theta) = 1 - \tanh[(L + 1)\theta] \tanh(\theta/2). \quad (3)$$

Fig. 1(a) shows $f(e^\theta)$ plotted as a function of θ . The plot shows (and it is easily verified by a calculation) that $f(e^\theta)$ is continuous and monotonically decreasing, and is guaranteed to intersect a horizontal line at $f(e^\theta) = s$ (at finite θ if $s > 0$, and at $\theta \rightarrow \infty$ if $s = 0$). This gives exactly one solution to the eigenvalue equation, which we denote θ_0 . The corresponding eigenvalue and eigenvector are similarly labelled λ_0 and ψ_0 .

B. Complex z solutions

Next, in the case where z is complex with unit modulus we can write $z = e^{i\theta}$, which gives the eigenvalue and (unnormalised) eigenvector:

$$\lambda = 1 - s \cos \theta, \quad [\psi]_k = \cos[(L - k + 1/2)\theta], \quad (4)$$

where θ is the solution to the equation:

$$s = f(e^{i\theta}) = 1 + \tan[(L + 1)\theta] \tan(\theta/2). \quad (5)$$

If θ is a solution to Eq. 5 then it is clear that $\theta + 2\pi m$ is also a solution for any $m \in \mathbb{Z}$, since $z = e^{i(\theta+2\pi m)} = e^{i\theta}$. However, replacing $\theta \rightarrow \theta + 2\pi m$ in the expressions for the eigenvalue and eigenstate in Eq. 4 shows that these solutions all correspond to the same eigenvalue and eigenvector. We may therefore restrict to solutions to Eq. 5 in any 2π range, say $\theta \in [-\pi, \pi)$. Also, if θ is a solution to Eq. 5 then so is $-\theta$, since $f(e^{i\theta}) = f(e^{-i\theta})$. But again, replacing $\theta \rightarrow -\theta$ in Eq. 4 shows that this does not give a distinct solution to the eigenvalue equation. All distinct solutions may therefore be found in the range $\theta \in [0, \pi]$. In Fig. 1(b) we plot $f(e^{i\theta})$ as a function of θ in this range. The function $f(e^{i\theta})$ diverges for certain values of θ . From Eq. 5 we see that these divergences occur at the points $\theta = (2l - 1)\pi/[2(L + 1)]$, for $l = 1, \dots, L$, marked by grey vertical lines in Fig. 1(b).

Moreover, in the interval $\theta \in \left[\frac{(2l-1)\pi}{2(L+1)}, \frac{(2l+1)\pi}{2(L+1)}\right]$ between two consecutive divergences the function $f(e^{i\theta})$ increases continuously from $-\infty$ to $+\infty$ and will therefore cross a horizontal line at $f(e^{i\theta}) = s$. Since there are L such intervals in the range $\theta \in [0, \pi]$ we are guaranteed L solutions, which we denote θ_l where $l = 1, \dots, L$. The corresponding eigenvalues and eigenvectors are λ_l and ψ_l . Since the eigenvalue $\lambda = 1 - s \cos \theta$ is an increasing function of θ for $\theta \in [0, \pi]$ we are also guaranteed that the eigenvalues are labelled in increasing order $\lambda_1(s) \leq \lambda_2(s) \leq \dots \leq \lambda_L(s)$.

Combining the solution θ_0 obtained for real z with the L solutions $\{\theta_1, \dots, \theta_L\}$ for complex z gives a complete set of $L + 1$ eigenvalues and eigenvectors of $H(s)$.

V. APPROXIMATIONS

Although we have identified the complete set of $L + 1$ solutions to the eigenvalue equation, we cannot solve the transcendental equations 3 and 5 to find explicit solutions. However, progress can be made by finding approximate solutions.

A. Ground state approximation

We begin with the ground state eigenvalue $\lambda_0 = 1 - s \cosh \theta_0$ and eigenvector $[\psi_0]_k = \cosh[(L - k + 1/2)\theta_0]$, where θ_0 is the solution to $s = f(e^{\theta_0}) = 1 - \tanh[(L + 1)\theta_0] \tanh(\theta_0/2)$. When $(L + 1)\theta_0 \gg 1$ we have $\tanh[(L + 1)\theta_0] \approx 1$, which gives $\theta_0 \approx 2 \tanh^{-1}(1 - s) = \ln\left(\frac{2}{s} - 1\right)$. With this approximation the ground state eigenvalue is:

$$\begin{aligned} \lambda_0(s) &\approx 1 - s \cosh \left[\ln \left(\frac{2}{s} - 1 \right) \right] \\ &= \frac{s(1 - s)}{2 - s} \equiv \lambda_0^{\text{approx}}(s), \end{aligned}$$

