Automatic Generation of Grover Quantum Oracles for Arbitrary Data Structures

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Abstract—The steadily growing research interest in quantum computing - together with the accompanying technological advances in the realization of quantum hardware - fuels the development of meaningful real-world applications, as well as implementations for well-known quantum algorithms. One of the most prominent examples till today is Grover’s algorithm, which can be used for efficient search in unstructured databases. Quantum oracles that are frequently masked as black boxes play an important role in Grover’s algorithm. Hence, the automatic generation of oracles is of paramount importance. Moreover, the automatic generation of the corresponding circuits for a Grover quantum oracle is deeply linked to the synthesis of reversible quantum logic, which - despite numerous advances in the field - still remains a challenge till today in terms of synthesizing efficient and scalable circuits for complex boolean functions.

In this paper, we present a flexible method for automatically encoding unstructured databases into oracles, which can then be efficiently searched with Grover’s algorithm. Furthermore, we develop a tailor-made method for quantum logic synthesis, which vastly improves circuit complexity over other current approaches. Finally, we present another logic synthesis method that considers the requirements of scaling onto real world backends. We compare our method with other approaches through evaluating the oracle generation for random databases and analyzing the resulting circuit complexities using various metrics.

Index Terms—quantum computing, oracle generation, grover’s algorithm, quantum logic synthesis

I. INTRODUCTION

A. General Remarks

The field of quantum computing has seen a significant rise in interest over the past two years since the quantum supremacy announcement from Google [1] and will continue to be of great interest, among other things, due to the recent supremacy announcements regarding chinese quantum hardware designs [2], [3], [4]. Yet some of the well known algorithms that are representative for the potential of quantum computing are still far from being implementable for meaningful applications on today’s quantum hardware. Especially noteworthy are Shor’s algorithm that could play a significant role in cryptography and cybersecurity as well as Grover’s algorithm. The latter was initially designed for searching through large unstructured databases [5] but also has applications in cryptography [6] (e.g. for the search of encryption keys in the context of symmetric cryptographic algorithms), optimization problems [7], [8], [9] - that can even be beneficial for material discovery [10] - as well as applications for challenging problems in the domain of data structure and hash function design [11].

The focus of the research presented in this paper relates to the scalable synthesis of quantum oracles used in the context of Grover database search. The need for automatic oracle generation for Grover’s algorithm was extensively discussed in one of our previous research works [12]. After a thorough analysis, [12] clearly states that there is a paramount requirement for automatically generated oracles as inputs for Grover’s algorithm, in order to be able to provide function/procedure APIs (Application Programming Interfaces) to developers and that way seamlessly integrate quantum computing into existing software development projects (e.g. telecom supporting systems, web shops and other kinds of applications) and processes. In order to address this urgent need, we present the design and implementation of a fully automated programming framework for the complete Grover based search process, including the generation of the belonging quantum oracles. This involves the conversion of arbitrary data into boolean functions that are encoded in truth tables, the synthesis of Grover oracles from these truth table expressions and the direct integration into the initialization and diffusion steps of Grover’s algorithm.

B. Problem Statement

The following constitutes a tangible list of aspects that summarize the targeted problem:

- The creation of oracles for Grover’s search algorithm is a challenging task.
- The creation of quantum oracles containing the input for a Grover search needs to be done on a case-by-case basis depending on the database/list to search in and the object/value to search for.
- As of the current state-of-the art there is no accessible computer scientist’s alike API for functions/procedures (e.g. int grover(int f, list_to_search_in, int value_to_search_for)) that allows for effortless submission of a database/list and an object/value to search for in this database/list.
- Hence, Grover’s algorithm is almost impossible to apply for the execution of standard tasks in the course of programing IT components and products in different application domains.
In order to address the above issues, our current research paper presents a solution, such that efficient and convenient I/O procedures to Grover’s algorithm are enabled. The following sub-section outlines the specific contributions of our paper which address the posed problem statement and belonging research challenge.

C. Contributions

The following key contributions are the result of our research work, which is presented in the current paper towards progressing on the topic of automatic generation of Grover quantum oracles for arbitrary data structures:

1) The current paper presents an overall structure of a procedure for the automatic generation of Grover oracles, which is based on truth tables and belonging quantum logic synthesis. This procedure enables Grover quantum search of arbitrary databases.

2) We present a high level complexity analysis of this general structure/procedure and clearly identify the benefits and the need for improvements of the algorithms and the approach itself.

3) Subsequently, we present a flexible method for implementing similarity searches over a database thereby steering the oracle generation correspondingly. Within a similarity search it is possible to utilize Grover’s algorithm to identify database items which have a certain degree of resemblance compared to a particular item we are searching for.

4) Moreover, we survey the topic of quantum logic synthesis and adapt different available algorithms - such as the Reed-Muller Expansion and the Gray Synthesis in order to improve their efficiency in the workflow of oracle generation.

5) We present a new Phase Tolerant Synthesis method, a streamlined version of the established Gray Synthesis, which (asymptotically) halves the required resources.

6) Another critical issue is constituted by the scaling of logic synthesis methods which quickly requires extremely fine phase gates. In order to address this issue we introduce the method of CSE-synthesis.

7) Finally, we present a number of benchmarking results which confirm the efficiency of our approaches and algorithms for quantum logical synthesis and in general for automatic Grover oracle generation.

The above items constitute clear contributions, which to the author’s knowledge are the first attempt so far to enable the efficient and convenient input of databases and objects to search for with Grover’s algorithm with the goal to make it usable for different tasks in modern IT components and products (e.g. web portals, search engines, network operation centers etc.).

D. Structure of the Paper

The rest of this paper is organized as follows: In section (II) we present an overview of the state-of-the-art in oracle synthesis work. In the subsequent section (III) our method for automatic oracles generation is presented. In section (IV), we give an introduction into different methods for reversible quantum logic synthesis and elaborate on our improved version for Grover oracle generation that we denote as phase tolerant synthesis. This is then further discussed in the context of scalable logic synthesis circuit design in section (V). Section (VI) describes the tests and results we obtained by comparing existing oracle generation methods with the one we developed in terms of circuit complexity. Finally, section (VII) contains a summary of the research presented in this paper as well as some brief discussion about our future research plans.

II. OVERVIEW AND BACKGROUND

To provide an initial overview, section (II) reviews Grover’s algorithm for efficient item search in unstructured databases on a higher level without going into the mathematical details and proofs. Afterwards, some recent research works from the domain of Reversible Quantum Logic Synthesis are presented. These activities and related results are of particular importance for our approach to the automated generation of Grover quantum oracles. Besides specific applications for Grover’s algorithm, proof of concepts for experimental realizations [13] and low-scale prototype implementations on current quantum hardware [14], a really important field of research lies in the scalable generation of Grover oracles and quantum oracles for black box algorithms in general [12].

A. Grover’s Algorithm

At the heart of Grover’s algorithm lies a quantum oracle, which phase-tags only the winner items. For now we leave the specifics of generating said oracle from the database to the subsequent sections and simply assume it has the following functionality:

\[ O |i\rangle = (-1)^{f(i)} |i\rangle \quad \text{with} \quad f(i) = \begin{cases} 0, & \text{if } i \not\in \{ w_j \} \\ 1, & \text{if } i \in \{ w_j \}. \end{cases} \quad (1) \]

Note that for the oracle, we don’t need to explicitly know \( w_j \) but we only need a valid function \( f \) for the search problem. Also for an explicit construction of such oracles, one generally needs an auxiliary qubit register to store intermediate results into which has to be uncomputed later on\(^1\). The role of this auxiliary qubit register and belonging operations is further discussed in section (III).

In order to evaluate Grover’s algorithm with this oracle, we initialize the system in the fiducial state \( |\Psi\rangle = |0\rangle^\otimes n \). Grover’s algorithm starts by setting all qubits into an equal superposition state \( |s\rangle \)

\[ H^\otimes n |0\rangle^\otimes n = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle = |s\rangle. \quad (2) \]

Here, the integer states \( |i\rangle \) directly relate to corresponding binary encoded states in the computational basis.

