

Symbolic Reasoning about Quantum Circuits in Coq

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Abstract A quantum circuit is a computational unit that transforms an input quantum state to an output state. A natural way to reason about its behavior is to compute explicitly the unitary matrix implemented by it. However, when the number of qubits increases, the matrix dimension grows exponentially and the computation becomes intractable.

In this paper, we propose a symbolic approach to reasoning about quantum circuits. It is based on a small set of laws involving some basic manipulations on vectors and matrices. This symbolic reasoning scales better than the explicit one and is well suited to be automated in Coq, as demonstrated with some typical examples.

Keywords Symbolic reasoning · Quantum circuits · Dirac notation · Coq.

1 Introduction

A quantum circuit is a natural model of quantum computation [20]. It is a computational unit that transforms an input quantum state to an output state. Once a quantum circuit is designed to implement an algorithm, it is indispensable to analyze the circuit and ensure that it indeed conforms to the requirements of the algorithm. When a large number of qubits are involved, manually reasoning about a circuit's behavior is tedious and error-prone. One way of reasoning about quantum circuits (semi-) automatically and reliably is to mechanize the reasoning procedure in an interactive theorem prover, such as the Coq proof assistant [7]. For example, Paykin et al. [22] verified a few quantum algorithms in Coq, using some semi-automated strategies to generate machine-checkable proofs.

Existing approaches have apparent drawbacks in both efficiency and human readability. Quantum states and operations are represented and computed using matrices explicitly, and their comparison is made in an element-wise way, thus is highly non-scalable with respect to qubit numbers. Furthermore, as the system dimension grows,

it is almost impossible for human beings to read the matrices printed by the theorem prover.

In this paper, we propose a symbolic approach to reasoning about the behavior of quantum circuits in Coq, which improves both efficiency of the reasoning procedure and readability of matrix representations. The main contributions of this paper include:

- A matrix representation in Coq using the Dirac notation [10], which is commonly used in quantum mechanics. Matrices are represented as combinations of $|0\rangle$, $|1\rangle$, scalars, and a set of basic operators such as tensor product and matrix multiplication. Here $|0\rangle$ and $|1\rangle$ are the Dirac notation for 2-dimensional column vectors $[1\ 0]^T$ and $[0\ 1]^T$, respectively. In this way, we have a concise representation for sparse matrices, commonly used in quantum computation.
- A tactic library for (semi-)automated symbolic reasoning about matrices. The tactics are based on a small set of inference laws (lemmas in Coq). The key idea is to reduce matrix multiplications in the form of $\langle i|j\rangle$ into scalars, and simplify the matrix representation by absorbing ones and eliminating zeros. In this way, our approach reasons matrices by (semi-)automated rewriting instead of actually computing matrices, and outperforms the computational approach of Paykin et al. [22], as shown in proving the functional correctness of some typical quantum algorithms in Section 6.

We illustrate the intuition of our tactics by the following simple example which computes the result of applying the Pauli-X gate to the $|0\rangle$ state. In an explicit matrix-vector multiplication form, it reads as follows:

$$X |0\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \times 1 + 1 \times 0 \\ 1 \times 1 + 0 \times 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle$$

and four multiplications are required for the whole computation. By contrast, if we use the Dirac notation for X and apply distribution and associativity laws, then

$$\begin{aligned} X |0\rangle &= (|0\rangle \langle 1| + |1\rangle \langle 0|) |0\rangle \\ &= |0\rangle \langle 1|0\rangle + |1\rangle \langle 0|0\rangle \\ &= 0 |0\rangle + 1 |1\rangle \\ &= |1\rangle. \end{aligned}$$

Note that the two terms $\langle 1|0\rangle$ and $\langle 0|0\rangle$ are reduced (symbolically) to 0 and 1, respectively. Consequently, no multiplication is required at all.

The rest of the paper is structured as follows. In Section 2 we recall some basic notation from linear algebra and quantum mechanics. In Section 3 we introduce a symbolic approach to reasoning about quantum circuits. In Section 4 we discuss some problems in representing matrices using Coq's type system and our solutions. In Section 5 we propose two notions of equivalence for quantum circuits. In Section 6 we conduct a few case studies. In Section 7 we discuss some related work. Finally, we conclude in Section 8.

The Coq scripts of our tactic library and the examples used in our case studies are available at the following link

<https://github.com/Vickyswj/DiracRepr>.

2 Preliminaries

For the convenience of the reader, we briefly recall some basic notions from linear algebra and quantum theory which are needed in this paper. For more details, we refer the reader to [20].

2.1 Basic linear algebra

A *Hilbert space* $\mathcal{H}$ is a complete vector space equipped with an inner product

$$\langle \cdot | \cdot \rangle : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$$

such that

1. $\langle \psi | \psi \rangle \geq 0$ for any $|\psi\rangle \in \mathcal{H}$, with equality if and only if $|\psi\rangle = 0$;
2. $\langle \phi | \psi \rangle = \langle \psi | \phi \rangle^*$;
3. $\langle \phi | \sum_i c_i |\psi_i\rangle = \sum_i c_i \langle \phi | \psi_i \rangle$,

where $\mathbb{C}$ is the set of complex numbers, and for each $c \in \mathbb{C}$, c^* stands for the complex conjugate of c . A vector $|\psi\rangle \in \mathcal{H}$ is *normalised* if its length $\sqrt{\langle \psi | \psi \rangle}$ is equal to 1. Two vectors $|\psi\rangle$ and $|\phi\rangle$ are *orthogonal* if $\langle \psi | \phi \rangle = 0$. An *orthonormal basis* of a Hilbert space $\mathcal{H}$ is a basis $\{|i\rangle\}$ where each $|i\rangle$ is normalised and any pair of them is orthogonal.

Let $\mathcal{L}(\mathcal{H})$ be a set of linear operators on $\mathcal{H}$. For any $A \in \mathcal{L}(\mathcal{H})$, A is *Hermitian* if $A^\dagger = A$ where $A^\dagger$ is the adjoint operator of A such that $\langle \psi | A^\dagger | \phi \rangle = \langle \phi | A | \psi \rangle^*$ for any $|\psi\rangle, |\phi\rangle \in \mathcal{H}$. The fundamental *spectral theorem* states that the set of all normalised eigenvectors of a Hermitian operator in $\mathcal{L}(\mathcal{H})$ constitutes an orthonormal basis for $\mathcal{H}$. That is, there exists a so-called spectral decomposition for each Hermitian A such that

$$A = \sum_i \lambda_i |i\rangle \langle i|$$

where the set $\{|i\rangle\}$ constitutes an orthonormal basis of $\mathcal{H}$, $\{\lambda_i\}$ denotes the set of eigenvalues of A , and $|i\rangle \langle i|$ is the projector to the corresponding eigenspace of λ_i . A linear operator $A \in \mathcal{L}(\mathcal{H})$ is *unitary* if $A^\dagger A = AA^\dagger = I_{\mathcal{H}}$ where $I_{\mathcal{H}}$ is the identity operator on $\mathcal{H}$. The *trace* of A is defined as $\text{tr}(A) = \sum_i \langle i | A | i \rangle$ for some given orthonormal basis $\{|i\rangle\}$ of $\mathcal{H}$. It is worth noting that the trace function is actually independent of the orthonormal basis selected. It is also easy to check that the trace function is linear and $\text{tr}(AB) = \text{tr}(BA)$ for any $A, B \in \mathcal{L}(\mathcal{H})$.

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces. Their *tensor product* $\mathcal{H}_1 \otimes \mathcal{H}_2$ is defined as a vector space consisting of linear combinations of the vectors $|\psi_1 \psi_2\rangle = |\psi_1\rangle |\psi_2\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$ with $|\psi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle \in \mathcal{H}_2$. Here the tensor product of two vectors is defined by a new vector such that

$$\left(\sum_i \lambda_i |\psi_i\rangle \right) \otimes \left(\sum_j \mu_j |\phi_j\rangle \right) = \sum_{i,j} \lambda_i \mu_j |\psi_i\rangle \otimes |\phi_j\rangle.$$

Then $\mathcal{H}_1 \otimes \mathcal{H}_2$ is also a Hilbert space where the inner product is defined in the following way: for any $|\psi_1\rangle, |\phi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle, |\phi_2\rangle \in \mathcal{H}_2$,

$$\langle \psi_1 \otimes \psi_2 | \phi_1 \otimes \phi_2 \rangle = \langle \psi_1 | \phi_1 \rangle_{\mathcal{H}_1} \langle \psi_2 | \phi_2 \rangle_{\mathcal{H}_2}$$

where $\langle \cdot | \cdot \rangle_{\mathcal{H}_i}$ is the inner product of $\mathcal{H}_i$. For any $A_1 \in \mathcal{L}(\mathcal{H}_1)$ and $A_2 \in \mathcal{L}(\mathcal{H}_2)$, $A_1 \otimes A_2$ is defined as a linear operator in $\mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ such that for each $|\psi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle \in \mathcal{H}_2$,

$$(A_1 \otimes A_2)|\psi_1\psi_2\rangle = A_1|\psi_1\rangle \otimes A_2|\psi_2\rangle.$$

2.2 Basic quantum mechanics

According to von Neumann's formalism of quantum mechanics [27], an isolated physical system is associated with a Hilbert space which is called the *state space* of the system. A *pure state* of a quantum system is a normalised vector in its state space, and a *mixed state* is represented by a density operator on the state space. Here a density operator ρ on Hilbert space $\mathcal{H}$ is a positive linear operator such that $\text{tr}(\rho) = 1$. Another equivalent representation of a density operator is an ensemble [20] of pure states. In particular, given an ensemble $\{(p_i, |\psi_i\rangle)\}$ where $p_i \geq 0$, $\sum_i p_i = 1$, and $|\psi_i\rangle$ are pure states, then $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ is a density operator. Conversely, each density operator can be generated by an ensemble of pure states in this way. Finally, a pure state can be regarded as a special mixed state.

The state space of a composite system (for example, a quantum system consisting of many qubits) is the tensor product of the state spaces of its components. Note that in general, the state of a composite system cannot be decomposed into a tensor product of the reduced states on its component systems. A well-known example is the 2-qubit state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle).$$

This kind of state is called an *entangled state*. Entanglement is an important feature of quantum mechanics which has no counterpart in the classical world, and is the key to many quantum information processing tasks.

Let $|\psi\rangle$ be a state vector and θ a real number. In quantum mechanics, the state $e^{i\theta}|\psi\rangle$ is considered to be equal to $|\psi\rangle$, up to the global phase factor $e^{i\theta}$. The reason is that from an observational point of view, global phases are irrelevant to the observed properties of the physical system under consideration and can thus be ignored as far as quantum states are concerned [20].

The evolution of a closed quantum system is described by a unitary operator on its state space. If the states of the system at times t_1 and t_2 are $|\psi_1\rangle$ and $|\psi_2\rangle$, respectively, then $|\psi_2\rangle = U|\psi_1\rangle$ for some unitary operator U which depends only on t_1 and t_2 . A convenient way to understand unitary operators is in terms of their matrix representations. In fact, the unitary operator and matrix viewpoints turn out to be completely equivalent. An m by n complex unitary matrix U with entries U_{ij} can be considered as a unitary operator sending vectors in the vector space $\mathbb{C}^n$ to the vector space $\mathbb{C}^m$, under matrix multiplication of the matrix U by a vector in $\mathbb{C}^n$.

We often denote a single qubit as a vector $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ parameterized by two complex numbers satisfying the condition $|\alpha|^2 + |\beta|^2 = 1$. A unitary operator for a qubit is then described by a 2×2 unitary matrix. Quantum circuits are a popular model for quantum computation, where quantum gates usually stand for basic unitary operators whose mathematical meanings are given by appropriate unitary matrices. Some commonly used quantum gates to appear in the current work include the 1-qubit Hadamard gate H , the Pauli gates I_2, X, Y, Z , the controlled-NOT gate CX performed on two qubits, and the 3-qubit Toffoli gate. Their matrix representations are given below:

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad TOF = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

For example, in Figure 1 we display a circuit that can generate the 3-qubit Greenberger–Horne–Zeilinger state (GHZ state) [13], which is $\frac{|000\rangle + |111\rangle}{\sqrt{2}}$. In the circuit, a Hadamard gate is applied on the first qubit, then two controlled-NOT gates are used, with the first qubit controlling the second, which in turn controls the third.

