

# Improved Gap Estimates for Simulating Quantum Circuits by Adiabatic Evolution\*

Percy Deift<sup>†</sup>

Courant Institute of Mathematical Sciences, 251 Mercer St., New York, NY 10012  
deift@courant.nyu.edu

Mary Beth Ruskai<sup>‡</sup>

Department of Mathematics, Tufts University, Medford, MA 02155  
Marybeth.Ruskai@tufts.edu

Wolfgang Spitzer

Department of Physics, International University of Bremen  
Campus Ring 8, 28759 Bremen, Germany  
w.spitzer@iu-bremen.de

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## Abstract

We use elementary variational arguments to prove, and improve on, gap estimates which arise in simulating quantum circuits by adiabatic evolution.

There are several models for quantum computation [5]. The quantum Turing machine model and the quantum circuit model, are equivalent in the sense that any algorithm that runs in polynomial time in one requires only polynomial time in the other. There are also several “one-way” measurement-based models [3], such as the cluster state model [6], which can simulate any polynomial time quantum circuit in polynomial time.

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In [2], Farhi, et al introduced quantum computation by adiabatic evolution of a Hamiltonian and showed that it could be simulated *by* a suitable quantum circuit. In this model, the time required is assumed to depend inversely on the square of the eigenvalue gap.<sup>1</sup> In [1], a method was given for simulating an arbitrary quantum circuit with  $L$  gates by the adiabatic evolution of a Hamiltonian in time which is polynomial in  $L$ , using a simple “clock” model to construct the Hamiltonian. Some modifications [4, 7] of the Hamiltonian construction have been considered without introducing different techniques for estimating the gap.

In [1], the techniques used to prove the gap estimates are rather complicated. In this note we show that very elementary techniques suffice, and that one of the bounds can be improved by a factor of  $L$ . To make precise statements, we need some notation.

Let  $|e_k\rangle$  denote the standard basis for  $\mathbf{C}^d$ ; in particular,  $|e_1\rangle = (1, 0, \dots, 0)^T$ . Let  $-\Delta_d$  denote the discrete Laplacian with Neumann boundary conditions, i.e.,

$$-\Delta_d = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & 0 & 0 & \cdots & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & \cdots & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -\frac{1}{2} & 1 & -\frac{1}{2} \\ 0 & \cdots & 0 & 0 & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}. \quad (1)$$

The Hamiltonian used in Lemma 3.5 of [1] can be written as

$$H_0(s) = s(-\Delta_d) + (1-s)I_d - (1-s)|e_1\rangle\langle e_1| \quad (2)$$

and the block diagonal Hamiltonian in Lemma 3.12 as

$$\mathbb{H}(s) = \bigoplus_{j=0}^{2^m-1} H_j(s), \quad (3)$$

where

$$H_j(s) = s(-\Delta_d) + (1-s)I_d + [b_j - (1-s)]|e_1\rangle\langle e_1|. \quad (4)$$

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<sup>1</sup>This assumption does not take into account the fact that higher order terms in the asymptotic expansion may be needed, or their possible growth as the Hamiltonian changes with the size of the problem [8]. Although this may affect the time estimates, it seems unlikely to do more than change the order of the polynomial. In this note, we deal only with gap estimates and not with time estimates. For further details and references on issues involved see the report of the workshop at [http://www.perimeterinstitute.ca/activities/scientific/PI-WORK-6/related\\_links.php](http://www.perimeterinstitute.ca/activities/scientific/PI-WORK-6/related_links.php)

with  $b_j$  an integer  $\geq 1$  for  $j \geq 1$ , and  $b_0 \equiv 0$ . Let  $\lambda_1(s) < \lambda_2(s) \dots$  denote the eigenvalues of  $H_0(s)$  and  $\Lambda_k(s)$  the eigenvalues of  $\mathbb{H}(s)$  also in increasing order. One is interested in  $g(s) = \lambda_2(s) - \lambda_1(s)$  and  $G(s) = \Lambda_2(s) - \Lambda_1(s)$ , the energy gaps between the two lowest states of these Hamiltonians.

The eigenvalue equation  $H_j|u\rangle = \lambda|u\rangle$  written in terms of the vector components  $u_k$  of  $|u\rangle$  is

$$\frac{s}{2}(u_{k-1} + u_{k+1}) = (1 - \lambda)u_k \quad k = 2, 3, \dots, d-1 \quad (5)$$

subject to the boundary conditions

$$u_1(b_j + \frac{s}{2} - \lambda) = \frac{s}{2}u_2 \quad (1 - \frac{s}{2} - \lambda)u_d = \frac{s}{2}u_{d-1}. \quad (6)$$

This is a second order difference equation with constant coefficients subject to boundary conditions. It can be solved exactly by elementary methods entirely analogous to those used to solve the ‘‘particle in a box’’ boundary value problem. For general  $s, b_j$  the algebra can become somewhat tedious and we need only bounds on the lowest eigenvalues, not the full spectrum. Good estimates on the gaps can be obtained from one special case and a simple variational argument.