\(^1\) Uncompilation is the process of Garbage Collection with respect to qubits, i.e. during an uncomputation the corresponding qubits are systematically reset to their initial states through the belonging reversible mathematical operations.
After phase-tagging the winner states - i.e. the states representing the values we search for in the unstructured database - Grover’s algorithm implements a so called diffusion operator \( U_d = 2|s\rangle\langle s| \) - I that amplifies the amplitudes for measuring the winner states. The phase-tagging and diffusion steps can geometrically be considered as two successively performed reflections, and thus as a single rotation in a 2D-plane. Each such rotation corresponds to a single Grover iteration that gradually rotates \(|s\rangle\) closer to \(|w_j\rangle\). At the end of the algorithm, a measurement in the computational basis is performed and the searched and potentially found items can be identified by distinct peaks in the distribution of the measured results. It is important to remark that in literature \([15]\) there is a derived optimal number of Grover iterations (i.e. amplification and oracle application) that results in \(|s\rangle\) being rotated the closest to \(|w_j\rangle\). This optimal number of iterations yields the best measurement results. Thus, performing more or less rotations is expected to lead to increasingly worse search results. A more in-depth discussion about Grover iterations will be given in section (III). To summarize briefly: searching \(M\) items within an unstructured database needs at most \(O(\sqrt{\frac{N}{M}})\) iterations by Grover’s algorithm. Hence there is a noticeable advantage over classical search algorithms, which are known to perform in \(O(N)\) for a linear search.

B. Reversible Quantum Logic Synthesis

Technically, there is a deep interconnection between generating quantum oracles and synthesizing reversible quantum circuits from classical logic expressions. Therefore, in section (III) we describe the application of state-of-the-art quantum logic synthesis procedures for our approach to Grover oracle synthesis. In the following paragraph, we conduct a brief introduction to related research and development activities from the area.

As Reversible Quantum Logic Synthesis is an active field of research for more than 20 years \([16]\), more efficient methods in terms of gate counts and the usage of ancilla qubits arise frequently \([17]\). While many of them are available in the tweedledum \([18]\) library, a fairly recent method of interest is denoted as resource-efficient oracle synthesis (ROS) and was initially presented in \([19]\). It is built on the LUT-based hierarchical reversible logic synthesis framework (LHRS) \([20]\) and improves the LUT-network approach by adding a special quantum aware k-LUT mapper, involving specially truncated XAGs \([21]\) and a more efficient SAT-based quantum garbage management technique \([22]\), which offers control over the number of qubits used in the synthesized circuits. This method can be considered as a reasonable competitor and thus constitutes an interesting research work for comparison to our synthesis methods. Additionally, there are some implementations for oracle generation in the established software frameworks like Qiskit \([22]\) and Q# \([23]\). The Qiskit implementation will be tested and compared to our approach in section (V). Apart from the above mentioned activities, there are no further comparable methods to the best of our knowledge.

III. METHOD FOR AUTOMATIC ORACLE GENERATION

We will now present our method of turning arbitrary databases into oracles. The basic idea is to deploy a computationally effective labeling function, which turns the data into bitstrings of suited length. For a database \(D\), this labeling will be denoted as:

\[
l : D \rightarrow \mathbb{F}_2^k
\]

where \(k \in \mathbb{N}\) stands for the label size, which has to be chosen according to the specifics of the problem (more to that in section (III-A)). The method of obtaining these bitstrings is in principle also free to choose as long as it only takes local information from the database, i.e. the bitstring of each element is independent from the rest of the database. For example, in our Python implementation, the native hash function generates an integer hash value for a wide class of objects, which we convert to the belonging binary representation and clip the bitstring to a length of \(k\).

As a result, the labels provide a sequence of bitstrings representing the database, which eventually can be used to form a logical truth table (see table (1a) for an example). Subsequently, this truth table is turned into a quantum circuit using a suited quantum logic synthesis algorithm. Given two registers (the index and the label register) this yields a unitary mapping \(U_D\) which acts as

\[
U_D |i\rangle |0\rangle = |i\rangle |l(e(i))\rangle.
\]

where \(l(e(i))\) is the label of the database entry \(e\) with index \(i\). It is important to note that the synthesis process only has to be done once per database. The resulting circuit can then be used for subsequent searches and only needs to be updated at changes to the database entries. We leave the challenge of efficient updating for database circuits as an open research question, which we are going to address in the near future.

Based on the above considerations, in order to query the index \(i_q\) for a given database element \(e_q\), we combine the synthesized truth table with a phase-tag of the bitstring \(l(e_q)\), which can be calculated with very small effort from \(e_q\). The phase-tag is realized using a multi-controlled \(|z\rangle\) gate which is enclosed by \(X\) gates at the appropriate qubits. Finally, the label variable has to be uncomputed again. Denoting the tagging function of label \(l(e)\) with \(T(l(e))\), the mathematical description of the actions of the oracle \(O(e_q) = U_D^\dagger T(l(e))U_D\) of the element \(e_q\) is as follows:

\[\mathbb{F}_2\] is the Galois field with two elements, i.e. the field of operation for traditional boolean algebra. The arithmetic operations are all carried out \(\mod 2\), i.e. \(1 + 1 \equiv 0 \mod 2\). We will use the \(\oplus\) notation for additions in the \(\mathbb{F}_2\) space.
with the particular bitstring of why we use a heuristic approach to estimate M which is precisely the functionality we required O(e_q) to have in eq. (1).

A. Hash collisions

As can be seen in table (14), it can happen that two elements have the same label (here: Grace & Bob). This poses not that much of a problem, since after running Grover’s algorithm a classical search can be applied on the (heavily reduced) result space. Another insight is constituted by the fact that the probability for a hash collision is well controlled by increasing/decreasing the label size (i.e. the size of the binary string). A second maybe more subtle problem is that in order to determine the optimal amount of Grover iterations R, the amount of tagged states has to be known according to (24).

\[
R \leq \left\lceil \frac{\pi}{4} \sqrt{\frac{N}{M}} \right\rceil
\]  

with M being the amount of elements sharing the labeling bitstring l(e_q) and N the amount of elements contained in the database D. This might seem only like a minor inconvenience, because on first sight this could result in only a few extra-iterations. However, as described in the previous section, the results get worse if continuing with iterations after the optimal prescribed number. A possible quantum algorithm, which can determine M, is presented in [25]. Unfortunately, it requires exponentially many oracle calls, which is untenable for an efficient database and fast system reaction times. In addition, all these oracle calls have to be controlled, which implies that every CNOT gate is turned into a Toffoli gate\(^\text{6}\) leading to another factor of 6 in the CNOT count. Due to these disadvantages, the approach is not feasible in practice, which is why we use a heuristic approach to estimate M. In detail, we determine the expected value of another element e_i with the particular bitstring of e_0. For this we assume that the bitstrings are uniformly distributed over the label space \(E^2_k\). This is the setup for a Bernoulli-Process with \(n = N - 1\) tries with a probability of \(p = 2^{-k}\). The resulting model is constituted by the binomial distribution and the expected value therefore takes the very simple form of

\[
E(\#\text{collisions}) = np = (N - 1)2^{-k}.
\]  

Since there is at least one element sharing the bitstring of \(e_0\) (i.e. \(e_0\) itself) we add a 1 to acquire the expected value for M:

\[
E(M) = 1 + (N - 1)2^{-k}.
\]  

This formula captures the intuitive relationship between the label size k and the number of estimated hash collision M. It shows that by decreasing the label size k, one can increase M, while in parallel decreasing the amount of Grover iterations (see eq. (5)) to be executed and synthesis tasks to be performed. This would be interesting in future hybrid use cases, where quantum resources are available at a similar cost as classical resources but still not capable of solving complex problems on their own. In this hybrid scenario, the search space would first be drastically lowered by a factor of \(O(2^{-k})\) by the quantum computer and then reduced to 1 with a classical search.

B. Algorithmic View on Oracle Generation

We want to continue by summarizing the overall procedure for the automated oracle generation from an algorithmic point of view. Thereby, we provide an overall structure of the steps which are required to generate an oracle for Grover’s algorithm from a random database. These are structured in two sub-algorithms, namely the one responsible for database encoding (i.e. algorithm (1)) and the second one, which is responsible for automatic definition of the oracle based on the encoded database (i.e. algorithm (2)). Based on those two sub-algorithms, time complexity estimations are provided, in order to give a feeling regarding the applicability and the open research issues relating to the topic of automatic oracle generation.