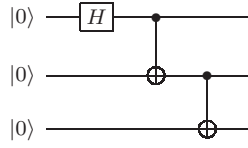


Fig. 1 A circuit for creating the 3-qubit GHZ state

A quantum *measurement* is described by a collection $\{M_m\}$ of measurement operators, where the indices m refer to the measurement outcomes. It is required that the measurement operators satisfy the completeness equation $\sum_m M_m^\dagger M_m = I_{\mathcal{H}}$. If the state of a quantum system is $|\psi\rangle$ immediately before the measurement, then the probability that result m occurs is given by

$$p(m) = \langle \psi | M_m^\dagger M_m | \psi \rangle,$$

and the state of the system after the measurement is $\frac{M_m |\psi\rangle}{\sqrt{p(m)}}$. If the states of the system at times t_1 and t_2 are mixed, say ρ_1 and ρ_2 , respectively, then $\rho_2 = U \rho_1 U^\dagger$ after the unitary operation U is applied on the system. For the same measurement $\{M_m\}$ as

Scalars:	$\mathbb{C}$
Basic vectors:	$ 0\rangle, 1\rangle$
Operators:	$\cdot, \times, +, \otimes, \dagger$
Laws:	L1 $\langle 0 0\rangle = \langle 1 1\rangle = 1, \langle 0 1\rangle = \langle 1 0\rangle = 0$ L2 Associativity of $\cdot, \times, +, \otimes$ L3 $0 \cdot A_{m \times n} = \mathbf{0}_{m \times n}, c \cdot \mathbf{0} = \mathbf{0}, 1 \cdot A = A$ L4 $c \cdot (A + B) = c \cdot A + c \cdot B$ L5 $c \cdot (A \times B) = (c \cdot A) \times B = A \times (c \cdot B)$ L6 $c \cdot (A \otimes B) = (c \cdot A) \otimes B = A \otimes (c \cdot B)$ L7 $\mathbf{0}_{m \times n} \times A_{n \times p} = \mathbf{0}_{m \times p} = A_{m \times n} \times \mathbf{0}_{n \times p}$ L8 $I_m \times A_{m \times n} = A_{m \times n} = A_{m \times n} \times I_n, I_m \otimes I_n = I_{mn}$ L9 $\mathbf{0} + A = A = A + \mathbf{0}$ L10 $\mathbf{0}_{m \times n} \otimes A_{p \times q} = \mathbf{0}_{mp \times nq} = A_{p \times q} \otimes \mathbf{0}_{m \times n}$ L11 $(A + B) \times C = A \times C + B \times C, C \times (A + B) = C \times A + C \times B$ L12 $(A + B) \otimes C = A \otimes C + B \otimes C, C \otimes (A + B) = C \otimes A + C \otimes B$ L13 $(A \otimes B) \times (C \otimes D) = (A \times C) \otimes (B \times D)$ L14 $(c \cdot A)^\dagger = c^* \cdot A^\dagger, (A \times B)^\dagger = B^\dagger \times A^\dagger$ L15 $(A + B)^\dagger = A^\dagger + B^\dagger, (A \otimes B)^\dagger = A^\dagger \otimes B^\dagger$ L16 $(A^\dagger)^\dagger = A$

Table 1 Terms and laws

above, if the system is in the mixed state ρ , then the probability that measurement result m occurs is given by

$$p(m) = \text{tr}(M_m^\dagger M_m \rho),$$

and the state of the post-measurement system is $\frac{M_m \rho M_m^\dagger}{p(m)}$ provided that $p(m) > 0$.

3 Symbolic reasoning

In this section, we first introduce the terms that will appear in our symbolic reasoning and some laws that are useful for reducing terms. Then we present in detail the strategies that we developed to simplify circuits.

3.1 Terms and laws

Our symbolic reasoning is based on terms constructed from scalars and basic vectors using some constructors:

- Scalars are complex numbers. We write $\mathbb{C}$ for the set of complex numbers. Our formal treatment of complex numbers is based on the definitions and lemmas in the library of Paykin et al. [22] for complex numbers, which, in turn, is adapted from the Coquelicot library [5].
- Basic vectors are the base states of a qubit, i.e., $|0\rangle$ and $|1\rangle$ in the Dirac notation. Mathematically, $|0\rangle$ stands for the vector $[1 \ 0]^T$ and $|1\rangle$ for $[0 \ 1]^T$.
- Constructors include the scalar product $\cdot$, matrix product $\times$, matrix addition $+$, tensor product $\otimes$, and the conjugate transpose $A^\dagger$ of a matrix A .

In Dirac notations, $\langle 0|$ represents the dual of $|0\rangle$, i.e. $|0\rangle^\dagger$; similarly for $\langle 1|$. The term $\langle j| \times |k\rangle$ is abbreviated into $\langle j|k\rangle$, for any $j, k \in \{0, 1\}$. This notation introduces an intuitive explanation of quantum operation. For example, the effect of the X operator is to map $|0\rangle$ into $|1\rangle$ and $|1\rangle$ into $|0\rangle$. Thus we define X in Coq as $|0\rangle\langle 1| + |1\rangle\langle 0|$, instead of $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. Then it is obvious that $X|0\rangle = |1\rangle\langle 0|0\rangle + |0\rangle\langle 1|0\rangle = |1\rangle$ and similarly for $X|1\rangle$.

Some commonly used vectors and gates can be derived from the basic terms. For example, we define the vectors $|+\rangle$ and $|-\rangle$ as follows.

$$|+\rangle = \frac{1}{\sqrt{2}} \cdot |0\rangle + \frac{1}{\sqrt{2}} \cdot |1\rangle \quad |-\rangle = \frac{1}{\sqrt{2}} \cdot |0\rangle + \left(-\frac{1}{\sqrt{2}}\right) \cdot |1\rangle$$

We also define four simple matrices $B_0, \dots, B_3$.

$$B_0 = |0\rangle \times \langle 0| \quad B_1 = |0\rangle \times \langle 1| \quad B_2 = |1\rangle \times \langle 0| \quad B_3 = |1\rangle \times \langle 1| \quad (1)$$

The Hadamard matrix H is a combination of the four matrices above.

$$H = \frac{1}{\sqrt{2}} \cdot B_0 + \frac{1}{\sqrt{2}} \cdot B_1 + \frac{1}{\sqrt{2}} \cdot B_2 + \left(-\frac{1}{\sqrt{2}}\right) \cdot B_3$$

Similarly, the Pauli-X gate and the controlled-NOT gate CX are given as follows.

$$X = B_1 + B_2 \quad CX = B_0 \otimes I_2 + B_3 \otimes X \quad (2)$$

Notice that tensor products of matrices from $\{B_j : j = 0, 1, 2, 3\}$ constitute an orthonormal basis for the space of all matrices of dimension 2^n , for all $n \geq 1$. Thus any matrix that appeared in the computation of a quantum circuit can be represented as a term.

Suppose the state of a quantum system is represented by a vector. The central idea of our symbolic reasoning is to employ the laws in Table 1 to rewrite terms, trying to put together the basic vectors and simplify them using the laws in L1. Technically, we design a series of strategies for that purpose.

3.2 Soundness of the laws

Let $T_1 = T_2$ be a law that relates two terms T_1 and T_2 . We say that the law is sound if both terms can be reduced to exactly the same matrix, after their metavariables (e.g., $|0\rangle$) are instantiated by concrete matrices (e.g., $[1 \ 0]^T$). We define a strategy called `orthogonal_reduce` to verify that the laws in L1 are sound. In this case, we explicitly represent $|0\rangle$ and $|1\rangle$ as matrices. Both of them are 2×1 matrices, so we can use matrix multiplication to prove that the corresponding elements in the matrices on both sides of the equation are the same. For example, the law $\langle 0|0\rangle = 1$ is actually shown via $[1 \ 0] \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 1$. We add the laws in L1 to the set named `S_db`. The laws in L2-16 are also proved through explicit matrix representation.

Theorem 1 *All the laws in Table 1 are sound.*

We have given a formal soundness proof in Coq for each of the laws in Table 1. We collect the soundness properties in a library that contains many useful properties about matrices.

3.3 Strategy for basic matrices

The four matrices $B_0, \dots, B_3$ defined in (1) are the basic building blocks to represent 2×2 matrices, and are intensively used in our symbolic reasoning. We design a strategy called `base_reduce` to prove some equations about them acting on the base states $|0\rangle$ and $|1\rangle$. For example, let us consider the equation $B_0 \times |0\rangle = |0\rangle$. We first represent B_0 by $|0\rangle \times \langle 0|$, then use the associativity of matrix multiplication to form the subterm $\langle 0| \times |0\rangle$. Now we can use the proved laws in **L1** to rewrite $\langle 0| \times |0\rangle$ into 1. The last step is to deal with scalar multiplications. We add these equations to the set named `B_db`.

3.4 Strategy for the Pauli and Hadamard gates

The Pauli and Hadamard gates are probably the most widely used single-qubit gates. We introduce a strategy called `gate_reduce` to prove some equations about the matrices I_2, X, Y, Z, H acting on base states. For example, consider the equation $X \times |0\rangle = |1\rangle$. We first expand X into $B_1 + B_2$. In order to prove the equation $(B_1 + B_2) \times |0\rangle = |1\rangle$, we use the distributivity of matrix multiplication over addition to rewrite the left hand side of the equation into the sum of $B_1 \times |0\rangle$ and $B_2 \times |0\rangle$. Then we employ the proved laws in `B_db` to rewrite them. Eventually, we deal with scalar multiplications and cancel zero matrices. We add these equations to the set named `G_db`.

Furthermore, we add into `S_db` and `G_db` some commonly used equations about the matrices $B_0, \dots, B_3$ and I_2, X, Y, Z, H acting on states $|+\rangle$ and $|-\rangle$. For example, we have $H|+\rangle = |0\rangle$ and $H|-\rangle = |1\rangle$, etc.

3.5 Strategy for circuits

We propose a strategy called `operate_reduce` that puts together all the results above to reason about circuits applied to input states represented in the vector form. We will have a close look at the strategy by using an example. Let us revisit the 3-qubit GHZ state. The state can be generated by applying the circuit in Figure 1 to the initial state $|0\rangle \otimes |0\rangle \otimes |0\rangle$. We would like to verify that the output state is indeed what we expect by establishing the following equation.

$$\begin{aligned} & (I_2 \otimes CX) \times (CX \otimes I_2) \times (H \otimes I_2 \otimes I_2) \times (|0\rangle \otimes |0\rangle \otimes |0\rangle) \\ &= \frac{1}{\sqrt{2}} \cdot (|0\rangle \otimes |0\rangle \otimes |0\rangle) + \frac{1}{\sqrt{2}} \cdot (|1\rangle \otimes |1\rangle \otimes |1\rangle) \end{aligned} \quad (3)$$

We first use the right associativity of tensor product and matrix multiplication to change the expression on the left hand side in (3) into

$$(I_2 \otimes CX) \times ((CX \otimes I_2) \times ((H \otimes (I_2 \otimes I_2)) \times (|0\rangle \otimes (|0\rangle \otimes |0\rangle)))) \quad (4)$$

Then we calculate the inner layer matrix multiplications in sequence. We first calculate $(H \otimes (I_2 \otimes I_2)) \times (|0\rangle \otimes (|0\rangle \otimes |0\rangle))$. We exploit the law in **L13** to change a matrix product of tensored terms into a tensor product of matrix multiplications. Then we employ the laws established in `G_db` and `B_db` to rewrite terms. This transformation is as follows:

$$\begin{aligned} & (H \otimes (I_2 \otimes I_2)) \times (|0\rangle \otimes (|0\rangle \otimes |0\rangle)) \\ &= (H \times |0\rangle) \otimes ((I_2 \times |0\rangle) \otimes (I_2 \times |0\rangle)) \\ &= |+\rangle \otimes (|0\rangle \otimes |0\rangle) \end{aligned}$$

