Abstracting Entanglement

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Abstract

In quantum computation, entanglement is a fundamental phenomenon that significantly affects the behaviour and correctness of quantum programs. One of the most striking effects of such a phenomenon arises from its interplay with quantum measurement. A non-classical correlation between the entangled qubits, which is related to a non-local action, makes the measurement of one qubit of an entangled pair instantaneously affect also the other. This leads to potential problems in the execution of a quantum program where variables become entangled during a computation since unintended measurements may cause erroneous results. A static analysis detecting such critical situations is, therefore, necessary to guarantee the correct execution of a quantum program. To pursue this objective, we introduce a novel abstract domain specifically designed to analyse and manage entanglement in quantum programs.

CCS Concepts: • **Theory of computation** → **Abstraction**; **Program analysis**; • **Computer systems organization** → **Quantum computing**; • **Software and its engineering** → **Automated static analysis**.

Keywords: Entanglement, Quantum Computing, Static Analysis Abstract Interpretation, Quantum Languages

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1 Introduction

With the rapid progress in quantum technology, driven by the efforts of many companies that have been working for years to build a large-scale quantum computer, and the growing number of applications where quantum computers are used for practical industrial use cases, the study of quantum programming languages is becoming increasingly important.

The use of quantum programming languages poses unique challenges due to the special nature of quantum computation. In these languages, variables represent information contained in quantum states (i.e. vectors in a Hilbert space).

Quantum computation is characterised by two fundamental principles: superposition and entanglement. Unlike the classical case, a quantum state can exist in a superposition of classical states; in fact, it corresponds to a linear combination in a complex vector space with the classical states as base vectors (or dimensions). Entanglement occurs when, as a result of a computation, two particles become so strongly correlated that they form a single state that cannot be separated into two individual ones. This means that any change in the state of one particle influences the other. Entanglement is a crucial resource in many quantum algorithms (e.g. quantum factorisation[9, Chapter 7]) and quantum communication protocols (e.g. quantum teleportation[9, Chapter 5]). However, in quantum programming, entanglement can cause problems in some cases. For example, when combined with the principle of implicit measurement [10, Section 4.4], entanglement may have some negative effects on the result of the computation. This forces us to carefully deal with auxiliary quantum variables, which must be properly "reset" before the program ends to avoid the side effects of entanglement. Therefore, analysing and tracking entanglement is fundamental to reason about quantum languages.

In this paper, we introduce an abstract domain for the static analysis of entanglement. In particular, we are interested in detecting when a variable (typically a temporary variable) becomes entangled with another one during a computation so as to compromise the final results. An obstacle in the formalisation of quantum entanglement is that, as a property of quantum states, it is not transitive, i.e. if q_1 and q_2 are entangled and q_2 and q_3 are entangled, it is not always the case that q_1 and q_3 are entangled. As it is well known, the transitivity of an abstract property or, more precisely, the fact that it can be expressed by an equivalence relation guarantees the existence of a best approximation for any concrete element [7, 15]. Thus, we will consider an abstract property, which is a transitive abstraction of entanglement. We define this property, which we call *non-separability*, as a relation between sets of variables.

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We also propose a refinement of our domain, which is able to distinguish a particular case of entanglement corresponding to states of the form $\alpha\,|00\ldots0\rangle + \beta\,|11\ldots1\rangle$. These states, called GHZ from the names of their inventors[1], are particularly interesting because they can be 'disentangled' in a very easy way.

2 Quantum Computation

In this section, we briefly recall the main aspects of quantum computation at the basis of the entanglement phenomenon. In doing so, we will refer to the circuit model of computation. In a quantum circuit, wires represent quantum bits, or qubits, rather than bits. Thus, a qubit replaces the classical unit of information (the bit) in the quantum computation model, generalising the two only possible values 0 and 1 of a bit to any vector in a complex Hilbert space (the quantum system), with 0 and 1 as basis vectors. The typical notation of such vectors (or states of a qubit) is the Dirac *ket* notation, according to which $|0\rangle$ is the column vector $(1,0)^T$ and $|1\rangle$ is the column vector $(0,1)^T$ and, in general, $|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$ denote a linear combination or *superposition* state. The numbers α and β are complex numbers called probability amplitudes since, from them, we can infer the probability of the state resulting in 0 or 1 after measuring the system. Such probabilities are obtained as $|\alpha|^2$ and $|\beta|^2$, which explains why quantum states must be unitary, i.e. $|\alpha|^2 + |\beta|^2 = 1$ must hold.