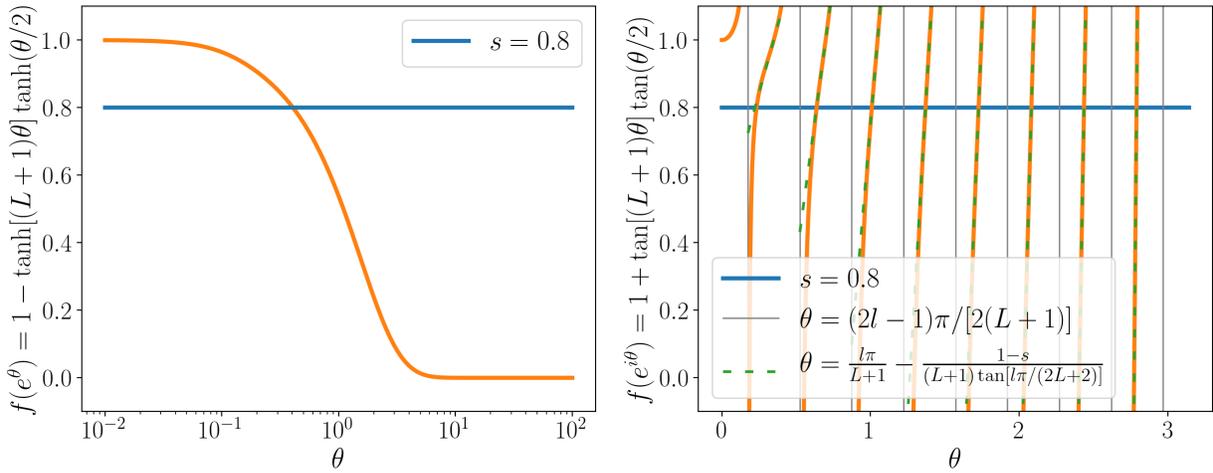


FIG. 1. Solutions to the transcendental equations Eq. 3 (left figure) and Eq. 5 (right figure) are found when $f(z) = s$. Plotted for $L = 8$.

and the eigenvector elements are:

$$[\psi_0]_k \approx \frac{1}{2} \left[\left(\frac{2}{s} - 1 \right)^{L-k+1/2} + \left(\frac{2}{s} - 1 \right)^{-L+k-1/2} \right] \equiv [\psi_0^{\text{approx}}]_k.$$

In Fig. 2 we compare the exact ground state and its eigenvalue (found by numerical diagonalisation of H) with the approximation.

We note that the approximation $\tanh[(L+1)\theta_0] \approx 1$ overestimates $\tanh[(L+1)\theta_0]$, and so underestimates θ_0 . The approximation therefore overestimates the eigenvalue $\lambda_0(s)$ and is an upper bound to the true eigenvalue, $\lambda_0^{\text{approx}}(s) \geq \lambda_0(s)$.

B. Excited state approximations

We next approximate the excited state eigenvalues $\lambda_l = 1 - s \cos \theta_l$ and eigenvectors $[\psi_l]_k = \cos[(L-k+1/2)\theta_l]$, where θ_l are the L solutions to $s = f(e^{i\theta}) = 1 + \tan[(L+1)\theta] \tan(\theta/2)$ in the range $\theta \in (0, \pi)$. In section IV B we showed that the l 'th solution θ_l lies in the range $\theta_l \in \left[\frac{(2l-1)\pi}{2(L+1)}, \frac{(2l+1)\pi}{2(L+1)} \right]$ between two consecutive divergences of $f(e^{i\theta})$. A lower bound to the true value of θ_l is therefore found by choosing the smallest value in this range, i.e., $\theta_l \approx (2l-1)\pi/[2(L+1)]$. Since $\lambda = 1 - s \cos \theta$ is an increasing function of θ for $\theta \in [0, \pi]$, a lower bound to the eigenvalue λ_l can be obtained using this lower bound for θ_l :

$$\lambda_l(s) \geq 1 - s \cos \frac{(2l-1)\pi}{2(L+1)}.$$

This lower bound will be useful in the next subsection when we derive a lower bound on the spectral gap. However, in terms of the error with respect to the true value of θ_l , the approximation $\theta_l \approx (2l-1)\pi/[2(L+1)]$ begins

to break down as s increases or as l increases. This can be seen in Fig. 1(b), where the approximations (the thin vertical grey lines) depart from the true values (the solid orange lines) as s increases or as l increases. However, the approximation may be improved by observing that for $s \approx 1$ or for $l \approx L$, the function $f(e^{i\theta})$ is well approximated by the linear expansion around the solutions to $f(e^{i\theta}) = 1$, i.e., around $\theta = l\pi/(L+1)$. This gives:

$$s = f(e^{i\theta}) \approx 1 + \left[\theta - \frac{l\pi}{L+1} \right] (L+1) \tan \frac{l\pi}{2(L+1)},$$

which we can easily solve for θ to obtain $\theta_l \approx l\pi/(L+1) - (1-s)/[(L+1) \tan[l\pi/2(L+1)]]$. These linear approximations are plotted in the green dashed lines in Fig. 1(b). The two approximations for θ_l may be combined in a single approximation:

$$\theta_l \approx \max \left\{ \frac{(2l-1)\pi}{2(L+1)}, \frac{l\pi}{L+1} - \frac{1-s}{(L+1) \tan[l\pi/(2L+2)]} \right\} \equiv \theta_l^{\text{approx}}.$$