Correspondingly, the expression in (4) turns into

$$(I_2 \otimes CX) \times ((CX \otimes I_2) \times (|+\rangle \otimes (|0\rangle \otimes |0\rangle))).$$

The inner layer matrix multiplication to be calculated next is the following expression: $(CX \otimes I_2) \times (|+\rangle \otimes (|0\rangle \otimes |0\rangle))$. Different from the calculation of the previous layer, we have to expand the multiple-qubit quantum gates first. Here is the CX gate. After this step, we use the distributivity of tensor product and matrix product over addition to rewriting it. We also exploit the law in **L13** as well as the equations in `G_db` and `B_db`. So the inference goes as follows:

$$\begin{aligned} & (CX \otimes I_2) \times (|+\rangle \otimes (|0\rangle \otimes |0\rangle)) \\ &= ((B_0 \otimes I_2 + B_3 \otimes X) \otimes I_2) \times (|+\rangle \otimes (|0\rangle \otimes |0\rangle)) \\ &= ((B_0 \otimes I_2 \otimes I_2 + B_3 \otimes X \otimes I_2) \times (|+\rangle \otimes (|0\rangle \otimes |0\rangle))) \\ &= ((B_0 \otimes (I_2 \otimes I_2)) \times (|+\rangle \otimes (|0\rangle \otimes |0\rangle))) + ((B_3 \otimes (X \otimes I_2)) \times (|+\rangle \otimes (|0\rangle \otimes |0\rangle))) \\ &= ((B_0 \times |+\rangle) \otimes (I_2 \times |0\rangle) \otimes (I_2 \times |0\rangle)) + ((B_3 \times |+\rangle) \otimes (X \times |0\rangle) \otimes (I_2 \times |0\rangle)) \\ &= \frac{1}{\sqrt{2}} \cdot (|0\rangle \otimes (|0\rangle \otimes |0\rangle)) + \frac{1}{\sqrt{2}} \cdot (|1\rangle \otimes (|1\rangle \otimes |0\rangle)) \end{aligned}$$

Other laws such as the associativity and distributivity of scalar multiplication may also be used in the inference, though they are not demonstrated in this example.

We continue in this way until no more matrix multiplication is possible. It is worth noting that if there is a zero matrix in the summands of a certain layer of calculation, it can be eliminated immediately, without being carried into the next layer of calculation. Finally, we simplify the expressions about complex numbers.

The above steps appear a bit complex, but they can be fully automated in Coq, fortunately. The script for implementing the strategy `operate_reduce` is as follows:

```
Ltac inner_reduce :=
  unfold_operator;
  kron_plus_distr;
  isolate_scale;
  assoc_right;
  try repeat rewrite Mmult_plus_distr_l;
  try repeat rewrite Mmult_plus_distr_r;
  repeat rewrite <- Mscale_kron_dist_r;
  repeat mult_kron;
  repeat rewrite Mscale_mult_dist_r;
  repeat (autorewrite with G_db);
  repeat cancel_0;
  repeat rewrite Mscale_kron_dist_r;
  repeat rewrite <- Mmult_plus_distr_l.
```

```

Ltac operate_reduce :=
  assoc_right;
  repeat inner_reduce;
  reduce_scale;
  unified_base.

```

In summary, using the strategy `operate_reduce`, we can formally prove the equation in (3) automatically.

As we can see, our general framework is to formalize circuits symbolically as terms, and simplify terms involving matrices by (semi-)automated term rewriting instead of actually computing the matrices. The strategies in Sections 3.2-3.5 are designed with the common goal: to reduce matrix multiplications in the form of $\langle i|j \rangle$ into scalars, and simplify the matrix representation by absorbing ones and eliminating zeros. This symbolic approach of reasoning about circuits turns out to be effective; see Section 6.7 for more detailed discussion.

3.6 Density matrices as quantum states

Although it is very intuitive to represent pure quantum states by vectors, there is an inconvenience. In quantum mechanics, the global phase of a qubit is often ignored. For example, we would not distinguish $|\psi\rangle$ from $e^{i\theta}|\psi\rangle$ for any θ . However, when written in vector form, $|\psi\rangle$ and $e^{i\theta}|\psi\rangle$ may be different because of the coefficient $e^{i\theta}$ present in the latter but not in the former. Therefore, we use the symbol $\approx$ to denote such an equivalence, i.e. $e^{i\theta}|\psi\rangle \approx |\psi\rangle$. As a matter of fact, we can be more general and define an observational equivalence for matrices, as given below.

```

Definition obs_equiv {m n : nat} (A B : Matrix m n) : Prop :=
  exists c : C, Cmod c = R1 /\ c .* A = B.

Infix "≈" := obs_equiv.

```

In the above definition, the condition $\text{Cmod } c = R1$ means that the norm of the complex number c is one and $c .* A = B$ says that the matrix A is equal to B after a scalar product with the coefficient c . See Section 6.1 for more concrete examples that use the relation $\approx$.

Note that if quantum states are represented by density matrices, we have

$$(e^{i\theta}|\psi\rangle)(e^{i\theta}|\psi\rangle)^\dagger = (e^{i\theta}|\psi\rangle)(e^{-i\theta}\langle\psi|) = |\psi\rangle\langle\psi|.$$

Therefore, the discrepancy entailed by the global phase disappears: the two vectors $e^{i\theta}|\psi\rangle$ and $|\psi\rangle$ correspond to the same density matrix $|\psi\rangle\langle\psi|$. Representing states by density matrices can thus omit unnecessary details and in some cases simplify our reasoning. This is a small but useful trick in formal verification of quantum circuits, which does not seem to have been exploited in the literature. In Sections 6.2 and 6.3, we give two examples where the input and output quantum states of the circuits are given in terms of density matrices.

If the state of a quantum system is represented by a density matrix, the reasoning strategies discussed above can still be used. For instance, suppose a system is in the initial state given by density matrix ρ . After the execution of a quantum circuit implementing some unitary transformation U , the system changes into the new

state $\rho' = U\rho U^\dagger$. Let $\rho = \sum_j \lambda_j |j\rangle\langle j|$ be its spectral decomposition, where λ_j are eigenvalues of ρ and the vectors $|j\rangle$ the corresponding eigenvectors. It follows that

$$\rho' = U\left(\sum_j \lambda_j |j\rangle\langle j|\right)U^\dagger = \sum_j \lambda_j U|j\rangle(U|j\rangle)^\dagger. \quad (5)$$

Therefore, we can first simplify $U|j\rangle$ into a vector, take its dual and then obtain ρ' easily. Our approach to symbolic reasoning also applies in this setting.

We define two functions `density` and `super` in advance. The former converts states in the vector form into corresponding states in the density matrix form. The latter formalizes the transformation process between states in the density matrix form.

```
Definition density {n} (phi : Matrix n 1) : Matrix n n := phi × phi†.
Definition super {m n} (M : Matrix m n) : Matrix n n -> Matrix m m :=
  fun rho => M × rho × M†.
```

We introduce the simplification strategy called `super_reduce` for states in the density matrix form.

```
Ltac super_reduce:=
  unfold super, density;
  (* Expand super and density *)
  match goal with
  (* Match the pattern of target
   with U × phi × phi† × U† *)
  ||-context [ (?A × ?B) × ?A† ] =>
    match B with
    | (?C × ?C†) =>
      transitivity ((A × C) × (C† × A†))
  (* Cast uniform types *)
  end
end;
[repeat rewrite <- Mmult_assoc; reflexivity|..];
rewrite <- Mmult_adjoint;
(* Extract adjoint *)
let Hs := fresh "Hs" in
  match goal with
  ||-context [ (?A × ?B) × ?C† ] =>
    match C with
    | ?A × ?B => assert (A × B = D) as Hs
    end
  end;
end;
(* Use operate_reduce to prove vector states
and rewrite it in density matrix form *)
[try reflexivity; try operate_reduce |
repeat rewrite Hs; reflexivity].
```

In the above strategy, we first expand the `density` and `super` functions in the target. Next, we match the pattern of the target to see whether it is in the form $U \times |\psi\rangle \times \langle\psi| \times U^\dagger$ (the middle of the equation in (5)) and cast uniform types, for the reasons to be discussed in Section 4. Then we exploit the law in **L14** to extract adjoint of multiplication terms so the target becomes $U \times |\psi\rangle \times (U \times |\psi\rangle)^\dagger$ as in the right hand side of the equation in (5). Finally, we use the strategy `operate_reduce` to conduct the proof for states in vector form and rewrite it back in density matrix form. Note that we omit dimensions for presentation purpose, in practice we need to specify these implicit arguments.

3.7 Mixed state

As mentioned in Section 2.2, the mixed state $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ is an ensemble $\{(p_i, |\psi_i\rangle)\}$ of pure states $|\psi_i\rangle$, where p_i is the probability of the pure state $|\psi_i\rangle$ with $\sum_i p_i = 1$. In Coq, we use a list of pairs of real numbers and density operators to define mixed states.

```
Definition Pure n := (R * (Matrix n n)).
Definition Mix n := (list (Pure n)).
```

Recall that the application of unitary operator U on the mixed state ρ is in the following form:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \xrightarrow{U} U\rho U^\dagger = \sum_i p_i U|\psi_i\rangle\langle\psi_i|U^\dagger. \quad (6)$$

We formalize (6) in Coq as follows.

```
Fixpoint UnitMix {n} (A : Matrix n n) (m : Mix n) : Mix n :=
  match m with
  | [] => []
  | a :: b => (match a with
    | (x , y) => (x , super A y)
    end) :: (UnitMix A b)
  end.
```

After a measurement, results can be expressed with mixed states, as introduced in Section 2.2. For simplicity, we use projection measurements, so for each measurement operator M_m we have $M_m^\dagger M_m = M_m$. We first define the measurement operators of any dimension as follows, where the two parameters n and k stand for the space dimension and the position of an active qubit.

```
Definition Mea0 (n k : N) := (I (2^k) ⊗ |0⟩⟨0| ⊗ I (2^(n-k))).
Definition Mea1 (n k : N) := (I (2^k) ⊗ |1⟩⟨1| ⊗ I (2^(n-k))).
Definition Mea (n k : N) := Mea0 n k .+ Mea1 n k.
```

Then we formalize measurements on the mixed state in Coq as follows. Note that a pure state ρ can be regarded as a special mixed state $[(1, \rho)]$.

```
Fixpoint MeaMix {n} (m k : N) (l : Mix n) : Mix n :=
  match l with
  | [] => []
  | a :: b => match a with
    | (x , y) =>
      [((x * (trace((Mea0 m k) × y))), / (trace ((Mea0 m k) × y)) * super(Mea0 m k) y);
      ((x * (trace((Mea1 m k) × y))), / (trace ((Mea1 m k) × y)) * super(Mea1 m k) y)]
    end ++ (MeaMix m k b)
  end.
```

4 Problems from Coq's type system and our solution

In principle, the Dirac notation is fully symbolic, i.e. no matter how we formalize it, the relevant laws and their proofs should remain unchanged. However, it turns out that different design choices in formalization do make a difference.

In Coq, there are three kinds of equivalence between expressions: (1) syntactic equality, (2) $\beta\eta$ -reduction, and (3) provable equivalence. Specifically, a and b are syntactically equal if they are the same Coq expression. If a and b are not the same Coq expression, it is still possible for them to be $\beta\eta$ -reducible to the same term.¹ In that case, a and b can be used interchangeably in Coq, i.e. if $P(a)$ is a well-typed proposition, then so is $P(b)$, and every proof of $P(a)$ is also a proof of $P(b)$. Moreover, if $T(a)$ is a legal Coq type, then so is $T(b)$, and every element of $T(a)$ is also an element of $T(b)$. If a and b are not $\beta\eta$ -equivalent, it is still possible for them to be provably equivalent. For example, the two expressions $(1 + n)$ and $(n + 1)$ are not $\beta\eta$ -equivalent in Coq for a general variable n but they are provably equal to each other. In other words, a proof of $P(1 + n)$ is NOT necessarily a proof of $P(n + 1)$ although we can always derive a proof of $P(n + 1)$ from a proof of $P(1 + n)$. Moreover, if $T(1 + n)$ is a type, its element is not necessarily an element of type $T(n + 1)$.

