Crushing runtimes in adiabatic quantum computation with Energy Landscape Manipulation (ELM): Application to Quantum Factoring

Richard Tanburn
\(^{1}\)

\(^{1}\)Mathematical Institute, Oxford University, OX2 6GG, Oxford, UK.

Oliver Lunt
\(^{2}\)

\(^{2}\)Department of Physics, Oxford University, OX1 3PU, Oxford, UK.

Nikesh S. Dattani
\(^{3,4}\)

\(^{3}\)School of Materials Science and Engineering, Nanyang Technological University, 639798, Singapore, and

\(^{4}\)Fukui Institute for Fundamental Chemistry, 606-8103, Kyoto, Japan

We introduce two methods for speeding up adiabatic quantum computations by increasing the energy between the ground and first excited states. Our methods are even more general. They can be used to shift a Hamiltonian’s density of states away from the ground state, so that fewer states occupy the low-lying energies near the minimum, hence allowing for faster adiabatic passages to find the ground state with less risk of getting caught in an undesired low-lying excited state during the passage. Even more generally, our methods can be used to transform a discrete optimization problem into a new one whose unique minimum still encodes the desired answer, but with the objective function’s values forming a different landscape. Aspects of the landscape such as the objective function’s range, or the values of certain coefficients, or how many different inputs lead to a given output value, can be decreased or increased. One of the many examples for which these methods are useful is in finding the ground state of a Hamiltonian using NMR. If it is difficult to find a molecule such that the distances between the spins match the interactions in the Hamiltonian, the interactions in the Hamiltonian can be changed without changing the ground state at all. We apply our methods to an AQC algorithm for integer factorization, and the first method reduces the maximum runtime in our example by up to 754%, and the second method reduces the maximum runtime of another example by up to 250%. These two methods may also be combined.

PACS numbers: 06.20.Jr, 31.30.jh, 31.50.Bc, 95.30.Ky

I. INTRODUCTION

It has been proven that an adiabatic quantum computer (AQC) can simulate any circuit-based quantum computation with only polynomial overhead \(^{[1, 2]}\), but so far it has been far easier to build devices that implement adiabatic quantum algorithms than circuit-based ones. For example, the most famous circuit-based quantum algorithm (Shor’s algorithm \(^{[3, 4]}\)) has been celebrated for more than 20 years, but never implemented with more than 7 qubits \(^{[5, 6]}\). Contrarily, quantum annealing devices have been used to find the ground states of Hamiltonians with over 1000 qubits, and for many of the problems solved on annealing devices such as in \(^{[2, 9]}\), no classical computer has ever found the solutions faster. Circuit-based quantum algorithms have had nowhere near this level of success.

It is also strikingly easier to design an algorithm under the AQC model of computation than the circuit-based model, for many problems. For example, turning integer factorization into a Hamiltonian whose ground state represents the prime factors can easily be understood with only high-school education, or even less \(^{[5, 10]}\): In fact, the whole algorithm can be explained in less than half a page, including a fully worked example \(^{[5]}\).

However, implementing an AQC algorithm is still not trivial:

1. The runtime increases significantly as the energy between the ground state(s) and the lowest excited state(s) of the Hamiltonian becomes small compared to the full range of the Hamiltonian’s energies.

2. If plenty of eigenstates of the Hamiltonian have energies close to the ground state, the runtime for finding the ground state can be much longer than if all excited states are at the highest energy levels.

3. The required energy levels of the qubits, and the coupling strengths between them, can be difficult to achieve in a real physical system.

We will show in this paper that it is possible to manipulate the size of the energy gap between ground and excited states, or the number of states at a given energy level, or the required coupling strengths between the qubits. We refer to this as ELM (Energy Landscape Manipulation).
Various classical algorithms for solving discrete optimization problems will also find a given problem easier or harder to solve depending on the energy landscape of the Hamiltonian, except one may want to call the Hamiltonian that needs to be minimized the “objective function” and the energy landscape as the “values that the objective function attains”. For example, the simulated annealing algorithm of \cite{11} performs better when the range of the energy landscape is increased (contrary to AQC, where it is usually preferred for the energy landscape to have a small range). ELM can therefore also benefit classical discrete optimization algorithms.

Simply put, ELM can provide a new Hamiltonian (or objective function) whose minimum still occurs at the same place, but is much easier to find.