**Algorithm 1 Database encoder**

**Input:** Iterable database \(D\), labeling function  
**Output:** Encoding circuit \(U_D\)

1: list bitstrings = []  
2: for \(e\) in \(D\) do
   3: bitstrings.append(Label(e))  
5: TruthTable tt = TruthTable(bitstrings)
6: return QuantumLogicSynthesis(tt)

Algorithm (1) describes the steps required to encode an arbitrary database for the purposes of Grover’s search algorithm. The only requirement here is, that it should be possible to iterate over the content of the database. Thereby, no order of the content is presumed. Hence, the database can contain arbitrary objects.

The other ingredient, which is required as an input to algorithm (1), is the labeling function. This function needs to have the capability to take an arbitrary object from the database and assign it a label, that does not have to be unique. In fact, hash functions as known in computer science are natural choices as labeling functions. Hash functions in general do not provide unique labels (i.e. hash collisions). However, even with non-unique labels of the database objects, Grover search

\(\text{6A Toffoli gate is a a controlled CNOT gate (or CCNOT). This gate can be synthesized using 6 CNOT gates.}\)
can be used to search for labels and that way reduce the overall search complexity by collapsing the search space only to those objects/entries, which have been assigned a particular label.

As can be seen in the listing of algorithm (1), a for-cycle is required that iterates over the database objects and assigns a label to each of them. This cycle has the time complexity of $O(N)$, with $N$ being the number of entries in the database. Each label is presumed to be a binary string and is stored in a corresponding list, which is used to initially prepare a truth table for Grover oracle. This truth table consists of simply listing and preparing the label bitstrings in such a way they can be used for quantum logic synthesis. Hence, the truth table creation has again complexity of $O(N)$ and and leaves the previous complexity estimation unchanged.

The quantum logic synthesis in the last step of algorithm (1) is the most critical part of the process. This step can be conducted by various algorithms and procedures, which is further focused on in the following sections of this paper, in which some fitting methods from literature are applied and evaluated and subsequently own methods are presented. As we will see in the upcoming section (IV) this step can be performed quite efficiently using an algorithm called Fast Hadamard-Walsh Transform [27] which has classical time complexity $O(N \times \log(N))$ per truth table column. In our case we synthesize about $k \approx O(\log_2(N))$ in order to prevent excessive hash collisions, yielding an classical time complexity of $O(N \times \log(N)^2)$.

However, as algorithm (1) has to be executed only once per fixed database, Grover’s algorithm can be executed for different values to search for on the prepared database quantum circuit. Thus, the time complexity can be relieved this way with regard to the application of algorithm (1).

After the steps from algorithm (1) have been conducted, algorithm (2) must be executed every time before a new object/value is being searched for in the database entries. Algorithm (2) contains the required instructions towards preparing a specific quantum oracle encoding the database and the search value. This specific quantum oracle is then embedded in Grover’s algorithm for the subsequent search on the quantum computer side. We see the following components.
Algorithm 2 Query oracle generator

Input: Encoded database circuit \( U_D \), query element \( e_q \), labeling function
Output: Oracle circuit \( O \)

1: string qlabel = Label\((e_q)\)
2: QuantumCircuit \( O = \text{QuantumCircuit}(\text{index register, label register}) \)
3: \( O . \text{apply}(U_D) \)
4: \( O . \text{apply}((\text{PhaseTag}(\text{qlabel}, \text{label register}))) \)
5: \( O . \text{apply}(U_D^\dagger) \)
6: return \( O \)

In algorithm 2: The creation of a QuantumCircuit object, in which the quantum circuit encoding the database (result from Algorithm 1) is immediately embedded (i.e. \( O . \text{apply}(U_D) \)) and finally \( O . \text{apply}(U_D^\dagger) \) followed by the application of a phase tag (i.e. \( O . \text{apply}((\text{PhaseTag}(\text{qlabel, label register}))) \)) for marking the value/object to search for. The steps in the first component are dominated by the embedding of the quantum encoded database circuit (i.e. \( O . \text{apply}(U_D) \)) and finally \( O . \text{apply}(U_D^\dagger) \) which can be considered linear with respect to the number of gates in the database quantum circuit. As we will see in the upcoming sections, the Gray synthesis method has a quantum gate complexity of \( O(N) \) per truth table column, implying a quantum gate complexity of \( O(N \times \log(N)) \) for \( k \approx O(\log(N)) \) columns. The phase tag (i.e. \( O . \text{apply}((\text{PhaseTag}(\text{qlabel, label register}))) \)) and the diffuser can also be synthesized using Gray synthesis i.e. \( O(N) \). As we require \( O(\sqrt{N}) \) Grover iterations, the overall quantum gate complexity is

\[
O(N^{1.5} \times \log(N)).
\]

(9)

On first sight this seems like a decrease in Grover’s efficiency \( O(\sqrt{N}) \) however we have to keep in mind that this is the complexity in oracle calls the oracle evaluation itself will have a non-constant complexity in almost any other comparable scenario.

Even though currently not more efficient than classical database search, our results open many research directions which could ultimately lead to an increase in database search efficiency.

Having briefly discussed this, the following sections continue with the presentation and deepen the discussion on various methods for quantum logic synthesis and for establishing Grover oracles and the search procedures in a flexible way.

C. Similarity Search

The method presented so far can be generalized to a technique, which also allows for searching bitstrings similar to the query, i.e., not the exact item but rather one that is very close according to some metric. In the case, where the oracle has been generated from labeled data, this can obviously only work if the labeling function preserves the similarities between the database elements. Another application scenario for a similarity search could be the case where the labels themselves constitute the data.

The general idea of encoding the similarity of two bitstrings into the quantum oracle is to replace the tagging function \( T^{\text{sim}}\) with a circuit that performs phase shifts based on the Hamming-Distance. One such circuit is given by the application of RZ gates on the label register. In more detail:

\[
T^{\text{sim}}(l(e_q)) = \bigotimes_{j=0}^{k-1} \text{RZ}_j \left( \frac{(-1)^j l_j(e_q)}{k} \right). \tag{10}
\]

For a single RZ gate acting on a qubit in a computational basis state we have

\[
\text{RZ}\left( \frac{(-1)^j x \pi}{2} \right) |y\rangle = \exp \left( \frac{i \phi}{2} (-1)^{x \pi} \right) |y\rangle. \tag{11}
\]

Applying the similarity tag \( T^{\text{sim}}(l(e_q)) \) to the multi-qubit state \( |l(e)\rangle \) therefore yields:

\[
T^{\text{sim}}(l(e_q)) |l(e)\rangle = \exp \left( \frac{i \pi}{k} \sum_{j=0}^{k-1} (-1)^j l_j(e_q) \Delta l_j(e) \right) |l(e)\rangle. \tag{12}
\]

To get an intuition of the effect of this, we now consider what happens when \( l(e) = l(e_q) \). In this case we have:

\[
l_j(e_q) \Delta l_j(e) = 0 \quad \forall j < k \tag{13}
\]

implying that the sum over \( j \) evaluates to \( k \). Therefore the applied phase is simply \( \pi \), i.e., exactly what we have in the case of a regular phase-tag. If \( l(e) = l(e_q) \) for all but one \( j \)-index, the sum evaluates to \( k-2 \). Hence, the applied phase is \( \pi (1 - \frac{1}{k}) \) which is “almost” the full phase-tag. An example application of the similarity search can be found in fig. (1a).