Matrix definition. When it comes to matrix definitions. The first problem is to decide whether $2^{n+1} \times 2^{n+1}$ matrices and $2^{1+n} \times 2^{1+n}$ matrices are $\beta\eta$ -equivalent Coq types or not. Intuitively, since these two kinds of matrices are mathematically the same object, they should be used interchangeably. However, $(1 + n)$ and $(n + 1)$ are not $\beta\eta$ -equivalent. Thus, we have to carefully define the Coq type of matrices so that those two kinds above are $\beta\eta$ -equivalent types. We follow the approach used in QWIRE [22] and define matrices (no matter how large they are) to be functions from two natural numbers (row and column numbers) to complex numbers:

Definition Matrix (m n : N) := nat -> nat -> C.

But still, there are two problems that need to be solved.

The elements outside the range of a matrix. Intuitively, this definition above says that, given a pair of numbers (k, l) , if $k < m$ and $l < n$ then the entry of the matrix in the k -th row and l -th column is a complex number determined by the mapping. However, if $k \geq m$ or $l \geq n$ then the number determined by the mapping does not correspond to a valid entry in the matrix. In manual proofs we can simply ignore those elements.

$$A_{m \times n} = \begin{bmatrix} a_{00} & \cdots & a_{0(n-1)} & 0 \cdots \\ \vdots & & \vdots & \vdots \\ a_{(m-1)0} & \cdots & a_{(m-1)(n-1)} & 0 \cdots \\ 0 & \cdots & 0 & 0 \cdots \\ \vdots & & \vdots & \vdots \end{bmatrix} \quad (7)$$

¹ Coq is an extension of the lambda calculus. The $\beta\eta$ -reduction here means the $\beta\eta$ -reduction of the underlying lambda calculus.

$$B_{m \times n} = \begin{bmatrix} a_{00} & \cdots & a_{0(n-1)} & 1 & \cdots \\ \vdots & & \vdots & \vdots & \\ a_{(m-1)0} & \cdots & a_{(m-1)(n-1)} & 1 & \cdots \\ 1 & \cdots & 1 & 1 & \cdots \\ \vdots & & \vdots & \vdots & \end{bmatrix} \quad (8)$$

For example, in (7) and (8) we give two mappings in the form of two infinite-dimensional matrices $A_{m \times n}$ and $B_{m \times n}$, respectively. Basically, $A_{m \times n}$ is the same as $B_{m \times n}$ except that all the elements with rows (resp. columns) greater than or equal to m (resp. n) are 0 in the former but they are 1 in the latter. In computer-aided proofs, we could choose to only reason about *well-formed* matrices whose “outside elements” are all zero like $A_{m \times n}$ above. Rand et al. [22] heavily used this approach in their work. They would consider $A_{m \times n}$ well-formed but $B_{m \times n}$ ill-formed. However, only reasoning about well-formed matrices imposes a heavy burden for formal proofs because the condition of well-formedness needs to be checked each time we manipulate matrices. In our development, we choose a relaxed notion of matrix equivalence, which also appeared in [22], so that two matrices are deemed to be equivalent if they are equal component-wisely within the desired dimensions, and outside the dimensions the corresponding elements can be different. For instance, this notion of equivalence allows us to identify $A_{m \times n}$ with $B_{m \times n}$. With a slight abuse of notation, we still use the symbol $=$ to denote the newly defined matrix equivalence², and prove its elementary properties about scale product, matrix product, matrix addition, tensor product and conjugate transpose. Reasoning about matrices modulo that equivalence turns out to be convenient in Coq. Specifically, the automation of the rewriting strategies mentioned above does not require side condition proofs about well-formedness.

Coq type casting for rewriting. In math, $|0\rangle \otimes |0\rangle$ is a 4×1 matrix and it is only verbose to say it is a $(2 \cdot 2) \times (1 \cdot 1)$ matrix. Even though $(2 \cdot 2) \times (1 \cdot 1)$ is convertible to 4×1 , these two typing claims are not syntactically identical in Coq but only $\beta\eta$ -equivalent to each other. This difference is significant in rewriting. For example, the associativity of matrix multiplication is usually described as follows:

$$A \times (B \times C) = (A \times B) \times C.$$

But more formally, the associativity means for any natural numbers m, n, o, p and $m \times n$ matrix A , $n \times o$ matrix B and $o \times p$ matrix C ,

$$A \underset{m,n,p}{\times} (B \underset{n,o,p}{\times} C) = (A \underset{m,n,o}{\times} B) \underset{m,o,p}{\times} C$$

where we use subscripts under $\times$ to indicate matrices’ dimensions. These parameters do appear (implicitly) in Coq’s formalization of matrix multiplication’s associativity.

² Nevertheless, we keep our Coq script in the repository at Github more rigid. There we use $\equiv$ to stand for the relaxed notion of matrix equivalence and reserve $=$ for the stronger notion of equivalence in the sense that $A = B$ means the two matrices A and B are equal component-wisely both within and outside their dimensions.

$XX = I_2$	$\frac{1}{\sqrt{2}} \cdot (X + Z) = H$
$YY = I_2$	$H_2 \times CX \times H_2 = CZ$
$ZZ = I_2$	$CX \times X_1 \times CX = X_1 \times X_2$
$HH = I_2$	$CX \times Y_1 \times CX = Y_1 \times X_2$
$CX \times CX = I_4$	$CX \times Z_1 \times CX = Z_1$
$HXH = Z$	$CX \times X_2 \times CX = X_2$
$HYH = -Y$	$CX \times Y_2 \times CX = Z_1 \times Y_2$
$HZH = X$	$CX \times Z_2 \times CX = Z_1 \times Z_2$

Fig. 2 More laws

Thus rewriting does not work in the following case:

$$A \underset{1,1,1}{\times} (B \underset{1 \cdot 1, 1, 1 \cdot 1}{\times} C)$$

because rewriting uses an exact syntax match. This problem of type mismatch often occurs after we use the law **L13** for rewriting. We choose to build a customized rewrite tactic to overcome this problem. Using the example above, we want to rewrite via the associativity of multiplication. We first do a pattern matching for expressions of the form

$$A \underset{m, n_1, p_1}{\times} (B \underset{n_2, o, p_2}{\times} C)$$

no matter whether n_1 and p_1 coincide with n_2 and p_2 , respectively. We then use Coq's built-in unification to unify n_1, p_1 with n_2, p_2 . This unification must succeed or else the original expression of matrix computation is not well-formed. After the expression is changed to

$$A \underset{m, n_1, p_1}{\times} (B \underset{n_1, o, p_1}{\times} C)$$

we can use Coq's original rewrite tactic via the associativity of multiplication.

We handle the above mentioned type problems silently and whoever uses our system to formalize his/her own proof will not even feel these problems.

5 Equivalences of circuits

In order to judge whether two circuits have the same behavior, we need to formally define reasonable notions of equivalence for circuits in the first place. In this section, we propose two candidate relations: one is called matrix equivalence and the other observational equivalence.

5.1 Matrix equivalence

A natural way of interpreting a quantum circuit without measurements is to consider each quantum gate as a unitary matrix and the whole circuit as a composition of matrices that eventually reduces to a single matrix. From this viewpoint, two circuits are equivalent if they denote the same unitary matrix, that is, matrix equivalence = suffices to stand for circuit equivalence.

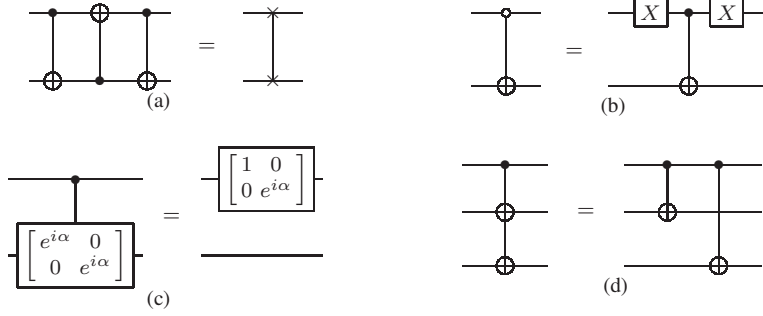


Fig. 3 Some equivalent circuits

Directly showing that two matrices are equivalent requires to inspect their elements and compare them component-wisely. Instead, we can take a functional view of matrix equivalence. Let A, B be two $2^m \times 2^m$ matrices, then $A = B$ if and only if $A|v\rangle = B|v\rangle$ for any vector $|v\rangle \in \mathcal{H}$, where $\mathcal{H}$ is the space of all m -qubit states.

```
Lemma MatrixEquiv_spec: forall {n} (A B: Matrix n n),
  A = B <-> (forall v: Vector n, A × v = B × v).
```

At first sight, it appears difficult to verify whether $A|v\rangle = B|v\rangle$ for all vectors $|v\rangle$, since there are infinitely many vectors in the state space $\mathcal{H}$. However, both matrices A and B represent linear operators, which means that it suffices to consider the vectors in an orthonormal basis of $\mathcal{H}$, where there are only 2^m vectors.

In Figure 2 we list some laws that are often useful in simplifying circuits before showing that they are equivalent. Let us verify the validity of the laws. Take the first one as an example. Its validity is stated in Lemma `unit_X`. In order to prove that lemma, we apply `MatrixEquiv_spec` and reduce it to Lemma `unit_X'`, which can be easily proved by the strategy `operate_reduce`.

```
Lemma unit_X : X × X = I_2.
```

```
Lemma unit_X' : forall v : Vector 2, X × X × v = I_2 × v.
```

In the right column of Figure 2, the subscripts of X, Y, Z and H indicate on which qubits the quantum gates are applied. For example, X_2 means that the Pauli-X gate is applied on the second qubit. Thus, the operation $Y_1 \times X_2$ actually stands for $(Y \otimes I_2) \times (I_2 \otimes X)$.

In Figure 3, we display some equivalent circuits. In diagram (a), on the right of $=$ is a schematic specification of swapping two qubits, which is implemented by the circuit on the left. Mathematically, the equality is described by Lemma `Eq1` below.

```
Definition SWAP := B0 ⊗ B0 .+ B1 ⊗ B2 .+ B2 ⊗ B1 .+ B3 ⊗ B3.
```

```
Definition XC := X ⊗ B3 .+ I_2 ⊗ B0.
```

```
Lemma Eq1 : SWAP = CX × XC × CX.
```

In diagram (b), there is a controlled operation performed on the second qubit, conditioned on the first qubit being set to zero. It is equivalent to a CX gate enclosed by two Pauli-X gates on the first qubit. The equality is specified by Lemma `Eq2` below.

```
Definition not_CX := B0 ⊗ X .+ B3 ⊗ I_2.
```

```
Lemma Eq2 : not_CX = (X ⊗ I_2) × CX × (X ⊗ I_2).
```

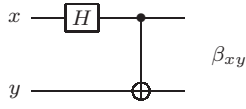



Fig. 4 The Bell states

$$\begin{aligned}
 |\beta_{00}\rangle &= \frac{1}{\sqrt{2}} \cdot |0\rangle \otimes |0\rangle + \frac{1}{\sqrt{2}} \cdot |1\rangle \otimes |1\rangle \\
 |\beta_{01}\rangle &= \frac{1}{\sqrt{2}} \cdot |0\rangle \otimes |1\rangle + \frac{1}{\sqrt{2}} \cdot |1\rangle \otimes |0\rangle \\
 |\beta_{10}\rangle &= \frac{1}{\sqrt{2}} \cdot |0\rangle \otimes |0\rangle - \frac{1}{\sqrt{2}} \cdot |1\rangle \otimes |1\rangle \\
 |\beta_{11}\rangle &= \frac{1}{\sqrt{2}} \cdot |0\rangle \otimes |1\rangle - \frac{1}{\sqrt{2}} \cdot |1\rangle \otimes |0\rangle
 \end{aligned}$$

In diagram (c), the controlled phase shift gate on the left is equivalent to a circuit for two qubits on the right. Lemma Eq3 gives a description of this equality.