II. THE METHOD

A. Terminology

Suppose the solution to our problem is represented by the ground state of the Hamiltonian $H$. We use $|0\rangle, |1\rangle, \ldots, |n\rangle$ to denote the ground, 1st excited, and $n$th excited states of $H$ respectively, and their associated eigenvalues (energies) are denoted: $E_{|0\rangle}, E_{|1\rangle}, \ldots, E_{|n\rangle}$ respectively. When there are multiple states with the same eigenvalue, the number of states associated with eigenvalue $n$ is given by $N_n$. We also define $E_{\text{max}}$ to be the largest eigenvalue, and $E_{\text{width}} = E_{\text{max}} - E_{|0\rangle}$ to be the spectral width of the Hamiltonian (range of the objective function). Likewise, $E_{\text{gap}} = E_{|1\rangle} - E_{|0\rangle}$ will be the spectral gap of the Hamiltonian, and the spectral ratio will be $\mathcal{R} = E_{\text{width}}/E_{\text{gap}}$. For time-dependent Hamiltonians, we will use the notation $E_{\text{gap}}(t)$.

B. Motivation

1. Theoretical bound on the runtime of an adiabatic quantum computation

In 1928, Born and Fock reported the adiabatic theorem, which is that if a system is in a ground state of a Hamiltonian, and the Hamiltonian is changed slowly enough, the system will stay in a ground state (of the new Hamiltonian as it changes) \cite{12}. But if the Hamiltonian quickly changes into one in which one of its excited states has the same energy as the ground state energy level of the original Hamiltonian, the system might not have enough time to release the energy required to stay in a ground state, and it will find itself in an excited state. Therefore, one might wonder how slowly one must change the Hamiltonian, in order to ensure that the system is in the ground state encoding the solution to the problem, after the Hamiltonian has at last been fully transformed.

If the Hamiltonian is transformed from $H_{\text{init}}$ to $H_{\text{final}}$ by the interpolant:

$$H(t) = \left(1 - \frac{t}{T}\right) H_{\text{init}} + \frac{t}{T} H_{\text{final}},$$

over a total “runtime” of time $T$, and we assume that the system begins in $|\psi(0)\rangle$ a ground state of $H(0) \equiv H_{\text{init}}$, and we assume that the system evolves according to the non-relativistic Schrodinger equation, the current best lower bound for the runtime was derived in 2007 \cite{13}. We present it in the notation of \cite{2}:

$$T \geq \max_t \frac{\|H_{\text{final}} - H_{\text{init}}\|^2}{\epsilon E_{\text{gap}}(t)^3},$$

which ensures that $|\psi(T)\rangle$, the solution to the Schrodinger equation at time $T$, is close enough to the ground state $|0\rangle$ of $H_{\text{final}}$ according to:

$$\sqrt{\langle\psi(T)|}\langle\psi(T)\rangle \leq \epsilon.$$

The matrix norm used is the spectral norm:

$$\|H\| = \sqrt{\text{max eigenvalue}(H^*H)}.$$

The starting Hamiltonian $H_{\text{init}}$ is usually chosen to be one for which the ground state is easy to realize in an experiment, so when attempting to reduce the runtime, one generally has more freedom to manipulate $H_{\text{final}}$ than $H_{\text{init}}$. With this in mind, we look for ways to reduce $T$ by changing only the properties of $H_{\text{final}}$, while maintaining its defining property: the encoding of the solution to the factorization problem in its ground state.

One helpful fact is that in 2001, a bound for the largest eigenvalue of $H_{\text{final}} - H_{\text{init}}$ was determined by the individual eigenvalues of $H_{\text{final}}$ and $H_{\text{init}}$ \cite{14}:

$$\|H_{\text{final}} - H_{\text{init}}\| \leq \|H_{\text{final}}\| - \|H_{\text{init}}\|.$$  

We can also set the zero of energy at the ground state of $H_{\text{final}}$, in which case $\|H_{\text{final}}\| = E_{\text{width}}$. We also note that $\min_t (E_{\text{gap}}(t)) \leq E_{\text{gap}}(T) \equiv E_{\text{gap}}$, so Eq. \cite{2} leads to a less tight, but more clear bound:

$$T \geq \frac{E_{\text{width}}^2}{\epsilon E_{\text{gap}}^3} = O(\mathcal{R}).$$

Therefore we will make effort to reduce $E_{\text{width}}$ and to increase $E_{\text{gap}}$, to ultimately reduce $O(\mathcal{R})$ and hence reduce the lower bound on the runtime $T$.