Implementing significant and powerful quantum algorithms requires performing quantum computation on circuits which are more complex than a single qubit operation and involve n qubit states with $n > 1$. A n qubit state corresponds to a unitary vector in the 2^n-dimensional Hilbert space ($\mathcal{H}^{2^n}$), obtained by composing by tensor product ($\otimes$) the vector space of the single qubits, each living in a 2-dimensional complex Hilbert space ($\mathcal{H}^2$) [10, Chapter 2]. For instance, the space of two qubits is $\mathcal{H}^4 = \mathcal{H}^2 \otimes \mathcal{H}^2$ and a generic state $|\psi\rangle$ in $\mathcal{H}^4$ can be written as:

$$|\psi\rangle = \alpha_0\,|00\rangle + \alpha_1\,|01\rangle + \alpha_2\,|10\rangle + \alpha_3\,|11\rangle$$

where all α_i are complex numbers.

2.1 Entanglement and Measurement

The behaviour of quantum circuits is determined by the laws of quantum mechanics and undergoes the effect of an important quantum phenomenon with no classical counterparts, namely entanglement. This can be intuitively described as an application of the superposition principle to a system composed of two or more subsystems and occurs when statistically correlated measurement outcomes are observed as the effect of two subsequent quantum measurements, one on each subsystem.

[1]Danny Greenberg, Mike Horne and Anton Zeilinger experimentally created this three-particle entanglement showing that quantum mechanics is not compatible with Einstein's theory of 'hidden variables'.

Quantum measurement is an operation that allows us to extract a classical result from a quantum superposition $|\psi\rangle$. This operation transforms the quantum state into a classical one by breaking the quantum coherence (and so the quantum nature) of the state. Therefore, measurement is typically applied as the last operation in a quantum circuit to get the final (classical) result of the coherent (i.e. in superposition) evolution of the quantum system represented by the circuit.

That two particles x and y, forming a composite system, become entangled means that, as a result of some computation, the state of the entire system, which they are part of, is in a superposition of strongly correlated product states of x and y, so that there is no way to characterise either one of the two particles by itself without referring to the other as well. Consequently, if measurements are made on an entangled state $ab + cd$, where a and c are two possible states of x and b and d are two possible states of y, then if x is found in state a, y must be in state b; similarly if x is found in state c, y must be in state d.

As an example, the state $1/\sqrt{2}(|00\rangle + |11\rangle)$ in the Hilbert space $\mathcal{H}^2 \otimes \mathcal{H}^2$ is entangled because it cannot be expressed as a tensor product of the individual states of the two component qubits. In this state, if one qubit is measured and found to be in the state $|0\rangle$, the other qubit will instantaneously collapse to the state $|0\rangle$ as well, and similarly for the state $|1\rangle$. In some cases, measuring a qubit of an entangled pair alters the other, keeping it in a quantum state. For instance, consider the entangled state $1/2(|00\rangle+|01\rangle+|10\rangle-|11\rangle)$. If the first qubit is measured and found in the state $|0\rangle$, the other qubit will instantaneously collapse to the state $1/\sqrt{2}(|0\rangle + |1\rangle)$ and, similarly, if the first after the measurement collapses to $|1\rangle$, then the other will be in state $1/\sqrt{2}(|0\rangle - |1\rangle)$.