Definition CE (u: R) := B0 $\otimes$ I_2 .+ B3 $\otimes$ (Cexp u .+ B0 .+ Cexp u .+ B3) .

Lemma Eq3 : CE u = (B0 .+ Cexp u .+ B3) $\otimes$ I_2 .

In diagram (d), a controlled gate with two targets is equivalent to the concatenation of two CX gates. This is formalized by Lemma Eq4 below.

Definition CXX := B0 $\otimes$ I_2 $\otimes$ I_2 .+ B3 $\otimes$ X $\otimes$ X .

Definition CIX := B0 $\otimes$ I_2 $\otimes$ I_2 .+ B3 $\otimes$ I_2 $\otimes$ X .

Lemma Eq4 : CXX = CIX $\times$ (CX $\otimes$ I_2) .

The previous four lemmas can all be proved by using the strategy `operate_reduce` in conjunction with `MatrixEquiv_spec`.

In Section 3 we have formalized the preparation of the 3-qubit GHZ state (cf. Figure 1). Now let us have a look at the Bell states. Depending on the input states, the circuit in Figure 4 gives four possible output states. The correctness of the circuit is validated by the four lemmas below, where the states are given in terms of density matrices and the circuit is described by a super-operator. It is easy to prove them by using our strategy `super_reduce`.

Definition bl00 := $\frac{1}{\sqrt{2}}$.+ ($|0,0\rangle$) .+ $\frac{1}{\sqrt{2}}$.+ ($|1,1\rangle$) .

Definition bl01 := $\frac{1}{\sqrt{2}}$.+ ($|0,1\rangle$) .+ $\frac{1}{\sqrt{2}}$.+ ($|1,0\rangle$) .

Definition bl10 := $\frac{1}{\sqrt{2}}$.+ ($|0,0\rangle$) .+ ($-\frac{1}{\sqrt{2}}$) .+ ($|1,1\rangle$) .

Definition bl11 := $\frac{1}{\sqrt{2}}$.+ ($|0,1\rangle$) .+ ($-\frac{1}{\sqrt{2}}$) .+ ($|1,0\rangle$) .

Lemma pb00 : super (CX $\times$ (H $\otimes$ I_2)) (density $|0,0\rangle$) = density bl00 .

Lemma pb01 : super (CX $\times$ (H $\otimes$ I_2)) (density $|0,1\rangle$) = density bl01 .

Lemma pb10 : super (CX $\times$ (H $\otimes$ I_2)) (density $|1,0\rangle$) = density bl10 .

Lemma pb11 : super (CX $\times$ (H $\otimes$ I_2)) (density $|1,1\rangle$) = density bl11 .

5.2 Observational equivalence

An alternative way of interpreting a quantum circuit without measurements is to consider it as an operator that changes input quantum states to output states and abstracts away unobservable details. Therefore, we reuse the notion of matrix equivalence $\approx$ introduced in Section 3 and call it observational equivalence for quantum circuits. The rationale of using $\approx$ is that from an observational point of view, global phases are irrelevant to the observed properties of the physical system under consideration and can be ignored as far as quantum states are concerned.

The following lemma provides a functional view of observational equivalence. It is a counterpart of `MatrixEquiv_spec` given in Section 5.1. Let A, B be two operators, we have $A \approx B$ if and only if $A|\psi\rangle \approx B|\psi\rangle$ for any state $|\psi\rangle$.

```

Lemma ObsEquiv_operator: forall {n} (A B: Matrix n n),
  A ≈ B <-> (forall ψ: Matrix n 1, A × ψ ≈ B × ψ).

```

Furthermore, two states are equal modulo a global phase, i.e. $|\psi\rangle \approx |\phi\rangle$ if and only if their density matrices are exactly the same, i.e. $|\psi\rangle\langle\psi| = |\phi\rangle\langle\phi|$. We formally prove this property as it motivated us to introduce density matrices to represent quantum states in Section 3.6.

```

Lemma ObsEquiv_state: forall {n} (ψ φ: Matrix n 1),
  ψ ≈ φ <-> ψ × (ψ†) = φ × (φ†) .

```

Although both matrix equivalence $=$ and observational equivalence $\approx$ can be used for relating circuits, the former is strictly finer than the latter in the sense that $A = B$ implies $A \approx B$ but not the other way around. Therefore, in the rest of the paper, we relate circuits by $=$ whenever possible, as they are also related by $\approx$. Moreover, it is not difficult to see that $=$ is a congruence relation. For example, if A, B are two quantum gates and $A = B$, then we can add a control qubit to form controlled- A and controlled- B gates, which are still identified by $=$. However, the relation $\approx$ does not satisfy such kind of congruence property. To see this, note that $I \approx -I$. But the controlled- I gate is quite different from controlled- $(-I)$: the latter transforms $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ into $\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$ whereas the former keeps it unchanged. In Section 6.1 we will see a concrete example of using $\approx$, where quantum states are identified by purposefully ignoring their global phases.

6 Case studies

To illustrate the power of our symbolic approach of reasoning about quantum circuits, we conduct a few case studies and compare the approach with the computational one in [22].

6.1 Deutsch's algorithm

Given a boolean function $f : \{0, 1\} \rightarrow \{0, 1\}$, Deutsch [9] presented a quantum algorithm that can compute $f(0) \oplus f(1)$ in a single evaluation of f . The algorithm can tell whether $f(0)$ equals $f(1)$ or not, without giving any information about the two values individually. The quantum circuit in Figure 5 gives an implementation of the algorithm. It makes use of a quantum oracle that maps any state $|x\rangle \otimes |y\rangle$ to the state $|x\rangle \otimes |y \oplus f(x)\rangle$, where $x, y \in \{0, 1\}$. More specifically, the unitary operator U_f can be in one of the following four forms:

- if $f(0) = f(1) = 0$, then $U_f = U_{f00} = I_2 \otimes I_2$;
- if $f(0) = f(1) = 1$, then $U_f = U_{f11} = I_2 \otimes X$;
- if $f(0) = 0$ and $f(1) = 1$, then $U_f = U_{f01} = CX$;
- if $f(0) = 1$ and $f(1) = 0$, then $U_f = U_{f10} = B_0 \otimes X + B_3 \otimes I_2$.

We formalize Deutsch's algorithm in Coq and use our symbolic approach to prove its correctness. Let us suppose that $|\psi_0\rangle = |01\rangle$ is the input state. There are three

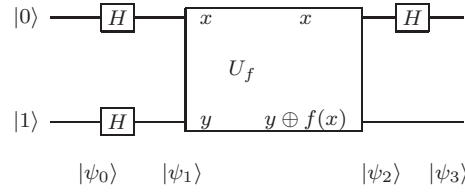


Fig. 5 Deutsch's algorithm

phases in this quantum circuit. The first phase applies the Hadamard gate to each of the two qubits. So we define the initial state and express the state after the first phase as follows:

Definition $\psi_0 := |0\rangle \otimes |1\rangle$.

Definition $\psi_1 := (H \otimes H) \times \psi_0$.

Lemma step1 : $\psi_1 = |+\rangle \otimes |-\rangle$.

Lemma step1 claims that the intermediate state after the first phase is $|+\rangle \otimes |-\rangle$. We can use the strategy `operate_reduce` designed in Section 3 to prove its correctness.

The second phase applies the unitary operator U_f to $|\psi_1\rangle$. Since U_f has four possible forms, we consider four cases.

Definition $\psi_{20} := (I_2 \otimes I_2) \times \psi_1$.

Definition $\psi_{21} := (I_2 \otimes X) \times \psi_1$.

Definition $\psi_{22} := CX \times \psi_1$.

Definition $\psi_{23} := (B0 \otimes X \text{ .+ } B3 \otimes I_2) \times \psi_1$.

Lemma step20 : $\psi_{20} = |+\rangle \otimes |-\rangle$.

Lemma step21 : $\psi_{21} = -1 \text{ .* } |+\rangle \otimes |-\rangle$.

Lemma step22 : $\psi_{22} = |-\rangle \otimes |-\rangle$.

Lemma step23 : $\psi_{23} = -1 \text{ .* } |-\rangle \otimes |-\rangle$.

Each of the above four lemmas corresponds to one case. They claim that the intermediate state $|\psi_2\rangle$ is $\pm 1 \cdot |+\rangle \otimes |-\rangle$ after the second phase when $f(0) = f(1)$, and $\pm 1 \cdot |-\rangle \otimes |-\rangle$ when $f(0) \neq f(1)$. We prove the four lemmas by rewriting $|\psi_1\rangle$ with Lemma step1 and using the strategy `operate_reduce` again.

The last phase applies the Hadamard gate to the first qubit of $|\psi_2\rangle$. So we still have four cases.

Definition $\psi_{30} := (H \otimes I_2) \times \psi_{20}$.

...

Lemma step30 : $\psi_{30} = |0\rangle \otimes |-\rangle$.

Lemma step31 : $\psi_{31} = -1 \text{ .* } |0\rangle \otimes |-\rangle$.

Lemma step32 : $\psi_{32} = |1\rangle \otimes |-\rangle$.

Lemma step33 : $\psi_{33} = -1 \text{ .* } |1\rangle \otimes |-\rangle$.

Observe that the only difference between $|\psi_{30}\rangle$ and $|\psi_{31}\rangle$ lies in the global phase -1 , which can be ignored. Similarly for $|\psi_{32}\rangle$ and $|\psi_{33}\rangle$. Formally, we can prove the following lemmas.

Lemma step31' : $\psi_{31} \approx |0\rangle \otimes |-\rangle$.

Lemma step33' : $\psi_{33} \approx |1\rangle \otimes |-\rangle$.

Therefore, after the last phase, we have $|\psi_3\rangle = |0\rangle \otimes |-\rangle$ when $f(0) = f(1)$, and $|\psi_3\rangle = |1\rangle \otimes |-\rangle$ when $f(0) \neq f(1)$. This is proved by using the intermediate results obtained in the first two phases and the strategy `operate_reduce`.

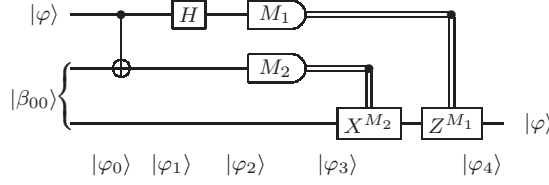


Fig. 6 Teleportation [20]

The above reasoning about the Deutsch's algorithm proceeds step by step and shows all the intermediate states in each phase. Alternatively, one may be only interested in the output state of the circuit once an input state is fed. In other words, we would like to show a property like

$$|\psi_{3ij}\rangle = (H \otimes I_2) \times U_{fij} \times (H \otimes H) \times |\psi_0\rangle.$$

Formally, we need to prove four equations depending on the forms of U_f .

```

Lemma deutsch00 :
  (H ⊗ I_2) × (I_2 ⊗ I_2) × (H ⊗ H) × (|0⟩ ⊗ |1⟩) = |0⟩ ⊗ |-⟩ .
Lemma deutsch01 :
  (H ⊗ I_2) × (I_2 ⊗ X) × (H ⊗ H) × (|0⟩ ⊗ |1⟩) = -1 .* |0⟩ ⊗ |-⟩ .
Lemma deutsch10 :
  (H ⊗ I_2) × CX × (H ⊗ H) × (|0⟩ ⊗ |1⟩) = |1⟩ ⊗ |-⟩ .
Lemma deutsch11 :
  (H ⊗ I_2) × (B0 ⊗ X .+ B3 ⊗ I_2) × (H ⊗ H) × (|0⟩ ⊗ |1⟩) = -1 .* |1⟩ ⊗ |-⟩ .

```

The second and fourth equations can be written in a simpler form as follows.

```

Lemma deutsch01' :
  (H ⊗ I_2) × (I_2 ⊗ X) × (H ⊗ H) × (|0⟩ ⊗ |1⟩) ≈ |0⟩ ⊗ |-⟩ .
Lemma deutsch11' :
  (H ⊗ I_2) × (B0 ⊗ X .+ B3 ⊗ I_2) × (H ⊗ H) × (|0⟩ ⊗ |1⟩) ≈ |1⟩ ⊗ |-⟩ .