In the following, a more formal proof is presented regarding why the above considerations work when applied within Grover’s algorithm. For this we assume that the oracle has tagged the uniform superposition \( |s\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{2^n-1} |x\rangle \) in such a way that the index register is in the state

\[
|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{2^n-1} \exp(i \phi(x)) \langle x|.
\]

(14)

We now apply the diffusion operator \( U_s = 2 |s\rangle \langle s| - \mathbb{I} \) on the above state:

\[
U_s |\psi\rangle = \frac{1}{\sqrt{N}} \exp(2 |s\rangle \langle s| - \mathbb{I}) \sum_{x=0}^{2^n-1} \exp(i \phi(x)) |x\rangle
\]

(15)

\[
= \frac{1}{\sqrt{N}} \sum_{x=0}^{2^n-1} \exp(i \phi(x)) (2 |s\rangle \langle s|x| - |x\rangle).
\]

Using \( \langle s|x| = \frac{1}{\sqrt{N}} \) gives

\[
= \frac{1}{\sqrt{N}} \left( \frac{2}{\sqrt{N}} \sum_{x=0}^{2^n-1} \exp(i \phi(x)) \right) |s\rangle - \sum_{x=0}^{2^n-1} \exp(i \phi(x)) |x\rangle.
\]

(16)

Next, we set

\[
r_{cm} \exp(i \phi_{cm}) := \frac{1}{N} \sum_{x=0}^{2^n-1} \exp(i \phi(x)),
\]

(17)
where $cm$ stands for the center of mass. Inserting the definition of $|s\rangle$ we get

$$
= \frac{1}{\sqrt{N}} \sum_{x=0}^{2^n-1} (2r_cm \exp(i\phi_cm) - \exp(i\phi(x))) |x\rangle
$$

Finally, we use the rules of polar coordinate addition

$$r_3 \exp(i\phi_3) = r_1 \exp(i\phi_1) + r_2 \exp(i\phi_2),$$

$$r_3 = \sqrt{r_1^2 + r_2^2 + 2r_1r_2 \cos(\phi_1 - \phi_2)}$$

$$\phi_3 = \arctan \left( \frac{r_1 \sin(\phi_1) + r_2 \sin(\phi_2)}{r_1 \cos(\phi_1) + r_2 \cos(\phi_2)} \right),$$

to determine the absolute values of the coefficients in order to find out about the amplification factor $A_x$

$$A_x = |2r_cm + \exp(i(\phi(x) - \phi_cm + \pi))|$$

$$= \sqrt{1 + 4r_cm^2 + 4r_cm \cos(\phi(x) - \phi_cm)}.$$  

From this we see that $A_x$ becomes maximal if $\phi(x) - \phi_cm = \pm \pi$, minimal if $\phi(x) - \phi_cm = 0$ and is monotonically developing in between, which is precisely the behavior we expected.

Even though the similarity tag allows a considerable cut in the CNOT count compared to the multi-controlled $Z$ gate, it comes with some drawbacks. The biggest problem is that the results of this method are very sensitive to the number of iterations. Applying the wrong amount of Grover iterations can lead to 0 instead of the query, get the same amplification as their inverted counterpart (assuming $\phi_cm = 0$ in eq. [22] - more to this assumption soon). For example if we query for the label 000000, the label 011111 would receive the same amplification as 100000. This can be explained by looking at equation [22]. If $l(e_q)$ and $l(e)$ differ on every single entry, we have

$$l(e_q)_i \oplus l(e)_i = 1 \ \forall i < k$$  

This results in the sum evaluating to $-k$ and yielding a phase of $-\pi$, which is equivalent to a phase of $\pi$. A similar effect can be observed, when only a single bit of the inverse is mismatching. In this case, we apply the phase $-\pi + \frac{1}{k}$. Even though this phase is not equivalent to $\pi - \frac{1}{k}$, its absolute value is, which is the feature of relevance according to equation [22].

D. Advanced Similarity Tags

In this section we will present a method which lifts the restriction of the similarity tags being confined to the Hamming distance. Instead, it will be possible to encode an extremely wide and flexible class of similarity measures (without any overhead compared to the regular multi-controlled $Z$ gate tags). If we denote the set of possible query objects with $Q$, any function with the following signature can be encoded as a similarity measure:

$$f : Q \times \mathbb{F}_2^k \to [0, 1].$$  

Here $\mathbb{F}_2^k$ again denotes the set of bitstrings with length $k$ and $[0, 1]$ the interval between 0 and 1 (endpoints included). So this function compares a query object $q \in Q$ with a bitstring and returns a real number between 0 and 1, which indicates how similar the two objects are. 1 means equivalent and 0 means no similarity. An example of such a similarity measure is the Dice coefficient. In this case we have

$$f : \mathbb{F}_2^k \times \mathbb{F}_2^k \to [0, 1],$$

$$((x_0, x_1, \ldots, x_k), (y_0, y_1, \ldots, y_k)) \mapsto \frac{2 \sum_{i=0}^k x_i y_i}{\sum_{i=0}^k (x_i + y_i)}.$$  

Note that the additions here are not denoted by $\oplus$ but the regular $+$ so they are not evaluated mod 2.

In order implement this advanced similarity tagging, we have to utilize the method of Gray synthesis which will be laid out in more detail in the coming section [V-B]. All we need to know about it here is that it can synthesize arbitrary diagonal (in the computational basis) unitary matrices: For a given $2^k$ tuple of real numbers $\phi = (\phi_0, \phi_1, \ldots, \phi_{2^k-1})$ a circuit $U_{gray}(\phi)$ can be synthesized such that for any computational basis state $|y\rangle$

$$U_{gray}(\phi) |y\rangle = \exp(i\phi_y) |y\rangle.$$  

Note that Gray synthesis requires only up to $2^k$ CNOT gates, implying such a similarity tag is computationally more efficient or of equivalent efficiency as tagging with a multi-controlled $Z$ gate.

We next show how applying Gray synthesis on the label register can be used to implement a tag, which acts as described in eq. [14]. Suppose we are given a similarity function $f$ of the type in eq. [14]. Then the similarity tag $T_f^{\text{sim}}(q)$ for the query object $q \in Q$ is given as:

$$T_f^{\text{sim}}(q) = U_{gray}(\phi_f^{\text{sim}}(q)),$$

where $(\phi_f^{\text{sim}}(q))_y = (-1)^y \pi f(q, y).$  

Next, we elucidate on the suitability of this operation as a similarity tag. For this we apply the similarity oracle consisting of the database encoding circuit $U_D$ and the similarity tag to the index register in a uniform superposition.

\footnote{Note that this circuit doesn’t necessarily has to encode a database but any other function calculating a binary value is also possible. One such alternative use case are optimization problems, which is under active research by the authors. Because of this we write $U_D |x\rangle |0\rangle = |x\rangle |y(x)\rangle$ instead of the $l(e(i))$ language used in the previous sections.}
We call this a similarity measure. Looking at the definition of \( \phi(x) \), where the above described aspects are clearly visible.

We see that this oracle has the effect we assumed in eq. [14] with \( \phi(x) = (\theta) \left( \prod_{i=1}^{n} \pi f(q, y(x))) \right) \). First of all, we note that (under reasonable assumptions about \( f \)) the alternating signs of the phases help getting \( \phi_{\text{cm}} \), close to zero. To see why this is the case, we assume that for the majority of \( x < 2^n \), the statement \( f(q, y(x)) \approx 0.5 \) holds or in other words: Only in a few cases we actually do have similarity. Looking at the definition of \( \phi_{\text{cm}} \), eq. [17], we observe the repeated addition of complex numbers mostly in the right half of the complex plane, which implies that the center of mass is most likely going to be in the right half of the complex plane. As the signs of the phases are alternating, we “balance” out the complex part by adding conjugates and non-conjugates which then implies \( \phi_{\text{cm}} \approx 0 \). If we now look at eq. [22], we see that the relation between the similarity measure \( f(q, y(x)) \) and the amplification factor \( A_x \) is monotonical, which results in the desired behavior. Note that this doesn’t imply that the amplification factor of \( x \) is proportional to the value of \( f \). Only the ordering is preserved, i.e.

\[
\text{if } f(q, y(x_1)) < f(q, y(x_2)) \quad \text{then } A_{x_1} < A_{x_2}. \tag{31}
\]

An example application of Grover’s algorithm to a similarity oracle implementing the Dice coefficient can be found in fig. [2a], where the above described aspects are clearly visible.