2. Properties that affect the runtime, but with no known bound (simulations required)

The bound on the runtime given in Eq. \cite{2} is still not very tight. For example, two Hamiltonians may have
the same spectral ratio, but if one of them has $N_1 = 1$ (i.e. only one eigenstate in the first excited energy level $E_{1(1)}$) while the other has $N_1 = 100$, intuition may expect that the runtime would be longer in the latter case. Likewise, if low-lying excited states (for example, $|2⟩$, $|3⟩$, $|4⟩$) lie very close to the ground state $|0⟩$, one can imagine that the runtime to find the ground state would be longer than if the distribution of energies was such that these states were much further away.

In the following sections, we present ways of changing the energy landscape, with the hope of shifting the density of states away from $E_{0(0)}$, and/or to increase the low-lying energy gaps $(E_{n(0)} - E_{0(0)})$ for small $n$ without increasing the spectral ratio $R$ too much and while not changing the ground state(s) of the Hamiltonian. Since it is not easy to analytically evaluate which changes to the energy landscape will be more important in reducing the runtime, we determine this by performing simulations.

C. ELM using deductions: deduc-ELM

Our first method uses a deduction to provide some control over the energy landscape. For example, suppose it is known that the solution to the problem requires $(x_0, x_1) = (0, 0), (0, 1)$ or $(1, 1)$. Such a deduction can be made by a local search, in which it is deduced that setting $(x_0, x_1) = (1, 0)$ will make it impossible to attain the minimum, which is what we are seeking. We have published two papers this year on such deductions in discrete optimization problems [5, 15]. This deduction is equivalent to the relation $x_0x_1 = x_0$, since it holds under the valid assignments and fails otherwise. With this relation, it is clear to see that we can add

$$\lambda(x_0x_1 - x_0)^2$$

(7)

to our Hamiltonian for any $\lambda > 0$, and the unique minimum will not change. We know that the minimum we are looking for has either $(x_0, x_1) = (0, 0), (0, 1)$ or $(1, 1)$, in which case adding Eq. (7) does not change the energy in any way. However for invalid assignments of $(x_0, x_1)$, namely $(x_0, x_1) = (1, 0)$, adding Eq. (7) only adds more energy to the Hamiltonian, which guarantees that such an assignment will not have the lowest energy. In fact we will move all such invalid states a distance of $\lambda$ further away from the global minimum, affecting a quarter of all states in the search space.

In general, if we are able to deduce that $f = g$ for some polynomials $f, g$ we can manipulate $H$ by adding $\lambda(f - g)^2$ for some $\lambda > 0$. This will move any state for which $f \neq g$ further away from the global minimum. The effectiveness of such an addition will be determined in turn by the energy landscape of $(f - g)^2$. For more details on forming the addition term see our previous paper which is entirely about using deductions (though not for ELM, but for eliminating multi-qubit interactions in the problem Hamiltonian without adding extra qubits) [16].

1. Application to the factoring problem

For this section we pick $\lambda = 1$ as the coefficient for all of our deductions. This is in part for simplicity but mostly because our aim is to move all of the states occupying $E_{1(1)}$ while minimizing our impact on the spectral width. Any larger choice of $\lambda$ would lead to a larger impact without pushing any more terms away from $E_{1(1)}$.

We illustrate our method with the factorization of 841 = 29 × 29 which can be obtained by solving the following simultaneous equations:

$$\begin{align*}
2p_1 + p_2 + q_2 &= 2z_{23} + 4z_{24} \\
2p_1 + p_1q_2 + p_3 + q_2 + z_{23} &= 2z_{34} + 4z_{35} + 1 \\
p_1p_3 + p_1q_3 + p_2q_2 + z_{24} + z_{34} &= 2z_{45} + 4z_{46} \\
2p_1 + p_2q_2 + p_3q_2 + z_{35} + z_{45} &= 2z_{56} + 4z_{57} \\
p_2 + p_3q_2 + q_2 + z_{46} + z_{56} &= 2z_{67} + 4z_{68} + 1 \\
p_3 + q_3 + z_{57} + z_{67} &= 2z_{68} + 4z_{79} \\
z_{68} + z_{79} &= 1.
\end{align*}$$

(8)–(14)

It should be noted that the above equations are the result of elementary simplification of the original factorization equations, as described in [5]. The Hamiltonian could also be simplified much further, but then we would not have enough qubits to keep this example interesting. See [5, 17] for details on forming the original equations.