```

Using our symbolic reasoning, these lemmas can be easily proved by `rewrite ObsEquiv_state` and `operate_reduce`. Thus, we know that the first qubit of the result state is $|0\rangle$ when $f(0) = f(1)$, and $|1\rangle$ otherwise. That is, $|\psi_{3ij}\rangle = |f(0) \oplus f(1)\rangle |- \rangle$ as expected.

6.2 Teleportation

Quantum teleportation [2] is one of the most important protocols in quantum information theory. It teleports an unknown quantum state by only sending classical information, by making use of a maximally entangled state. In particular, the algorithm involves performing intermediate measurements on the quantum state and then applying different operations on the intermediate measurement results represented by mixed states.

Let the sender and the receiver be *Alice* and *Bob*, respectively. The quantum teleportation protocol goes as follows, as illustrated by the quantum circuit in Figure 6.

1. *Alice* and *Bob* prepare an EPR state $|\beta_{00}\rangle_{q_2, q_3}$ together. Then they share the qubits, *Alice* holding q_2 and *Bob* holding q_3 .

2. To transmit the state $|\varphi\rangle$ of the quantum qubit q_1 , *Alice* applies a CX operation on q_1 and q_2 followed by an H operation on q_1 .
3. *Alice* measures q_1 and q_2 and sends the outcome x to *Bob*.
4. When *Bob* receives x , he applies appropriate Pauli gates on his qubit q_3 to recover the original state $|\varphi\rangle$ of q_1 .

We formalize the quantum teleportation protocol in Coq and use our symbolic approach to prove its correctness. Let $|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle$ be any vector used as a part of the input state. The other part is $|\beta_{00}\rangle$, which needs extra preparation. For simplicity, we directly represent $|\beta_{00}\rangle$ with a combination of $|0\rangle$ and $|1\rangle$. So we define the input state $|\varphi_0\rangle$ as follows.

```
Variables (α β : C).
Hypothesis Normalise: |α|^2 + |β|^2 = 1.
Definition φ : Vector 2 := α .* |0⟩ .+ β .* |1⟩.
Definition φ0 := φ ⊗ bl00.
```

The input state goes through the quantum circuit that comprises four phases. We can easily define the quantum pure state $|\varphi_2\rangle$ after the second phase as follows, and prove Lemma `tele1` by `operate_reduce`.

```
Definition φ2 := (H ⊗ I_2 ⊗ I_2) × (CX ⊗ I_2) × φ0.
Lemma tele1 : φ2 = α .* (|+⟩ ⊗ bl00) .+ β .* (|-⟩ ⊗ bl01).
```

In the third phase, due to the measurement with measurement operators $\{N_0, N_1\}$, where $N_0 = B_0$ and $N_1 = B_3$, there are four possible cases for the state $|\varphi_3\rangle$, and the probability for each case can be calculated as

$$\langle\varphi_2| \times (N_i \otimes N_j \otimes I_2)^\dagger \times (N_i \otimes N_j \otimes I_2) \times |\varphi_2\rangle = 1/4.$$

So we define p_{ij} and ρ_{3ij} as follows, where $i, j \in \{0, 1\}$ are the measurement outcomes for the top two qubits. Then we prove Lemma `tele2` about mixed states by `super_reduce` and some data processing. (We only consider projection operators as measurement operators, so we can replace $N^\dagger \times N$ with N).

```
Definition p0 := φ2 × (B0 ⊗ B0 ⊗ I_2) × φ2
Definition ρ30 :=
  1/p0 .* (super (B0 ⊗ B0 ⊗ I_2) (density φ2)).
...
Lemma tele2 :
  MeaMix 2 1 (MeaDen 2 0 (density φ2)) .:=
    [(1/4, 4 .* density (/√2 .* (|00⟩ ⊗ (α .* |0⟩ .+ β .* |1⟩))));
     (1/4, 4 .* density (/√2 .* (|01⟩ ⊗ (α .* |1⟩ .+ β .* |0⟩))));
     (1/4, 4 .* density (/√2 .* (|10⟩ ⊗ (α .* |0⟩ .+ -β .* |1⟩))));
     (1/4, 4 .* density (/√2 .* (|11⟩ ⊗ (α .* |1⟩ .+ -β .* |0⟩)))].
```

Finally, according to the different measurement results on the first two qubits, we apply corresponding Pauli gates on the third qubit. So the quantum state after the fourth phase becomes $|\varphi_{4ij}\rangle$. We can formalize it in Coq as follows.

$$|\varphi_{4ij}\rangle := (I_2 \otimes I_2 \otimes Z^i) \times (I_2 \otimes I_2 \otimes X^j) \times |\varphi_{3ij}\rangle$$

Definition $\rho_{40} := \rho_{30}$.
 Definition $\rho_{41} := \text{super } (I_2 \otimes I_2 \otimes X) \rho_{31}$.
 Definition $\rho_{42} := \text{super } (I_2 \otimes I_2 \otimes Z) \rho_{32}$.
 Definition $\rho_{43} := \text{super } ((I_2 \otimes I_2 \otimes Z) \times (I_2 \otimes I_2 \otimes X)) \rho_{33}$.

Lemma tele3 :

$$\begin{aligned} & [(1/4, \rho_{40}); [(1/4, \rho_{41}); [(1/4, \rho_{42}); [(1/4, \rho_{43})]]] := \\ & [(1/4, \text{density } (|0,0\rangle \otimes \psi); (1/4, \text{density } (|0,1\rangle \otimes \psi); \\ & [(1/4, \text{density } (|1,0\rangle \otimes \psi); (1/4, \text{density } (|1,1\rangle \otimes \psi))]. \end{aligned}$$

Using the simplification strategies discussed in Section 3, it is easy to prove that $|\varphi_{4ij}\rangle$ can be simplified to be $|i\rangle \otimes |j\rangle \otimes |\varphi\rangle$, and the probability of each case is $\frac{1}{4}$.

In summary, we can use the following equality to express the whole protocol.

$$\begin{aligned} |\varphi_{4ij}\rangle &= (I_2 \otimes I_2 \otimes Z^i) \times (I_2 \otimes I_2 \otimes X^j) \times (N_i \otimes N_j \otimes I_2) \\ &\quad \times (H \otimes I_2 \otimes I_2) \times (CX \otimes I_2) \times (|\varphi\rangle \otimes |\beta_{00}\rangle). \end{aligned}$$

It shows that the third qubit of the result state is always equal to $|\varphi\rangle$, the state to be teleported from Alice to Bob.

6.3 Simon's Algorithm

The Simon's problem was raised in 1994 [26]. Although it is an artificial problem, it inspired Shor to discover a polynomial time algorithm to solve the integer factorization problem.

Given a function $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$, suppose there exists a string $s \in \{0, 1\}^n$ such that the following property is satisfied:

$$f(x) = f(y) \Leftrightarrow x = y \text{ or } x \oplus y = s \quad (9)$$

for all $x, y \in \{0, 1\}^n$. Here $\oplus$ is the bit-wise modulo 2 addition of two n bit-strings. The goal of Simon's algorithm is to find the string s . The algorithm consists of iterating the quantum circuit and then performing some classical post-processing.

1. Set an initial state $|0\rangle^{\otimes n} \otimes |0\rangle^{\otimes n}$, and apply Hadamard gates to the first n qubits respectively.
2. Apply an oracle U_f to all the $2n$ qubits, where $U_f : |x\rangle|y\rangle \mapsto |x\rangle|f(x) \oplus y\rangle$.
3. Apply Hadamard gates to the first n qubits again and then measure them.

When $s \neq 0^n$, the probability of obtaining each string $y \in \{0, 1\}^n$ is

$$p_y = \begin{cases} 2^{-(n-1)} & \text{if } s \cdot y = 0 \\ 0 & \text{if } s \cdot y = 1. \end{cases}$$

Therefore, it can be seen that the result string y must satisfy $s \cdot y = 0$ and be evenly distributed. Repeating this process $n-1$ times, we will get $n-1$ strings $y_1, \dots, y_{n-1}$ so that $y_i \cdot s = 0$ for $1 \leq i \leq n-1$. Thus we have $n-1$ linear equations with n unknowns (n is the number of bits in s). The goal is to solve this system of equations to get s . We can get a unique non-zero solution s if we are lucky and $y_1, \dots, y_{n-1}$ are linearly independent. Otherwise, we repeat the entire process and will find a linearly independent set with a high probability.

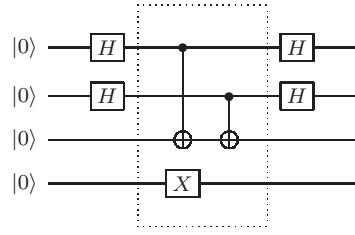


Fig. 7 Simon's algorithm with $n = 2$ and $s = 11$

As an example, we consider the Simon's algorithm with $n = 2$. The quantum circuit is displayed in Figure 7. We design the oracle as the gates in the dotted box $U_f = (I_2 \otimes CX \otimes I_2) \times (CIX \otimes X)$, where the gate CIX is defined in page 17. For this oracle, $s = 11$ satisfies property (9). The change of states can be seen as follows:

$$\begin{aligned}
 |0000\rangle &\xrightarrow{H \otimes H \otimes I_2 \otimes I_2} |++\rangle|00\rangle \\
 &\xrightarrow{U_f} \frac{1}{2}[(|00\rangle + |11\rangle)|01\rangle + (|01\rangle + |10\rangle)|11\rangle] \\
 &\xrightarrow{H \otimes H \otimes I_2 \otimes I_2} \frac{1}{2}[(|00\rangle + |11\rangle)|01\rangle + (|00\rangle - |11\rangle)|11\rangle]
 \end{aligned}$$

We can establish the following lemma with our symbolic approach and use the strategy `super_reduce` to prove it.

```

Lemma simon : super ((H ⊗ H ⊗ I_2 ⊗ I_2) × (I_2 ⊗ CX ⊗ I_2) ×
  (CIX ⊗ X) × (H ⊗ H ⊗ I_2 ⊗ I_2)) (density |0,0,0,0⟩) = density
  (/2 .* |0,0,0,1⟩ .+ /2 .* |1,1,0,1⟩ .+ /2 .* |0,0,1,1⟩ .+ -/2 .* |1,1,1,1⟩) .

```

We analyze the cases where the last two qubits are in the state $|01\rangle$ or $|11\rangle$. The corresponding first two qubits are in $|00\rangle$ or $|11\rangle$, each occurs with equal probability. By property (9), it means that $x \oplus y = 00$ or 11 , so we obtain that $s = 11$.

6.4 Grover's algorithm

In this section we consider Grover's search algorithm. The algorithm starts from the initial state $|0\rangle^{\otimes n}$. It first uses $H^{\otimes n}$ (the H gate applied to each of the n qubits) to obtain a uniform superposition state, and then applies the Grover iteration repeatedly. An implementation of the Grover iteration has four steps:

1. Apply the oracle O .
2. Apply the Hadamard transform $H^{\otimes n}$.
3. Perform a conditional phase shift on $|x\rangle$, if $|x\rangle \neq |0\rangle$.
4. Apply the Hadamard transform $H^{\otimes n}$ again.

Here the conditional phase-shift unitary operator in the third step is $2|0\rangle\langle 0| - I$. We can merge the last three steps as follows:

$$H^{\otimes n} \times (2|0\rangle\langle 0| - I) \times H^{\otimes n} = 2|\phi\rangle\langle \phi| - I$$



Fig. 8 The quantum circuit of different Oracle

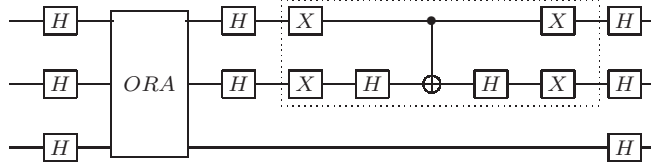


Fig. 9 the Grover's algorithm with two qubits

where $|\phi\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle$ with $N = 2^n$. Therefore, the Grover iteration becomes $G = (2|\phi\rangle\langle\phi| - I) \times O$.