### E. Contrast Functions

Since we are only interested in the ordering of the values of the similarity measure, we can improve some properties without changing information by applying a monotonically increasing function with signature

\[
\Lambda : [0, 1] \rightarrow [0, 1]. \tag{33}
\]

We call this a contrast function. In other words: For a given similarity measure \( f \) and a contrast function \( \Lambda \), instead of \( f \) we use \( \tilde{f} = \Lambda \circ f \) as similarity measure (the \( \circ \) denotes the composition). An example of a contrast function which improved the results in many cases can be found in fig. [2b]. Note that a large portion of the domain gets mapped to a value close to 0. This not only ensures the assumption

\[
\tilde{f}(q, y(x)) < 0.5 \quad \text{for most } x < 2^n \quad \text{(required for } \phi_{\text{cm}} \approx 0) \quad \text{but also yields } \tau_{\text{cm}} \approx 1 \quad \text{as in most cases } \phi(x) \approx 0 \quad \text{(compare eq. [17])}. \]

This in turn gives us a good amplification factor \( A_x \) for states that are supposed to be amplified but \( A_x \approx 0 \) for states that have only mediocre similarity (compare eq. [22]).

### IV. Quantum Logic Synthesis

As pointed out in the previous sections, an integral part of generating oracles is the logic synthesis. There is a multitude of approaches each having their benefits and drawbacks. In this section, we focus on the Reed-Muller Expansion and Gray Synthesis. Subsequently, a new synthesis method developed by us is introduced, which is significantly more efficient in terms of general gate count. Our approach is to relax the constraint of all outputs having the same phase. This does not interfere with the outcome of Grover’s algorithm as these phases cancel out during uncomputation. Finally, we derive and introduce another synthesis method, which addresses the pitfalls and requirements for scalable implementations of the belonging quantum circuits.

#### A. Reed-Muller Expansion

The very first and foremost approach to tackle the challenge of logic synthesis is the Reed-Muller Expansion. Even though it is by far the most efficient way to synthesize circuits for a quantum computer, it’s basic concepts will be helpful for further understanding of the proposed concepts. The belonging method is denoted as Positive Polarity Reed-Muller expansion synthesis [28] and is abbreviated as PPRM accordingly for the rest of the paper.

First, we note that due to their reversible architecture, quantum computers do not have direct access to the full range of tools as in traditional logic synthesis. For example, we can’t infer the input constellation of a classical AND gate by just looking at the output. However, reversibility is a fundamental requirement to any quantum operation as there are only reversible building blocks available to construct said operation. But there is a way to turn any non-reversible gate into a reversible one which is keeping the inputs in place and saving the result into a new qubit. Using an \( n \)-controlled \( X \) gate we can therefore compute a multi-\( AND \)-gate between \( n \)-qubits into a new qubit. Acting with another (multi-)controlled \( X \) gate on the same qubit, we can realize an \( XOR \) gate. Expressions of the type

\[
(x_0 \text{ AND } x_1 \text{ AND } x_2) \text{ XOR } (x_0 \text{ AND } x_1) \tag{34}
\]

are called XAG (XOR and \( AND \) Graphs) and can be described very conveniently by polynomials over the boolean algebra \( \mathbb{F}_2 \). The corresponding polynomial for eq. (34) would be

\[
p(x) = x_0 x_1 x_2 \oplus x_0 x_1 \tag{35}
\]

Using this, we can introduce a very basic approach to quantum logic synthesis: Given a single column truth table \( T \) depending
Fig. 2: (2a): Plot of the measurement probability of the index register after application of Grover’s algorithm to a similarity oracle using the Dice coefficient as similarity measure of an example database of 64 entries. (2b): The similarity measure (Dice coefficient) used in the oracle from fig. (2a). (2c): The same plot as fig. (2a) but the similarity function has been wrapped in a contrast function. (2d): The contrast function used in fig. (2c). The mathematical expression is 
\[ \Lambda(x) = (\exp(30(0.78 - x))) + 1 \]

TABLE I: Example decomposition into co-factors. Note that while \( T \) is depending on two boolean \( q \) variables, \( T_0 \) and \( T_1 \) are only depending on one variable.

| \( x_0 \) | \( x_1 \) | \( T \) | \( T_0 \) | \( T_1 \) |
|------|------|------|------|------|
| 0    | 0    | 0   | 0    | 0    |
| 0    | 1    | 1   | 1    | 1    |
| 1    | 0    | 1   | 1    | -    |
| 1    | 1    | 1   | 1    | 1    |

on \( n \) variables, its Reed-Muller expansion \( RM_T^n(x) \) is the polynomial which is recursively generated by the following equation

\[ RM_T^n(x) = x_0RM_{T_1}^{n-1}(x) \oplus (x_0 \oplus 1)RM_{T_0}^{n-1}(x) \]  

(36)

Here \( T_0, T_1 \) denote the co-factors of \( T \), i.e. the truth tables considering the entries of \( T \) where \( x_0 = 0 \) or \( x_0 = 1 \). This recursion cancels at \( n = 0 \) with \( RM_T^0(x) \) either equal to 0 or 1 depending on the value of \( T \). The resulting polynomial is unique for any given truth table [29]. Given such a polynomial, one can generate the corresponding circuit implementation for a truth table by setting up a multi-controlled X gate for every "summand" of the polynomial. While in principle sufficient, this method still has a lot of room for improvement as multi-controlled gates are computationally very expensive - [30] an \( n \)-controlled NOT gate requires \( (2n^2 - 2n + 1) \) CNOT gates. For this reason, the following sections investigate further methods towards a more resource efficient synthesis of boolean functions.

B. Gray Synthesis

A more efficient synthesis method can be achieved by taking advantage of the non-classical properties of a quantum computer. This method is called Gray Synthesis and a detailed description is given in [31]. The method works with three types of gates: CNOT, H and \( T_m \). While [31] also considers the possibility of directly synthesizing logic functions, these functions have to be \( \mathbb{F}_2 \)-linear, which is an impermissible restriction in our case of application. In this paper, the focus
on the possibility to synthesize a user-determined phase-shift for each computational basis state (now called “input state”). This in turn can then be used to efficiently synthesize a truth table \( T(x) \) by applying the method to the input register combined with the output qubit that is enclosed with \( H \)-gates. To illustrate how this works: consider that we synthesize a phase-shift of 0 for every input state that has a 0 in the output qubit and a phase-shift of \( \pi T(x) \) for every state that has a 1 in the output qubit. This leads to the following calculation towards the synthesis of the desired truth table:

\[
\begin{align*}
H_{\text{out}} U_{\text{gray}} H_{\text{out}} |x\rangle |0\rangle &= \frac{1}{\sqrt{2}} H_{\text{out}} U_{\text{gray}} |x\rangle (|0\rangle + |1\rangle) \\
&= \frac{1}{\sqrt{2}} H_{\text{out}} |x\rangle (|0\rangle + \exp(i\pi T(x)) |1\rangle) \\
&= \frac{1}{\sqrt{2}} H_{\text{out}} |x\rangle (|0\rangle + (-1)^T(x) |1\rangle) \\
&= |x\rangle |T(x)\rangle.
\end{align*}
\]

Here, the first ket \( |x\rangle \) represents the input register, the second ket \( |0\rangle \) the output qubit, and \( U_{\text{gray}} \) is the circuit which synthesizes the desired phases.

Since a good understanding of the phase synthesis method is a prerequisite to fully capture the power of phase tolerant synthesis, we will now go on to give a summary on how the phases are synthesized. A key concept in this context are parity operators, which basically are XOR expressions of different combinations of input variables e.g. \( x_0 \oplus x_2 \oplus x_3 \). Keep in mind, that we denote the XOR gates with the \( \oplus \) symbol, because additions over real numbers will occur now too. The value of a parity operator on a given input state can be “loaded” into a qubit by applying a sequence of CNOT gates (see fig. (3b) for an example). We can use the notion of parity networks to assign the desired phase to the input state by applying \( RZ \) gates onto the parity operators. Since \( RZ \) gates have the matrix representation \( \text{diag}(\exp(-\frac{i\theta}{2}), \exp(\frac{i\theta}{2})) \), the change of phase \( \Delta \phi \) after applying the gate \( RZ(\theta_p) \) to a qubit, which has the parity operator \( p \) loaded can be written as

\[
\Delta \phi = \begin{cases} 
-\frac{\theta}{2} & \text{if } p(x) = 0 \\
+\frac{\theta}{2} & \text{if } p(x) = 1 \\
\frac{1}{2}(-1)^p(x) \theta_p.
\end{cases}
\]  