We then create our first Hamiltonian

$$H_0 = (2p_1 + p_2 + q_2 - 2z_{23} - 4z_{24})^2 + ... + (z_{68} + z_{79} - 1)^2$$

(15)

which encodes the single ground state (note that there will only be one ground state since 841 is a perfect square). A summary of $H_0$’s energy landscape can be found in Table I.

To perform ELM by deductions, we first need some deductions. Our first set is obtained by looking at Eq. 8. We notice that if $z_{24} = 1$ then we must have $p_1 = p_2 = q_2 = 1$. This information can be encoded by

$$z_{24}(1 - p_1), z_{24}(1 - p_2), \text{ and } z_{24}(1 - q_2)$$

(16)

respectively. We can then consider

$$H_1 = H_0 + z_{24}(3 - p_1 - p_2 - q_2)$$

(17)

and analyze our impact on the energy landscape (see Table II).

Furthermore, we can then make an identical analysis of Eq. 13 to obtain our last Hamiltonian

$$H_2 = H_1 + z_{79}(4 - p_3 - q_3 - z_{57} - z_{67}).$$

(18)

With this we were able to manipulate the energy landscape of the problem enough to have a huge impact on the spectral ratio $R$, as can be seen in Table II.
We can also see that our set of deductions from Eq. 8 managed to push away two of the four states originally occupying energy level $E_{(1)}$, and even some states occupying other excited energy levels were pushed away, with a very small impact to the spectral width. Introducing the second set of deductions moves the remaining two states so that $R$ is almost halved from its initial value, with minimal impact on $E_{(\text{max})}$.

### D. ELM using multiplicity: multiplicity-ELM

Our second ELM method is useful for any problem that is built from a system of equations of discrete-valued variables. Suppose we begin with a solvable system of binary equations:

\[
\begin{align*}
    x_1 + x_2 &= x_3 + 1 \quad \text{(19)} \\
    x_1 + x_1 x_2 &= 2x_2 x_3 + x_2 + 1. \quad \text{(20)}
\end{align*}
\]

We know that we can form a Hamiltonian by moving all terms to the left side, then squaring and summing \[3\]:

\[
H_0 = (x_1 + x_2 - x_3 - 1)^2 + (x_1 + x_1 x_2 - 2x_2 x_3 - x_2 - 1)^2. \quad \text{(21)}
\]

$H_0$ will achieve its global minimum of 0 at exactly the solutions to the original equations. However, we do not need to add these equations with equal weight. For any positive $\lambda_1, \lambda_2$, an equally valid Hamiltonian would be:

\[
H_1 = \lambda_1 (x_1 + x_2 - x_3 - 1)^2 + \lambda_2 (x_1 + x_1 x_2 - 2x_2 x_3 - x_2 - 1)^2. \quad \text{(22)}
\]

Our first strategy is to choose $\lambda_1, \lambda_2$ such that the maximum energy contributed by each equation is the same. For example Eq. \[19\] contributes $(x_1 + x_2 - x_3 - 1)^2$ to the Hamiltonian, and therefore adds a maximum energy of $(0 + 0 - 1 - 1)^2 = 4$, and Eq. \[20\] contributes a maximum energy of $(0 + 0 - 2 - 1 - 1)^2 = 16$. To address this, we will set $\lambda_1 = 4\lambda_2$. In general the motivation for this method is that some equations contain few variables and small coefficients, so the largest energy contribution over the entire energy landscape will be quite small. We can then add more weight to these equations, hoping that we do not impact the spectral width too severely, whilst pushing many (hopefully low-energy) states further away from the ground state.

Specifically, let $E_1 = \max((x_1 + x_2 - x_3 - 1)^2 = 4$ be the maximum error contributed by the first equation, and similarly let $E_2 = 16$ be the maximum contribution of the second. Furthermore let $E_{\text{max}} = \max(E_1, E_2)$. We then choose $\lambda_1 = E_{\text{max}}/E_1 = 4$ and $\lambda_2 = E_{\text{max}}/E_2 = 1$. Then, by analyzing the energy landscape we see a great improvement in spectral ratio in Table II by using our method rather than the naive approach.