**Lemma 1.** *The lowest eigenvalue  $\mu_0$  of  $-\Delta_d + \frac{1}{2}|e_1\rangle\langle e_1|$  satisfies  $1 > \mu_0 > \frac{1}{d^2}$ .*

**Theorem 2.** *The energy gaps for the Hamiltonians given by (2) and (4) are both  $O(d^{-2})$ ; in fact,  $g(s) > 1/2d^2$ , and  $G(s) > 1/2d^2$ .*

When  $d = L + 1$ , part (a) is equivalent to Lemma 3.5 of [1] and part (b) improves Lemma 3.12 of [1] by a factor of  $L$ . Since we are interested in large  $d$ , we will henceforth not distinguish between estimates involving  $d$  and  $d \pm 1$ .

**Proof of Theorem 2:** Consider two simple trial functions using the ground states of  $H_0$  at the endpoints  $s = 0, 1$ . First,

$$\langle e_1, H_0(s)e_1 \rangle = s\langle e_1, (-\Delta_d)e_1 \rangle = \frac{1}{2}s. \quad (7)$$

Let  $|v\rangle$  denote the normalized constant vector with elements  $v_k = \frac{1}{\sqrt{d}}$ . Then

$$\langle v, H_0(s)v \rangle = (1 - s)\frac{d-1}{d} = (1 - s) - \frac{1}{d}(1 - s). \quad (8)$$

Thus,  $\lambda_1(s) \leq \min\{\frac{1}{2}s, (1 - s)\frac{d-1}{d}\}$  and the two curves cross at  $s_c$  where  $\frac{1}{2} < s_c = \frac{2d-2}{3d-2} < \frac{2}{3}$  for  $d > 2$ . Next, note that by the max-min principle

$$\lambda_2(s) \geq \inf_{u \in e_1^\perp} \langle u, H_0(s)u \rangle = (1 - s) + s\mu_0. \quad (9)$$

Since  $\mu_0 < \frac{3}{2}$ , one finds that  $\frac{1}{2}(2 - 3s) + s\mu_0$  is decreasing on  $[0, s_c]$  and attains its minimum at  $s_c$ . Thus

$$\begin{aligned} g(s) &= \lambda_2(s) - \lambda_1(s) \geq \begin{cases} \frac{1}{2}(2 - 3s) + s\mu_0 & s \leq s_c \\ \frac{1}{d}(1 - s) + s\mu_0 & s > s_c \end{cases} \\ &\geq s_c\mu_0 \geq \frac{1}{2d^2}. \end{aligned} \quad (10)$$

This proves part (a). To prove part (b) observe that the condition  $b_j \geq 1$  implies that for  $j \geq 1$  the Hamiltonian (4) satisfies

$$\begin{aligned} H_j(s) &\geq s(-\Delta_d) + (1 - s)I_d + s|e_1\rangle\langle e_1| \\ &\geq s(-\Delta_d + \frac{1}{2}|e_1\rangle\langle e_1|) + (1 - s)I_d \\ &\geq s\mu_0 + (1 - s). \end{aligned} \quad (11)$$

Now,  $\Lambda_2(s)$  is the minimum of  $\lambda_2(s)$  and the lowest eigenvalue of  $H_j(s)$  with  $j \geq 1$ . Therefore, (9) and (11) imply that  $\Lambda_2(s) \geq s\mu_0 + (1 - s)$  as well. Since  $\Lambda_1(s) = \lambda_1(s)$ , the argument above implies that gap for  $\mathbb{H}(s)$  satisfies  $G(s) \geq 1/2d^2$ .

**Proof of Lemma 1:** The eigenvalue problem for  $-\Delta_d + \frac{1}{2}|e_1\rangle\langle e_1|$  is equivalent to setting  $s = 1$ , and  $b = \frac{1}{2}$  in (5) and (6). We first look for solutions of the form  $u_k = e^{ik\theta} - e^{-ik\theta}$  with  $0 < \lambda < 2$ . When  $\lambda = 1 - \cos\theta$ , (5) and the first boundary condition are satisfied. One can verify that for  $\theta = \frac{2n-1}{2d+1}\pi$ , the second condition in (6) holds for  $n = 1, 2, \dots, d$ . Since this gives  $d$  linearly independent solutions in the range  $0 < \lambda < 2$ , the  $d$  eigenvalues are  $1 - \cos\left(\frac{2n-1}{2d+1}\pi\right)$  for  $n = 1, 2, \dots, d$ . The smallest eigenvalue is

$$\mu_0 = 1 - \cos\left(\frac{1}{2d+1}\pi\right) = \frac{\pi^2}{8d^2} - O\left(\frac{1}{d^4}\right) > \frac{1}{d^2}. \quad (12)$$

for  $d$  sufficiently large. **QED**

As a final remark, we note that  $-\Delta_d = \frac{1}{2}X^\dagger X$  with  $X = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ 0 & 1 & -1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & -1 \end{pmatrix}$

so that  $X|u\rangle$  has elements  $u_k - u_{k+1}$  and

$$\langle u, -\Delta_d u \rangle = \frac{1}{2} \langle Xu, Xu \rangle = \frac{1}{2} \sum_{k=1}^{d-1} |u_k - u_{k+1}|^2.$$

This lends itself to interpreting  $-\Delta_d$  as a lattice analogue of the kinetic energy, rather than as a 3-local potential as in [1]. Moreover, the interpolating Hamiltonians  $H_j$

are linear combinations of  $-\Delta$ , the Identity  $I$ , which can shift the spectrum but has no effect on the gap, and  $|e_1\rangle\langle e_1|$  whose only effect is to modify the first boundary condition.

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