As a concrete example, we consider the Grover's algorithm with two qubits. The size of the search space of this algorithm is four. So we need to consider four search cases with $x^* = 0, 1, 2, 3$. The oracle must satisfy that if $x = x^*$, then $f(x^*) = 1$, otherwise $f(x) = 0$. So in accordance with $x^* = 0, 1, 2, 3$, we design four oracles $ORA_0, \dots, ORA_3$, which are implemented by the four circuits in Figure 8.

Definition ORA0 := $B0 \otimes (B0 \otimes X \text{ .+ } B3 \otimes I_2) \text{ .+ } B3 \otimes I_2 \otimes I_2$.

Definition ORA1 := $B0 \otimes CX \text{ .+ } B3 \otimes I_2 \otimes I_2$.

Definition ORA2 := $B0 \otimes I_2 \otimes I_2 \text{ .+ } B3 \otimes (B0 \otimes X \text{ .+ } B3 \otimes I_2)$.

Definition ORA3 := $B0 \otimes I_2 \otimes I_2 \text{ .+ } B3 \otimes CX$.

The whole algorithm is illustrated by the circuit in Figure 9. The gates in the dotted box perform the conditional phase shift operation $2|0\rangle\langle 0| - I$. We then merge the front and back $H \otimes H$ gates to it and get the operation CPS as follows.

Definition MI := $(B0 \text{ .+ } B1 \text{ .+ } B2 \text{ .+ } B3) \otimes (B0 \text{ .+ } B1 \text{ .+ } B2 \text{ .+ } B3)$.

Definition CPS := $((1/2 \text{ .* } MI) \text{ .+ } (-1) \text{ .* } (I_2 \otimes I_2)) \otimes I_2$.

So we have the Grover iteration $G = (2|\phi\rangle\langle\phi| - I) \times O = CPS \times ORA_i$. Let the initial state be $|0\rangle \otimes |0\rangle \otimes |1\rangle$. After the Hadamard transform $H^{\otimes 3}$, we only perform Grover iteration once to get the search solution. In summary, we formalize the Grover's algorithm with two qubits in the vector form as follows, and use `operate_reduce` to prove them. The reasoning using density matrices can also be done.

Lemma Gro0:

$$(I_2 \otimes I_2 \otimes H) \times CPS \times ORA0 \times (H \otimes H \otimes H) \times |0, 0, 1\rangle = |0, 0, 1\rangle.$$

Lemma Gro1:

$$(I_2 \otimes I_2 \otimes H) \times CPS \times ORA1 \times (H \otimes H \otimes H) \times |0, 0, 1\rangle = |0, 1, 1\rangle.$$

Lemma Gro2:

$$(I_2 \otimes I_2 \otimes H) \times CPS \times ORA2 \times (H \otimes H \otimes H) \times |0, 0, 1\rangle = |1, 0, 1\rangle.$$

Lemma Gro3:

$$(I_2 \otimes I_2 \otimes H) \times CPS \times ORA3 \times (H \otimes H \otimes H) \times |0, 0, 1\rangle = |1, 1, 1\rangle.$$

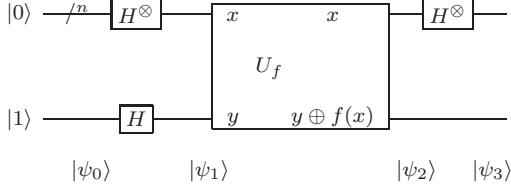
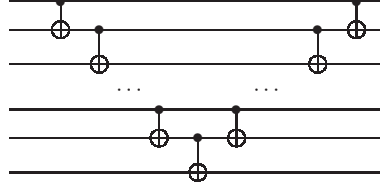


Fig. 10 Deutsch-Jozsa algorithm

Fig. 11 The circuit of U_f

For all the case studies in the current and previous subsections, we employ the same schema: first represent the quantum circuits and input states symbolically, and then apply the strategies developed in Section 3 to show that the output states are equal to our desired states. When the states are in the vector form, we use the strategy `operate_reduce`. When the states are in the density matrix form, we make use of the strategy `super_reduce`, which decomposes density matrices into multiplications of vectors and then essentially resort to `operate_reduce`, as discussed in Section 3. In addition, if it is necessary to identify states up to an ignorance of global phases, we have the extra task of rewriting terms with `ObsEquiv_state`.

6.5 Deutsch-Jozsa algorithm family

Representing a family of algorithms with unbounded qubit size, the Deutsch-Jozsa algorithm is a generalization application of the Deutsch algorithm on n qubits. Given a boolean function $f : \{0, 1\}^n \rightarrow \{0, 1\}$ as a quantum oracle, the algorithm judges whether f is a constant or a balanced function. Here $f(x)$ is balanced if it is equal to 1 for half of the input x , and 0 for the other half. As shown in Figure 10, the overall steps of the Deutsch-Jozas algorithm are as follows,

1. Apply Hadamard gates to all the $n + 1$ qubits respectively.
2. Apply the oracle U_f to the $n + 1$ qubits, where $U_f : |x\rangle|y\rangle \mapsto |x\rangle|y \oplus f(x)\rangle$.
3. Apply Hadamard gates to the first n qubits again and then measure them.

Suppose the input state is $|\psi_0\rangle = |0\rangle^{\otimes n} |1\rangle$. After each of the above three steps, we get three states $|\psi_1\rangle$, $|\psi_2\rangle$ and $|\psi_3\rangle$ respectively.

$$\begin{aligned}
 |\psi_1\rangle &:= \sum_{x=0}^{2^n-1} \frac{|x\rangle}{\sqrt{2^n}} |-\rangle \\
 |\psi_2\rangle &:= \sum_{x=0}^{2^n-1} \frac{(-1)^{f(x)} |x\rangle}{\sqrt{2^n}} |-\rangle \\
 |\psi_3\rangle &:= \sum_{x=0}^{2^n-1} \sum_{z=0}^{2^n-1} \frac{(-1)^{f(x)+x \cdot z} |z\rangle}{2^n} |-\rangle
 \end{aligned}$$

From $H^{\otimes n} |0\rangle^{\otimes n} = \sum_x |x\rangle / \sqrt{2^n}$, we easily get $|\psi_1\rangle$. Then due to the fact that $U_f |-\rangle = (-1)^{f(x)} |-\rangle$, we have $|\psi_2\rangle$. Finally, for a single qubit we know that

$H|x\rangle = \sum_z (-1)^{xz} |z\rangle / \sqrt{2}$, we obtain $|\psi_3\rangle$, where $x \cdot z$ is the bitwise inner product of x and z . After measuring the first n qubits, we analyse the probability of the event that the final result is $|0\rangle^{\otimes n}$. When $|z\rangle$ is $|0\rangle$, the coefficient of $|\psi_3\rangle$ is $\sum_x (-1)^{f(x)+x \cdot z} / 2^n |_{z=0}$, which is equal to $\sum_x (-1)^{f(x)} / 2^n$. Thus, when f is a constant function, the measurement result must be $|0\rangle^{\otimes n}$. Otherwise, when f is a balanced one, the result would not be $|0\rangle^{\otimes n}$. In summary, based on the measurement of the first n qubits, we can determine whether f is a constant or a balanced function and only query the oracle once.

In particular, consider the circuit of U_f shown in Figure 11, we specify U_f in Coq as follows,

```
Fixpoint Uf (n:nat) : Matrix (2*2^(N.of_nat n)) (2*2^(N.of_nat n)) :=
  match n with
  | 0 => I 2
  | S n' => (CX ⊗ I (2^(N.of_nat n'))) × (I 2 ⊗ (Uf n'))
           × (CX ⊗ I (2^(N.of_nat n')))
  end.
```

For convenience, we predefine an auxiliary function $kron_n\ n\ A$, which stands for $A^{\otimes n}$. When n is 1, it degenerates into I_1 , i.e. 1.

```
Fixpoint kron_n (n:nat) m1 m2 (A : Matrix m1 m2) :
  Matrix (m1^(N.of_nat n)) (m2^(N.of_nat n)) :=
  match n with
  | 0 => I 1
  | S n' => kron A (kron_n n' A)
  end.
```

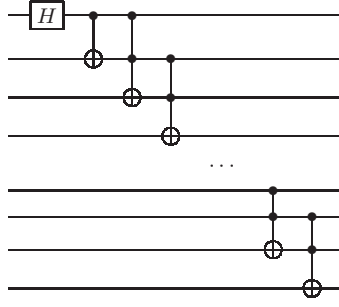
According to the above three steps, we use the following three lemmas to prove the correctness of the Deutsch-Jozsa algorithm.

```
Lemma DJ_0 :
  ((kron_n n H) ⊗ H) × ((kron_n n |0⟩) ⊗ |1⟩) = (kron_n n |+⟩) ⊗ |-⟩.
Lemma DJ_1 :
  (n > 0) % nat ->
  (Uf n) × ((kron_n n |+⟩) ⊗ |-⟩) = (kron_n n |+⟩) ⊗ |-⟩.
Lemma DJ_2 :
  ((kron_n n H) ⊗ H) × ((kron_n n |+⟩) ⊗ |-⟩) ≡ (kron_n n |0⟩) ⊗ |1⟩.
```

By using the proof assistant Coq, we can formalise the proof about n qubits with induction and rewriting strategies. Since the number of n is unbounded, the correctness of the algorithm is difficult to be prove without proof assistant platforms. As an example, we consider the second lemma. We first focus on the case of $n = 1$,

$$CX \times (I_2 \otimes I_2) \times CX \times (|+\rangle \otimes |-\rangle) = |+\rangle \otimes |-\rangle.$$

This case can be easily proved by `operate_reduce`. According to the inductive hypothesis, we assume that the algorithm is correct for the case of $n = k$. Then we are going to prove the case of $n = k + 1$ with it and some laws in Table 1. The proof



$$\begin{aligned}
 |000..00\rangle &\rightarrow \left[\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right] \otimes |00..00\rangle \\
 &\equiv \frac{1}{\sqrt{2}}(|000..00\rangle + |100..00\rangle) \\
 &\rightarrow \frac{1}{\sqrt{2}}(|000..00\rangle + |110..00\rangle) \\
 &\rightarrow \frac{1}{\sqrt{2}}(|000..00\rangle + |111..00\rangle) \\
 &\quad \dots \\
 &\rightarrow \frac{1}{\sqrt{2}}(|000..00\rangle + |111..10\rangle) \\
 &\rightarrow \frac{1}{\sqrt{2}}(|000..00\rangle + |111..11\rangle)
 \end{aligned}$$

Fig. 12 Preparing an entangled state

steps are as follows,

$$\begin{aligned}
 &U_f^{k+1} \times (|+\rangle^{\otimes(k+1)} \otimes |-\rangle) \\
 &= (CX \otimes I_{2^k}) \times (I_2 \otimes U_f^k) \times (CX \otimes I_{2^k}) \times (|+\rangle \otimes |+\rangle \otimes |+\rangle^{\otimes(k-1)} \otimes |-\rangle) \\
 &= (CX \otimes I_{2^k}) \times (I_2 \otimes U_f^k) \times ((CX \otimes I_{2^k}) \times (|+\rangle \otimes |+\rangle \otimes |+\rangle^{\otimes(k-1)} \otimes |-\rangle)) \\
 &= (CX \otimes I_{2^k}) \times (I_2 \otimes U_f^k) \times ((CX \times (|+\rangle \otimes |+\rangle)) \otimes (I_{2^k} \times (|+\rangle^{\otimes(k-1)} \otimes |-\rangle))) \\
 &= (CX \otimes I_{2^k}) \times ((I_2 \otimes U_f^k) \times (|+\rangle \otimes |+\rangle \otimes |+\rangle^{\otimes(k-1)} \otimes |-\rangle)) \\
 &= (CX \otimes I_{2^k}) \times ((I_2 \times |+\rangle) \otimes (U_f^k \times (|+\rangle^{\otimes k} \otimes |-\rangle))) \\
 &= (CX \otimes I_{2^k}) \times (|+\rangle \otimes (|+\rangle^{\otimes k} \otimes |-\rangle)) \\
 &= (CX \otimes I_{2^k}) \times ((|+\rangle \otimes |+\rangle) \otimes (|+\rangle^{\otimes k-1} \otimes |-\rangle)) \\
 &= (CX \times (|+\rangle \otimes |+\rangle)) \otimes (I_{2^k} \times (|+\rangle^{\otimes k-1} \otimes |-\rangle)) \\
 &= |+\rangle^{\otimes(k+1)} \otimes |1\rangle.
 \end{aligned}$$

After apply the Hadamard gates to the first n qubits, we can get that the first n qubits of the result is $|0\rangle^{\otimes n}$, So we know that the f described as U_f is a constant function.