In general, finding the absolute maximum energy contribution of an equation can be costly, since maximizing of an arbitrary polynomial over the integers is a hard problem \[18\]. However for the factorization problem, we are able to maximize them easily as each variable only appears once in each equation. To maximize the energy contribution of each equation, we first check that each side is fully expanded and that all of the coefficients are positive (by moving terms to the other side if necessary). We then maximize the left hand side by setting all of the variables to 1 and minimize the right hand side by setting all of its variables to 0. The difference between the sides can now be treated as a candidate for the maximum. The other candidate is obtained by setting the variables in the left hand side to 0 and the rest to 1. Squaring of the larger of these two candidate maxima gives us the maximum possible energy contribution of the equation.

It should be noted that in general, the ratio $E_{\text{max}}/E_i$ will not be an integer. For simplicity, in this paper we will only work with integer coefficients, and will therefore round all such ratios for all implementations of ELM. However, non-integer ratios are equally valid.

#### 1. Application to integer factorization

We exhibit the method on the factorization problem: $551 = 19 \times 29$. By generating the factorization equations and performing some very simple deductions to reduce the problem slightly (such as $x_1 + x_2 = 0$ implies that $x_1 = x_2 = 0$) we obtain the following set of simultaneous
Table III. Maximum energy contributed by each equation, for the factorization $551 = 19 \times 29$.

| Equation $(i)$ | Maximum Energy $E_i$ | $\lambda_i = [E_{\text{max}}/E_i]$ |
|----------------|----------------------|-----------------------------------|
| 23             | $\max(2,1)^2 = 4$    | 13                                |
| 24             | $\max(2,1)^2 = 4$    | 13                                |
| 25             | $\max(4,6)^2 = 36$   | 2                                 |
| 26             | $\max(6,6)^2 = 36$   | 2                                 |
| 27             | $\max(6,7)^2 = 49$   | 1                                 |
| 28             | $\max(5,6)^2 = 36$   | 2                                 |
| 29             | $\max(4,6)^2 = 36$   | 2                                 |
| 30             | $\max(3,2)^2 = 9$    | 6                                 |
| 31             | $\max(2,1)^2 = 4$    | 13                                |

We achieved a large reduction in the number of local minima close to the ground state. However, we have doubled the spectral gap and slightly more than doubled the spectral width, resulting in a slight increase in spectral ratio. This is undesirable for computation by an adiabatic quantum computer, so we present a small refinement.

We then form the naive Hamiltonian

$$H_0 = (p_1 + q_1 - 1)^2 + \ldots + (z_{79} + z_{89} - 1)^2.$$  

A quick check confirms that Eqs. 23-31 do not have any variables in both the left and right hand sides, even after our judgments, so we can carry out the algorithm described above for maximizing the energy contribution from each equation. We sum the appropriate coefficients and then choose $\lambda_i$ using the formula

$$\lambda_i = [E_{\text{max}}/E_i].$$

This results in the ELM-adjusted Hamiltonian:

$$H_1 = 13(p_1 + q_1 - 1)^2 + 13(p_2 + q_2 + 1) + 2(p_1 q_2 + p_2 q_1 + p_3 + q_3 - 2z_{34} - 4z_{35})^2 + 2(p_1 q_2 + p_2 q_1 + p_3 + q_3 - 2z_{34} - 4z_{35})^2 + 1(p_1 + p_2 q_3 + p_3 q_2 + q_1 + z_{35} + z_{45} - 2z_{36} - 4z_{57} - 1)^2 + 2(p_2 + p_3 q_3 + q_2 + z_{46} + z_{56} - 2z_{67} - 4z_{68})^2 + 2(p_3 + q_3 + z_{57} + z_{67} - 2z_{78} - 4z_{79})^2 + 6(z_{68} + z_{78} + 1 - 2z_{89})^2 + 13(z_{79} + z_{89} - 1)^2.$$  

Again, we show the spectral gap, width, ratio and nature of the first few excited states in Table IV.