Note that this is not a sum of \( \mathbb{F}_2 \) elements but of real numbers. We can therefore control what kind of phase each input state receives by carefully deciding on how to distribute the phase shifts \( \theta_p \). As each input state \( x \) can be uniquely identified by just looking at the set of parity operators, which return 1 when applied to \( x \), we can give each state a unique constellation of phase shifts by iterating over every possible parity operator. The next question is, how to determine the required \( \theta = (\theta_{x_0}, \theta_{x_1}, \theta_{x_0 \oplus x_1}, \ldots) \) phase shifts for a given sequence of desired overall phase shifts \( \phi = (\phi_0, \phi_1, \ldots) \)? In this regard, by successively writing down, which state receives which phase shift one can set up a system of linear equations. The resulting matrix is denoted as the \emph{parity matrix} \( D \). The corresponding system of equations therefore yields

\[
\phi = \frac{1}{2} D \theta.
\]  

This is achieved by ordering the rows according to the natural order of the input states (ie. 000, 001, 010, 011, 100, 101, 110, 111) and the columns according to an algorithmic solution of the Hamming TSP\(^9\) which visits all parity operators. The resulting matrix only depends on the number of input qubits. In the case of 3 input qubits, the phase applied on a given input state \( x = (x_0, x_1, \ldots x_n) \) after traversing the set of parity operators \( P \) can thus be summarized as

\[
\phi_x = \frac{1}{2} \sum_{p \in P} (-1)^p(x) \theta_p.
\]  

\(^9\)To see that this is true, consider two input states, where \( i \) is an index where the states differ. The parity operator \( x_i \) thus has differing values on the two states.

\(^{10}\)The Hamming TSP stands for a TSP (Travelling Salesman Problem) instance, where the Hamming distance is used as a distance measure between the involved entities/objects.
where

\[ \theta \phi = \frac{2 \Sigma H_n \phi}{N} \]

This can be interpreted as follows: \( \theta \) is the Hadamard-Walsh transform of \( \phi \) up to some permutation and factor. Fortunately, \( H_n \) doesn’t need to be explicitly calculated, since there is an algorithm called **Fast Hadamard Walsh Transformation** which performs the transformation in \( \mathcal{O}(\log(N)N) \) [27].

**C. Parity Operator Traversal**

As the space of parity operators is the dual space for the vector space \( \mathbb{F}_2^n \), it can be indexed by the natural numbers \( < 2^n \). Finding a parity operator traversal route therefore reduces to finding a solution to an integer programming [27] traveling salesman problem [33]. The restricting feature here is, that we need one CNOT gate per bit that is changed in a traversal step. A possible solution for this is the Gray-Codes [34]. The Gray-Code is a sequence of integers which traverse every single natural number \( < 2^n \) by only changing a single bit in every step. Even though it seems like this is precisely what is required, there is one drawback. As the Gray-Code traverses every parity operator, there is a considerable overhead, since only parity operators, which have a non-vanishing Hadamard-coefficient need to be traversed. This problem is addressed by a very simple heuristic solution. In order to ensure our traversal route ends where it started, we introduce a second salesman, which will meet the first after they both traversed the required integers. The resulting route will then be the route of the first salesman concatenated with the reversed route of the second salesman. Regarding the behavior of the individual salesmen, they always choose the closest parity operator, which has not been visited by either of them. We tried penalizing them for moving very far apart in order to reduce the reunification cost, which however didn’t lead to a significant reduction of the overall path length. Using this technique yields a (scale dependent) cut of about 10% in traversed parity operators, however it is significantly more expensive regarding the classical resources.

**D. Phase Tolerant Synthesis**

Even though Gray synthesis is already significantly cheaper in terms of CNOT gates than PPRM synthesis, there is an even bigger possible optimization with regard to the required quantum resources. During oracle application, we observe, that the label register always needs to be uncomputed after the winner state is tagged. This implies that we can be tolerant regarding the phases of the label variable as the tagging gate is not concerned with the involuntarily synthesized “garbage phases”. To be more explicit, the synthesis methods discussed so far applied to an index register in uniform superposition would result in the state

\[ \sum_{x=0}^{2^n-1} \chi_T(x) |x\rangle |T(x)\rangle. \]

However a state like

\[ \sum_{x=0}^{2^n-1} \exp(\mathcal{i} \chi_T(x)) |x\rangle |T(x)\rangle, \]

will be tagged in the correct way too and the “garbage-phases” \( \chi_T \) will be uncomputed, when the label register ism uncomputed. In order to understand how to synthesize with

\[ \text{The Hadamard TSP and the integer/binary programming TSP are closely related, given that within the Hamming TSP we have binary strings as the entities and the Hamming distance as the distance between those entities. In this regard, the integer programming constitutes the problem formulation as a combinatorial problem with an optimization function over integers/bitstrings.} \]
garbage-phases, we note that in this method of synthesis, the logical information is only captured in the phase differences of the 0 and 1 state of the output qubit. Following the principles applied on eq. (47), we arrive at:
\[
H(\exp(i\phi_0) |0\rangle + \exp(i\phi_1) |1\rangle) = \exp(i\phi_0)H(|0\rangle + \exp(i(\phi_1 - \phi_0)) |1\rangle) = \begin{cases} 
\exp(i\phi_0) |0\rangle & \text{if } \phi_1 - \phi_0 = 0 \\
\exp(i\phi_0) |1\rangle & \text{if } \phi_1 - \phi_0 = \pi.
\end{cases}
\]
(50)
This observation can now be used in combination with a view, consider the case that we are applying Gray synthesis to the parity network given in fig. (3b) visits every parity operator, which includes \( x_2 \) first and after that only operators which do not contain \( x_2 \). Furthermore directly after every parity operator which includes \( x_2 \) is visited, every circuit wire contains it’s very own parity operator, i.e. wire 0 contains the parity operator \( x_0 \), wire 1 contains \( x_1 \) and so on. Therefore, we can simply end the synthesis procedure at this point, because every bit of phase that is synthesized after, doesn’t differentiate between the \( |0\rangle \) and the \( |1\rangle \) state of the output qubit (which would be \( x_2 \) here), and therefore doesn’t contribute anything to the phase difference of the \( |0\rangle \) and the \( |1\rangle \) state.

To make this notion accessible from a more formal point of view, consider the case that we are applying Gray synthesis to the state of uniform superposition \( |s\rangle \):
\[
|s\rangle = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x\rangle.
\]
(51)

We factor out the output qubit
\[
|s\rangle = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} (|0\rangle + |1\rangle) |x\rangle.
\]
(52)
The “first step” in this view of Gray synthesis is synthesizing phases \( \phi_{(0,x)} \) and \( \phi_{(1,x)} \) on the output qubit
\[
U_{\text{gray}} \left| s \right\rangle = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} (\exp(i\phi_{(0,x)}) |0\rangle + \exp(i\phi_{(1,x)}) |1\rangle) |x\rangle \equiv |\psi\rangle.
\]
(53)
The second step would now be to synthesize a phase on the remaining qubits which could be seen as “correcting” the garbage phase \( \chi_x \). This however does not change the relative phase of the \( |0\rangle \) and \( |1\rangle \) state of the output qubit
\[
U_{\text{gray}} |\psi\rangle = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} \exp(-ix_x) (\exp(i\phi_{(0,x)}) |0\rangle + \exp(i\phi_{(1,x)}) |1\rangle) |x\rangle.
\]
(54)
The important point of phase tolerant synthesis is that the difference \( \phi_{(0,x)} - \phi_{(1,x)} \) determines the result of the logic output state:
\[
\phi_{(0,x)} - \phi_{(1,x)} = \begin{cases} 
0 & \text{if } T(x) = 0 \\
\pi & \text{if } T(x) = 1.
\end{cases}
\]
(55)
Note that while we in principle could determine the phases \( \chi_x, \phi_{(0,x)}, \phi_{(1,x)} \) from the user specified input phases \( \phi_0, \phi_1, \ldots, \phi_{2^n} \), it is neither necessary nor relevant. Just breaking the routine after the first step eq. (53) was performed, is sufficient.