6.6 Preparation of an entangled state

So far we have seen some simple examples with only a few qubits. Now let us consider a bigger example with a dozen qubits. The quantum circuit in Figure 12 can be used to create a maximally entangled state.

We start with the initial state $|000..00\rangle$ with 12 qubits. First, we apply the H gate on the first qubit q_1 to change the global state into $\left[\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right] \otimes |00..00\rangle$ with the first qubit in a superposition. It is equivalent to $\frac{1}{\sqrt{2}}(|000..00\rangle + |100..00\rangle)$. Then we apply the CX gate on the first and second qubits q_1 and q_2 , which leads to the state $\frac{1}{\sqrt{2}}(|000..00\rangle + |110..00\rangle)$. Then we apply the Toffoli gate on the first three qubits to yield $\frac{1}{\sqrt{2}}(|000..00\rangle + |111..00\rangle)$. In a similar way, we apply the Toffoli gate on the qubits q_i, q_{i+1} and q_{i+2} for $i \in 2, 3, \dots, n-2$ in turn. Eventually, we obtain a maximally entangled state $\frac{1}{\sqrt{2}}(|000..00\rangle + |111..11\rangle)$.

The correctness of the quantum circuit is stated by the following lemma.

	Deutsch	Simon	Teleportation	Secret sharing	QFT	Grover
Symbolic	3656	53795	39715	68919	25096	146834
Computational	25190	180724	46450	170490	68730	934570

Table 2 Comparison of two approaches with verification time in milliseconds

```

Lemma Entangled_state_12 :
  (I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ TOF )
  × (I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ TOF ⊗ I_2)
  × (I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ TOF ⊗ I_2 ⊗ I_2)
  × (I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ TOF ⊗ I_2 ⊗ I_2 ⊗ I_2)
  × (I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ TOF ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2)
  × (I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ TOF ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2)
  × (I_2 ⊗ I_2 ⊗ I_2 ⊗ TOF ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2)
  × (I_2 ⊗ TOF ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2)
  × (TOF ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2)
  × (CX ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2)
  × (H ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2 ⊗ I_2)
  × |0,0,0,0,0,0,0,0,0,0,0,0⟩
  ≡ /√2 .* |0,0,0,0,0,0,0,0,0,0,0,0⟩ .+ /√2 .* |1,1,1,1,1,1,1,1,1,1,1,1⟩.

```

By just using the strategy `operate_reduce`, we can prove the above property in half an hour. Note that this example cannot be handled by the computational approach — going beyond 6 qubits is very difficult for that approach.

6.7 Experiments

We have conducted experiments on Deutsch’s algorithm, Simon’s algorithm, quantum teleportation, quantum secret sharing protocol, quantum Fourier transform (QFT) with three qubits, and Grover’s search algorithm with two qubits. In Table 2, we record the execution time of those examples in milliseconds in CoqIDE 8.10.0 running on a PC with Intel Core i5-7200 CPU and 8 GB RAM. As we can see in the table, our symbolic approach always outperforms the computational one in [22].

The computational approach is slow because of the explicit representation of matrices and inefficient tactics for evaluating matrix multiplications. Let us consider a simple example. In the computational approach, the Hadamard gate H is defined by `ha` below:

```

Definition ha : Matrix 2 2 :=
  fun x y => match x, y with
  | 0, 0 => (1 / √2)
  | 0, 1 => (1 / √2)
  | 1, 0 => (1 / √2)
  | 1, 1 => -(1 / √2)
  | _, _ => 0
end.

```

Since H is unitary, we have $HH = I$ and the following property becomes straightforward.

```

Lemma H3_ket0: (ha ⊗ ha ⊗ ha) × (ha ⊗ ha ⊗ ha) × (|0,0,0⟩) = (|0,0,0⟩).

```

However, to prove the above lemma with the computational approach is far from being trivial. To see this, we literally go through a few steps. Firstly, we apply the associativity of matrix multiplication on the left hand side of the equation so to rewrite it into

$$(H \otimes H \otimes H) \times ((H \otimes H \otimes H) \times (|0\rangle \otimes |0\rangle \otimes |0\rangle)).$$

Secondly, each explicitly represented matrix is converted into a two-dimensional list and matrix multiplications are calculated in order. Finally, we need to show that each of the eight elements in the vector on the left is equal to the corresponding element on the right. Let $A_0 = (H \otimes H \otimes H) \times (|0\rangle \otimes |0\rangle \otimes |0\rangle)$ and $A_1 = (H \otimes H \otimes H) \times A_0$. With the computational approach, obvious simplifications such as multiplication and addition with 0 and 1 are carried out for the elements in A_0 and A_1 , and no more complicated simplification is effectively handled. So A_0 is a two-dimensional list with each element in the form $\frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}}$ and A_1 is a two-dimensional list whose first element is

$$\begin{aligned} & (\frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \times (\frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}})) \\ & + (\frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \times (\frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}})) \\ & + \dots \\ & + (\frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \times (\frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}} \times \frac{1}{\sqrt{2}})), \end{aligned}$$

which is a summation of eight identical summands with $\frac{1}{\sqrt{2}}$ multiplied with itself six times; other elements are in similar forms. From this simple example, we can already see that the explicit matrix representation and ineffective simplification in matrix multiplication make the intermediate expressions very cumbersome.

On the contrary, in the symbolic approach we have

$$\begin{aligned} A_1 &= (H \otimes H \otimes H) \times (H \otimes H \otimes H) \times (|0\rangle \otimes |0\rangle \otimes |0\rangle) \\ &= (H \otimes (H \otimes H)) \times ((H \otimes (H \otimes H)) \times (|0\rangle \otimes (|0\rangle \otimes |0\rangle))) \\ &= (H \otimes (H \otimes H)) \times ((H \times |0\rangle) \otimes ((H \times |0\rangle) \otimes (H \times |0\rangle))) \\ &= (H \otimes (H \otimes H)) \times (|+\rangle \otimes (|+\rangle \otimes |+\rangle)) \\ &= (H \times |+\rangle) \otimes ((H \times |+\rangle) \otimes (H \times |+\rangle)) \\ &= |0\rangle \otimes (|0\rangle \otimes |0\rangle). \end{aligned}$$

Notice that here we have kept the structure of tensor products rather than to eliminate them. In fact, we lazily evaluate tensor products because they are expensive to calculate and preserving more higher-level structures opens more opportunities for rewriting. The symbolic reasoning not only renders the intermediate expressions more readable, but also greatly reduces the time cost of arithmetic calculations.

In general, in the computational approach a multiplication of two $N \times N$ matrices of $O(k)$ -length expressions results in a matrix of $O(Nk)$ -length expressions, and those expressions are not effectively simplified. At the end of the computation, a matrix of $O(N^m)$ -length expressions is obtained if $m + 1$ matrices of size $N \times N$ are multiplied together, which takes exponential time to simplify. In our approach, we represent matrices symbolically and simplify intermediate expressions effectively on the fly, which has a much better performance.

7 Related work

Formal verification in quantum computing has been growing rapidly, especially in Coq. Boender et al. [4] presented a framework for modeling and analyzing quantum protocols using Coq. They made use of the Coq repository C-CoRN [8] and built a matrix library with dependent types. Cano et al. [6] specifically designed CoqEAL, a library built on top of ssreflect [18] to develop efficient computer algebra programs with proofs of correctness. They represented a matrix as a list of lists for efficient generic matrix computation in Coq but they did not consider optimizations specific for matrices commonly used in quantum computation. Rand et al. [22] defined a quantum circuit language Qwire in Coq, and formally verified some quantum programs expressed in that language [23,24]. Reasoning using their matrix library usually requires explicit computation, which does not scale well, as discussed in Section 6. Hietala et al. [14] developed a quantum circuit compiler VOQC in Coq, which uses several peephole optimization techniques such as replacement, propagation, and cancellation as proposed by Nam et al. [19] to reduce the number of unitary transformations. It is very different from our symbolic approach of simplifying matrix operations using the Dirac notation. Mahmoud et al. [17] formalized the semantics of Proto-Quipper in Coq and formally proved the type soundness property. They developed a linear logical framework within the Hybrid system [11] and used it to represent and reason about the linear type system of Quipper [12].

Our formalization of matrices is partly based on QWIRE [22]. We choose to use their formalization of matrices and matrix operations ($\cdot$, $\times$, $+$, $\otimes$, $\dagger$). For basic rules, QWIRE proves 30 out of 35 rules in Table 1³. But apart from that, our formalization of gates using Dirac notation, the notion of observational equivalence for circuits, and our systematic tactic library are novel.

Note that although sparse matrix computation is well studied in other areas of Computer Science, we are not aware of any library in Coq dedicated to sparse matrices. We consider the symbolic approach proposed in the current work as a contribution in this perspective. For example, let us consider the gate CX. It is represented as a sparse 4×4 matrix with 4 out of the 16 entries being non-zero (cf. Section 2.2). As we can see in (2), its symbolic representation is

$$B_0 \otimes I_2 + B_3 \otimes (B_1 + B_2) \quad (10)$$

using the terms I_2 and B_j ($j \in \{0, \dots, 3\}$). Those terms are the basic building blocks of our formalization of quantum circuits and our symbolic reasoning. The expression in (10) can be viewed as a compact way of representing the sparse matrix of gate CX.

Apart from Coq, other proof assistants have also been used to verify quantum circuits and programs. Liu et al. [15] used the theorem prover Isabelle/HOL [21] to formalize a quantum Hoare logic [28] and verify its soundness and completeness for partial correctness. Unruh [6] developed a relational quantum Hoare logic and implemented an Isabelle-based tool to prove the security of post-quantum cryptography

³ For the rest 5 rules, QWIRE proves 4 with additional well-formness assumptions and does not prove the associativity of tensor product.

and quantum protocols. Beillahi et al. [3] verified quantum circuits with up to 190 two-qubit gates in HOL Light. It relies on the formalization of Hilbert spaces in HOL Light proposed by Mahmoud et al. in [16], where a number of laws about complex functions and linear operators are proved. Although linear operators correspond to matrices in the finite-dimension case, our results are not implied by those in [3, 16]. For instance, a quantum state in [3] is necessarily a vector, which means that only pure states can be represented. In contrast, we can also deal with mixed states in the form of density matrices. Furthermore, one of our main contributions is to represent sparse matrices using Dirac notation, which is convenient for readability and cancelling zero matrices due to orthogonality of basic vectors.

Notice that the laws in Table 1 play an important role in our symbolic reasoning of quantum circuits. Although they resemble to some laws in a ring, the matrices under our consideration can be of various dimensions and they do not form a ring. It is also critical that the multiplication of two matrices, e.g. a row vector and a column vector, could be a scalar number (and even zero). Thus, rings are not enough here. The proof-by-reflection technique for rings might be useful but are usually hard to develop. We have shown that the tactic-based method is already efficient in our application scenario, and also flexible for both fully-automated and interactive proofs.

8 Conclusion and future work

We have proposed a symbolic approach to reasoning about quantum circuits in Coq. It is based on a small set of equational laws which are exploited to design some simplification strategies. According to our case studies, the approach is more efficient than the usual one of explicitly representing matrices and is well suited to be automated in Coq.

Dealing with quantum circuits is our intermediate goal. More interesting algorithms such as the Shor’s algorithm [25] also require classical computation. In the near future, we plan to formalize in Coq the semantics of a quantum programming language with both classical and quantum features.

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