2. Refinement

In the factoring problem, we know [5, 10] that the Hamiltonians always have the property that $E_{(i)} = 1$, so if we are able to shift $E_{(j)}$ up by just 1, while minimizing impact to $E_{\text{max}}$ at all costs, we may be more likely to reduce the spectral ratio. We present an alternative choice of $\lambda_i$ that achieves such a goal:

$$\lambda_i = \begin{cases} 
1, & E_i = E_{\text{max}} \\
2, & E_i \neq E_{\text{max}}.
\end{cases}$$

We then define the Hamiltonian produced according to this scheme:

$$H_2 = 2(p_1 + q_1 - 1)^2 + 2(p_2 + q_2 + 1) + 2(p_1 q_2 + p_2 q_1 + p_3 + q_3 - 2z_{34} - 4z_{35})^2 + 2(p_1 q_2 + p_2 q_1 + p_3 + q_3 - 2z_{34} - 4z_{35})^2 + 1(p_1 + p_2 q_3 + p_3 q_2 + q_1 + z_{35} + z_{45} - 2z_{36} - 4z_{57} - 1)^2 + 2(p_2 + p_3 q_3 + q_2 + z_{46} + z_{56} - 2z_{67} - 4z_{68})^2 + 2(p_3 + q_3 + z_{57} + z_{67} - 2z_{78} - 4z_{79})^2 + 2(z_{68} + z_{78} + 1 - 2z_{89})^2 + 2(z_{79} + z_{89} - 1)^2.$$
whose properties are described in Table IV.

On this occasion we have managed to reduce the spectral ratio as well as the number of local minima, as can be seen in the final column of Table IV.

III. CONCLUSION

We have presented two methods for manipulating the energy landscape of a Hamiltonian without changing the ground state, and without adding extra qubits: deducELM and multiplicityELM. We used these methods to increase the size of the energy gap between the ground state and lowest excited state of the Hamiltonian ($E_{\text{gap}}$), and to reduce the size of the gap between the ground state and highest excited state ($E_{\text{width}}$) for an adiabatic quantum computation algorithm for integer factorization.

For the first factorization example, deducELM was able to double $E_{\text{gap}}$ while increasing $E_{\text{width}}$ by only a factor of $\approx 1.03$ (see Table I). We showed that for the quantum computation to find a state that is a fixed distance away from the state that encodes the solution to the problem, the runtime is at most $E_{\text{width}}^3/E_{\text{gap}}^2$, so for this factorization example, the runtime would be decreased by at most a factor of 7.54, or 75.4% of the original maximum runtime. For the second factorization example, we applied multiplicityELM and were able to decrease the maximum runtime by at most 250%.

Our method is in fact more general, in that it does not need to increase $E_{\text{gap}}$ or decrease $E_{\text{width}}$. In general, it can provide a new Hamiltonian whose ground state(s) are the same. One may choose to manipulate the energy landscape of the Hamiltonian in such a way to decrease the size of $E_{\text{gap}}$ or increase the size of $E_{\text{width}}$, as would be useful for classical simulated annealing algorithms such as the one described in [11]. One may also choose to transform the Hamiltonian in such a way to change the couplings between the qubits, so that it is easier to map the Hamiltonian onto available hardware, such as in NMR-based AQC where it may be difficult to find a molecule where the distances between the spins match the couplings in the desired Hamiltonian.

ACKNOWLEDGMENTS

We would like to thank Emile Okada (Cambridge University, UK), Ilia Zintchenko & Matthias Troyer (ETH Zurich, Switzerland), and Ke Zj & Xinhua Peng (University of Science and Technology, China) for helpful discussions.

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Table IV. Energy landscape for a 17-qubit factorization of 511 for various Hamiltonians $H$ with equivalent ground states.

| $H$ | $E_{\text{gap}} = E_{\langle 1 \rangle}$ | $n_1$ | $E_{\langle 2 \rangle}$ | $n_2$ | $E_{\langle 3 \rangle}$ | $n_3$ | $E_{\langle 4 \rangle}$ | $n_4$ | $E_{\text{max}}$ | $R$ |
|-----|-------------------------------------|------|----------------------|------|----------------------|------|----------------------|------|----------------|------|
| $H_0$ | 1 | 2 | 2 | 20 | 3 | 60 | 4 | 113 | 133 | 17 689 |
| $H_1$ | 2 | 2 | 3 | 8 | 4 | 4 | 5 | 16 | 296 | 10 952 |
| $H_2$ | 2 | 2 | 3 | 12 | 4 | 8 | 5 | 35 | 238 | 7 081 |

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