2.2 Density Operator

Quantum mechanics can also be formulated in terms of density operators rather than state vectors [11, Chapter 2.4]. Given a state vector $|\psi\rangle$, the corresponding density operator is the matrix $\rho = |\psi\rangle\langle\psi|$, where $\langle\psi|$ is the conjugate transpose of $|\psi\rangle$ or 'bra' vector in Dirac's notation[2]. For instance, if $|\psi\rangle = 1/\sqrt{2}(|0\rangle - |1\rangle)$, the corresponding density operator is:

$$\rho = \begin{bmatrix} .5 & -.5 \\ -.5 & .5 \end{bmatrix}. \tag{1}$$

This formulation is mathematically equivalent to the state vector approach but is often more convenient for certain scenarios, particularly when dealing with quantum systems where the exact state is uncertain and can be in a statistical distribution of states $\{(p_i, |\psi_i\rangle)\}_i$, where p_i is the probability associated to the state $|\psi_i\rangle$. The density operator for this system is defined by $\rho \equiv \sum_i p_i\,|\psi_i\rangle\,\langle\psi_i|$. As an example, consider a quantum system in which there is a 50% probability

[2]If $|\psi_i\rangle$ is column vector $(\alpha,\beta)^T$, then $\langle\psi|$ is a row vector (α^*,β^*), where α^*, β^* are the complex conjugate of α, β

that the system is in the state $|0\rangle$ or in the state $|1\rangle$. The density matrix for this state is:

$$\rho = 0.5\,|0\rangle\langle 0| + 0.5\,|1\rangle\langle 1| = \begin{bmatrix} .5 & 0 \\ 0 & .5 \end{bmatrix}. \tag{2}$$

We note that in Equation 1, we represent a system where we know for sure the state it is in (that is a quantum superposition), while in Equation 2, the system is represented by a statistical distribution, so we do not know the exact state of the quantum system. In particular, when a quantum state is known with certainty, we say that the state is *pure*, while if the state of the system is in a statistical distribution of pure states, we say that the state is *mixed*.

The purity of a quantum state described by the density operator ρ can be checked considering its trace $\mathrm{Tr}(\rho) = \sum_i \langle i|\,\rho\,|i\rangle$, where $\{|i\rangle\}_i$ is any orthonormal basis [cf. Chapter 2][11]. In particular, if ρ is pure, then $\rho^2 = \rho$ and so $\mathrm{Tr}(\rho) = \mathrm{Tr}(\rho^2) = 1$. Instead, if ρ is mixed, $\rho^2 \neq \rho$ and $\mathrm{Tr}(\rho^2) < 1$.

The partial measurement of a state, i.e. removing a part of a quantum system by measuring it, can be performed by the partial trace operator. For two systems A and B and state $\rho_{A,B} \in \mathcal{H}_A \otimes \mathcal{H}_B$, the partial trace $\mathrm{Tr}_B(\rho_{A,B})$ gives the state ρ_A of A and $\mathrm{Tr}_A(\rho_{A,B})$ results in the state ρ_B of B. Mathematically, this is expressed as:

$$\mathrm{Tr}_A(\rho_{A,B}) = \sum_i (\langle i|_A \otimes I_B)\rho_{A,B}(|i\rangle_A \otimes I_B) = \rho_B,$$

where $\{|i\rangle_A\}_i$ is any orthonormal basis for the Hilbert space $\mathcal{H}_A$.

2.3 Entanglement and Quantum Programming

As explained in [1], a high-level approach to programming quantum computers requires particular care in dealing with variables that are abstractions of entangled qubits, in order to avoid incorrect results. Here, we introduce an abstract domain for the entanglement property, which can be used to detect entangled variables while analysing quantum programs. For the definition of our abstract domain, we will follow [17] and construct the space of values for the set $Q = \{q_i\}$ of all program's quantum variables as the Hilbert space $\mathcal{H}_Q = \bigotimes_i \mathcal{H}_{q_i}$ obtained by composing via tensor product the space of each variable. We write $|\psi\rangle_q$ to indicate that q represents the state $|\psi\rangle$ in $\mathcal{H}_q$. For entangled states, such as for example $^1/\sqrt{2}(|01\rangle + |10\rangle)$, we write $(^1/\sqrt{2}(|01\rangle + |10\rangle))_{p,q}$ to indicate that p and q represent, respectively, the first and the second qubit of the entangled pair. In this case, the state is a vector in the space $\mathcal{H}_p \otimes \mathcal{H}_q$.