In Fig. 2 we compare the approximate eigenvectors and eigenvalues with the exact ones (found numerically).

C. Lower bound for the gap

In section V A we found that an upper bound to the ground state eigenvalue is $\lambda_0(s) \geq s(1-s)/(2-s)$, and in section V B that a lower bound to the first excited state eigenvalue is $\lambda_1(s) \leq 1 - s \cos \epsilon$, where $\epsilon = \pi/(2L+2)$. This means that the spectral gap is bounded by:

$$\Delta(s) \geq 1 - s \cos \epsilon - \frac{s(1-s)}{2-s}. \quad (6)$$

Minimising over s gives:

$$\min_s \Delta(s) \geq 2\sqrt{2[1 + \cos \epsilon]} - 2[1 + \cos \epsilon] = \frac{\epsilon^2}{2} + \mathcal{O}(\epsilon^4), \quad (7)$$

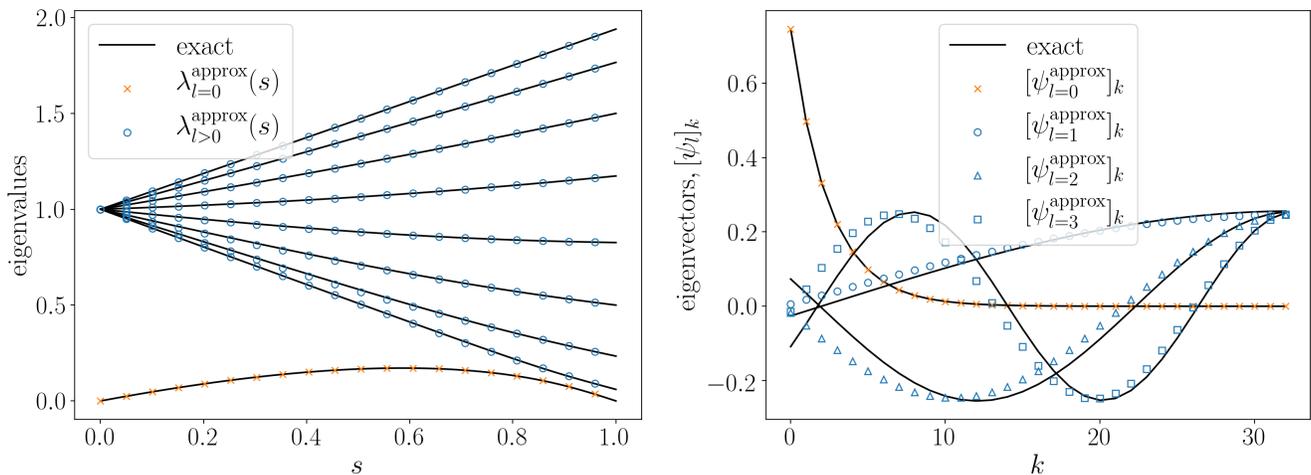


FIG. 2. Left: A comparison of the exact and the approximate eigenvalues for $L = 8$. Right: exact vs. approximate eigenstates (the 4 lowest) for $s = 0.8$ and $L = 32$.

where we have expanded the right hand side to leading order in ϵ . In the large L limit, our upper bound in Eq. 7 is a factor of $18\pi^2 \sim 177$ times larger than the bound $\min_s \Delta(s) \geq 1/144L^2$ that is given in Ref. [1]. Moreover, the proof here is more elementary than the one presented in Ref. [1]. With respect to the upper bound $\min_s \Delta(s) \geq 1/[2(L+1)]^2$ given in Ref. [4], ours is an improvement by a factor of approximately $\pi^2/4 \sim 2.5$.

VI. CONCLUSION

For the simulation of a quantum circuit with L computation steps by an adiabatic evolution by a Hamiltonian

$H(s)$, we have presented a relatively simple proof that the spectral gap of $H(s)$ is at least inverse quadratic in L . The derivation is reminiscent of the Bethe ansatz and opens up the possibility of using the well-developed techniques of Bethe ansatz to bound spectral gaps in generalisations of the adiabatic Hamiltonian considered here.

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