V. CSE SYNTHESIS

In this section, we present further progress beyond state-of-the-art from our research activities - the implementation of quantum logic synthesis under the consideration of restrictions in a real world setup. Phase tolerant Gray synthesis may be very resource friendly to both classical and quantum resources, however scaling on real devices is still challenging: Taking a look at eq. (47) we see that, because the only values of the entries of \( \phi \) that can appear in the scenario of logic synthesis are \( \pm \frac{\pi}{2} \). Therefore the values of the entries of \( \phi \) are integer multiples of \( \pm \frac{\pi}{2} \). This implies that if we want to encode an array with \( N \) entries, we will need reliant \( \frac{2^n}{N} \) RZ gates are. As this quantity will be central in the upcoming discussion, we will refer to the T-order of a circuit by the minimal number \( m \in \mathbb{N} \) such that every phase gate can be expressed as an integer multiple of a \( \frac{2^n}{N} \) phase gate.

Another ineffectiveness we observe is the fact that there is no usage of redundancy for the synthesis of multiple truth table columns even though we know that we will synthesize about \( \mathcal{O}(\log(N)) \) columns. In the worst case we have the same column twice which means two syntheses procedures, although one synthesis + 1 CNOT gate would be sufficient. This handmade solution requires about half the resources, raising the question for an automatisation of this procedure.

Both of these problems can be tackled with by an approach based on calculating intermediate results and intelligently optimizing the next synthesis steps accordingly. Such an approach has already been proposed in [19]. Even though the authors could effectively demonstrate a reduction in the T-order, their technique still does not consider redundancies, since they focus on synthesizing truth tables with only a single column. Even though very heavy on the classical resources side and moderate on the qubit count, our approach (presented in this paper) has been shown to significantly reduce the T-order (see table (III)). The basic idea lies in automated algebraic simplifications. As we saw in section (IV-A), a single column truth-table can be represented by a \( \mathbb{F}_2 \)-polynomial. Multi-column truth tables can be therefore be interpreted as tuples of \( \mathbb{F}_2 \) polynomials \( f(x) = (f_1(x), \ldots, f_n(x)) \). The key step is now to apply the common sub-expression elimination (CSE) algorithm of the computer algebra system (CAS) library sympy to these polynomials. This will give a sequence of intermediate values which reduce the overall resources required for the evaluation of \( f \). For example, given the truth table

---

13According to [55] it is possible to implement RZ gates virtually without any error and duration, however this might not be the case for every physical qubit realization

14According to [56] a logical qubit of a circuit of order \( m \) in fault tolerant implementation (using the punctured Reed-Muller Code) requires (up to) \( 2^{m+2} - 1 \) physical qubits

15SymPy CAS: https://www.sympy.org, as of 03.08.2021
We now apply the CSE algorithm, which yields two intermediate values. Another point we would like to highlight is that the resulting X gate in PPRM synthesis

16Note that basic PPRM synthesis can also be supported by phase tolerant Gray synthesis by outsourcing the synthesis of the multi-controlled gates to the phase tolerant algorithm.

VI. BENCHMARKING

A. Comparison of different synthesis methods

In order to provide meaningful data about synthesis performance, we first elaborate on our benchmarking method. We compare our method for synthesizing Grover oracles to the Qiskit implementation and algorithms from the synthesis library tweedledum [18].

The evaluation task is to synthesize a database circuit $U_D$ eq. 4 corresponding to an array of data which is randomly generated. The lengths of these arrays are discretely being increased in increments of powers of two, resulting in a range from 4 to 1024 data entries. We choose the label size $k$ equal to the bit amount of the truth table i.e. $k = \log_2(N)$.

The metrics of interest are the average CNOT count and the average amount of arbitrary unitary rotations contained in the individual circuits. The latter will be denoted as $U$ count from now on and is obtained by decomposing all occurring sub expressions do not have to be synthesized with PPRM but an arbitrary synthesis method. In our implementation, we select the method of lowest CNOT count from a pool of methods. This pool contained the Gray synthesis and PPRM synthesis implemented in tweedledum, as well as phase tolerant synthesis and a custom version of the PPRM synthesis, where multicontrolled X gates are being outsourced to a phase tolerant algorithm. For each step of the array oracle synthesis, each method from the pool of synthesis options is tested individually and the optimal method is selected by means of the lowest CNOT count. It showed, that either phase tolerant Gray synthesis or the custom phase tolerant supported PPRM synthesis are optimal in many steps of the synthesis process.

While our implementation might not be directly feasible due to its high demand for classical resources, the general idea seems to yield improvements. We therefore leave the search of an advanced common subexpression elimination algorithm specifically tailored for $\mathbb{F}_2$-polynomials as an open research question. Regarding the overhead in quantum resources we note that it is always possible to resubstitute equations back into each other. As this increases the T-order for the expressions in question, it is not directly clear in which cases doing this is viable. Another open question therefore arises for an automatic procedure, which decides whether an intermediate value is worth calculating.
we consider the CNOT counts obtained by the corresponding synthesis methods. For a database with $n$ entries, the qubit count and classical resources are selected as to provide a reasonable understanding regarding the efficiency of the methods under test. Hence, we have kept the sample fairly small and have not followed the path of statistical testing with the goal to show any statistical significance. The measured gate counts are rounded correspondingly to obtain reasonable results. Furthermore, we additionally show the savings in terms of CNOT counts by using the discussed solutions to the Hamming TSP instead of Gray-code in the phase tolerant synthesis. Those savings are more apparent in the case of smaller data sizes and smooth out when considering larger data sets. This does not have an impact on the classical resources now depend on the modified truth tables, additionally an average qubit count is given as well.

As a comparison of the complexity of arbitrary synthesized Grover oracles, we next check our phase tolerant Gray synthesis method against the TruthTableOracle class implemented in Qiskit Aqua. A brief description of this method can be seen in the official documentation and the source code is publicly available in the corresponding GitHub repository.

B. Comparison with Qiskits TruthTableOracle

As a comparison of the complexity of arbitrary synthesized Grover oracles, we next check our phase tolerant Gray synthesis method against the TruthTableOracle class implemented in Qiskit Aqua. A brief description of this method can be seen in the official documentation and the source code is publicly available in the corresponding GitHub repository.

In the previous section, we addressed the implementation of scalable logic synthesis with the assumption that the number of qubits will likely increase more than gate precision and circuit depth for upcoming quantum hardware. The data above shows a linear increase in the T-order with increasing data size together with rapidly growing $T_m$ counts. With this in mind, we test a last synthesis method using the common sub-expression elimination technique (CSE) as described before in a similar test scenario. The obtained results are depicted in Table II. As the qubit resources now depend on the modified truth tables, additionally an average qubit count is given as well.

We can only see a noticeable decrease in CNOT counts and $U$ counts at a data size of 64, whereas the qubit resources are several times larger. Since the qubit resources now depend on the modified truth tables and hence underlie some degree of variation, we have given the average results. For smaller data sizes, the $U$ counts are roughly on the same level as in the non CSE-supported synthesis methods and the CNOT counts have slightly increased in most of the analyzed cases. The main motivation for implementing the CSE method was to decrease the T-order and $T_m$ counts, which has proven to be highly successful as the T-order was kept constantly at 2 and the $T_m$ counts were reduced by up to 33%. Indeed, we traded a decrease in gate complexity through fewer and considerably less fine phase gates at the cost of an increase in the qubit count and classical resources for potential benefits in real-word applications.

### TABLE II: Comparison of average gate counts between our phase tolerant (PT) synthesis and the Tweedledum implementation of Gray synthesis.

| Data size | Average CNOT count | Average $U$ count | Average $T_m$ count (T-order) | Qubits |
|-----------|--------------------|-------------------|-----------------------------|--------|
|           | PT (Gray-code)    | PT (HTSP)         | Gray                        | Difference |
|           | Average          | Average           | Average                      |           |
|           | PT               | Gray             | Difference                   |           |
| 4         | 8                | 6                | 6                            | 0.0%      |
| 8         | 24               | 19               | 33                           | 73.7%     |
| 16        | 64               | 59               | 103                          | 74.6%     |
| 32        | 160              | 148              | 280                          | 89.2%     |
| 64        | 384              | 365              | 709                          | 94.9%     |
| 128       | 896              | 861              | 1713                         | 99.0%     |
| 256       | 2048             | 1979             | 3967                         | 100.5%    |
| 512       | 4608             | 4509             | 9022                         | 100.1%    |
| 1024      | 10240            | 10116            | 20126                        | 99.0%     |

The duration and amount of the experiments (30 per datasize) are selected as to provide a reasonable understanding regarding the efficiency of the methods under test. Hence, we have kept the sample fairly small and have not followed the path of statistical testing with the goal to show any statistical significance. The measured gate counts are rounded correspondingly to obtain reasonable results. Furthermore, we additionally show the savings in terms of CNOT counts by using the discussed solutions to the Hamming TSP instead of Gray-code in the phase tolerant synthesis. Those savings are more apparent in the case of smaller data sizes and smooth out when considering larger data sets. This does not have an impact on the classical resources now depend on the modified truth tables, additionally an average qubit count is given as well.

We can only see a noticeable decrease in CNOT counts and $U$ counts at a data size of 64, whereas the qubit resources are several times larger. Since the qubit resources now depend on the modified truth tables and hence underlie some degree of variation, we have given the average results. For smaller data sizes, the $U$ counts are roughly on the same level as in the non CSE-supported synthesis methods and the CNOT counts have slightly increased in most of the analyzed cases. The main motivation for implementing the CSE method was to decrease the T-order and $T_m$ counts, which has proven to be highly successful as the T-order was kept constantly at 2 and the $T_m$ counts were reduced by up to 33%. Indeed, we traded a decrease in gate complexity through fewer and considerably less fine phase gates at the cost of an increase in the qubit count and classical resources for potential benefits in real-word applications.

\[
U(\theta, \phi, \lambda) = \begin{pmatrix}
\cos \frac{\theta}{2} & -e^{i\lambda} \sin \frac{\theta}{2} \\
e^{i\phi} \sin \frac{\theta}{2} & e^{i(\phi + \lambda)} \cos \frac{\theta}{2}
\end{pmatrix}.
\] (59)

The duration and amount of the experiments (30 per datasize) are selected as to provide a reasonable understanding regarding the efficiency of the methods under test. Hence, we have kept the sample fairly small and have not followed the path of statistical testing with the goal to show any statistical significance. The measured gate counts are rounded correspondingly to obtain reasonable results. Furthermore, we additionally show the savings in terms of CNOT counts by using the discussed solutions to the Hamming TSP instead of Gray-code in the phase tolerant synthesis. Those savings are more apparent in the case of smaller data sizes and smooth out when considering larger data sets. This does not have an impact on the $U$ counts and the decrease in quantum resources comes of course at the cost of an increase in classical resources. When comparing our results to Tweedledum’s Gray synthesis implementation, we consider the CNOT counts obtained by the corresponding implementation of phase tolerant synthesis with the results obtained through the Hamming TSP based approach.

As can be seen from Table II, the comparison of both synthesis methods shows that the phase tolerant synthesis performs twice as good in terms of CNOT count when compared to the Gray synthesis implemented in Tweedledum. This is an impressive result that is confirmed after comparing the $U$ counts for both methods. For a database with $2^n$ entries, our phase tolerant synthesis as well as the standard Gray synthesis scale linear with the database size, which is an important property with regard to real world use cases. In the context of such real world use cases, it is not enough to look only at the general $U$ counts. Another interesting metric that can be extracted from the elementary single qubit rotations is the number of $T_m$ gates together with the T-order mentioned above. For this, we search for the $U_1$ rotations from the circuit data and extract the belonging angular parameters. These parameters are then represented in the most efficient sequence of $T_m$ gates. Thus, we can count all $T_m$ gates and compute the T-order corresponding to the largest occurring $m$ for each circuit. The corresponding data for both synthesis methods is shown in Table III.

17This means that we are using more qubits and that the computations of the quantum logic synthesis takes longer on the classical computer.

18At the time of preparing the current paper, this class is implemented in Qiskit Aqua 0.9.1 but due to a migration mainly to Qiskit Terra this is likely to change in the future.
The Qiskit-synthesized circuits can be further optimized by first minimizing the input truth table via the Quine-McCluskey\(^{19}\) algorithm \[39\], in order to find all the essential prime implicants and then by finding the exact cover via employing the DLX\(^{20}\) algorithm \[39\]. This is exponentially heavy on classical resources and it turns out that even with those optimizations, there is a huge gap in terms of CNOT counts and \(U\) counts. The qubit count can be additionally addressed through a given selection of options concerning the implementation of multi-controlled Toffoli gates, which have a noticeable impact on the CNOT counts and \(U\) counts as well. Hence, even when applying those optimizations for the Qiskit methods, we still get the same benchmarking results for the comparison between the different approaches.

We used the same test scenario as for the comparison of the synthesis methods above, however due to memory limitations\(^{21}\) during the synthesis and optimization process, we have limited the range in data size to a maximum of 64 data entries. The mode for constructing multi-controlled Toffoli gates was first set to the “basic” setting. The results for the CNOT counts and \(U\) counts can be seen in Table \[IV\].

The difference in circuit complexity between the TruthTable-Oracle and our method is in significant favour of our method and even more so, when considering the necessary number of qubits for the oracle circuits. The “basic” option for multi-controlled Toffoli construction delivers the best scaling behavior in terms of gate counts while using \(3n - 2\) qubits for the tested data with \(2^n\) entries, as opposed to our method using only \(2n\) qubits. The option leading to the lowest number of qubits - which is also given by \(2n\) - is the "noancilla" one. This method leads to a much worse scaling behavior as can be seen in Table \[IV\] below.

We also want to mention, that there is another implementation in Qiskit’s PhaseOracle class, which takes a boolean expression or a SAT problem in DIMACS CNF format \[40\] and passes this to the PPRM synthesis method implemented in tweedledum. Thus, we don’t give a further comparison between our method and the PhaseOracle class as we have tested the different synthesis methods implemented in tweedledum and identified the Gray synthesis as the most suited method and competitor in the context of array oracle generation for Grover’s algorithm.

### VII. Summary

The current paper provides a first successful attempt for enabling the convenient utilization of Grover’s search algorithm capabilities over traditional function/procedure APIs (e.g. `int grovertint [ ] list_to_search_in, int value_to_search_for`). The motivation for this research is based on observations in our previous work \[12\], in which the issues of constructing oracles for Grover database searches was discussed from a user perspective. Indeed, the only way to make quantum computing commercially viable is to provide accessible interfaces for programmers and end users to integrate quantum algorithms in their services and applications.

With regard to Grover’s algorithm, such APIs require for the automatic generation of the black box quantum oracles, which contain the database and the element to search for.

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\(^{19}\)The Quine-McCluskey procedure is a method for minimizing logical/boolean formulas based on a standard representation and the identification and elimination of redundant terms.

\(^{20}\)The DLX algorithm is an approach to solving the set cover problem through the methodology of dancing links \[39\] and was initially developed by Donald Knuth.

\(^{21}\)We ran the benchmark with a system memory of 32GB.
in this database. In this context, our current paper provides a methodology for automatically generating such quantum oracles for arbitrary databases. The generation consists of two main parts: 1) Mapping the database entries to a circuit \( U_D \) generated by logic synthesis and 2) tagging the query hash to create the query oracle. The first step is realized through the utilization of beyond state-of-the-art synthesis functions, while the second step can be realized either with the traditional multi-controlled \( Z \) gates or with our newly introduced similarity tags. In this regard, one of the main contributions of this paper is given by the phase tolerant enhancement of synthesis procedures, allowing for resource cuts up to 50\% within the context of Grover quantum oracle generation. Furthermore, we present a new synthesis method respecting the requirements of scaling the synthesis procedure for real world physical backends.

To summarize: this paper outlines a clear procedure for making the potentials of the powerful quantum algorithm by Grover available to programmers and end users for integration in everyday ICT-systems (e.g. online shops, telecommunication management systems, database search engines, web analytic systems ...). The methodology proposed in this paper generates the belonging quantum oracles automatically, thereby utilizing and leading to innovative methods for quantum logic synthesis. The computational complexity of the methodology is in general higher than the one of classical search. However, our future research works aims at optimizing this complexity through different heuristics, machine learning techniques and optimizations on the proposed approach. By continuously achieving such gradual improvements, one can see a clear path to a full-scale introduction and application of quantum algorithms based on oracles in current development processes and system architectures.

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