3 The Entanglement Property

To define an abstract domain that is able to capture the entanglement property of quantum variables, we will introduce a characterisation of this property by means of an equivalence relation on the domain of the variables values.

As intuitively explained before, entanglement is about the non-separability of states, and therefore, its characterisation necessarily involves a difficult problem in quantum information theory, namely the *separability problem*, which is a subject of current research. The problem has been shown to be NP-hard in [3, 5], so in general, determining if a state is separable is not straightforward.

We will limit our treatment to pure states and consider only the uncertainty within quantum mechanics (state superposition), thus avoiding the complication coming from the additional statistical information encoded in mixed states as a probability distribution (real convex combination) of pure states. For pure states in bipartite systems, described as vectors in the tensor product space $H_{q_1} \otimes H_{q_2}$ of variables q_1 and q_2 in Q, separability and entanglement can be easily defined as dual notions as follows.

Definition 1. A composite quantum state $|\psi\rangle_{q_1,q_2} \in \mathcal{H}_{q_1} \otimes \mathcal{H}_{q_2}$ is separable if and only if it can be written as $|\psi\rangle_{q_1,q_2} = |\phi_1\rangle \otimes |\phi_2\rangle$ for some states $|\phi_1\rangle \in \mathcal{H}_{q_1}$ and $|\phi_2\rangle \in \mathcal{H}_{q_2}$. A state $|\psi\rangle_{q_1,q_2}$ is entangled if and only if it is not separable.

However, when the space of the variables values is a composite system of $n \geq 3$ qubits, the situation becomes more complex. In this case, the entanglement of the full system corresponds to *full inseparability*, while other types of multipartite entanglement can be defined depending on the separability of the various subsystems.

A popular approach to capture the various degrees of separability of a multipartite system is to measure the amount of entanglement of its subsystems based on some particular functions called *entanglement monotones* and *entanglement measures*[16]. For example, in [2], a distance on the set of qubits of a given state $|\psi\rangle$ is defined in terms of an entanglement monotone function $E_{|\psi\rangle}(q_i, q_j)$. In this approach, $E_{|\psi\rangle}(q_i, q_j) = 0$ if and only if q_i and q_j are not entangled in the state $|\psi\rangle$. Generalising these functions to sets of variables, we can define two sets $\{p_i\}, \{q_i\}$ separable (equivalently, non-entangled) if and only if $E_{|\psi\rangle}(\{p_i\}, \{q_i\}) = 0$. Following the classification of [2], a multipartite state $|\psi\rangle_{q_1,q_2,q_3}$ can result in one of the following three cases:

- *Product states.* These are fully separable states that can be written as $|\psi\rangle_{q_1} \otimes |\psi\rangle_{q_2} \otimes |\psi\rangle_{q_3}$. In this case, for all $i, j, k \in \{1, 2, 3\}$ we get $E_{|\psi\rangle}(q_i, q_j) = 0$ and $E_{|\psi\rangle}(q_i, \{q_j, q_k\}) = 0$.
- *Bi-separable states.* These can be written as $|\psi\rangle_{q_1} \otimes |\psi\rangle_{q_2,q_3}$. In this case, we get $E_{|\psi\rangle}(q_1, q_2) = E_{|\psi\rangle}(q_1, q_3) = 0$ and $E_{|\psi\rangle}(q_1, \{q_2, q_3\}) = 0$, while $E_{|\psi\rangle}(q_2, q_3) \neq 0$ as well as $E_{|\psi\rangle}(q_2, \{q_1, q_3\}) \neq 0$ and $E_{|\psi\rangle}(q_3, \{q_1, q_2\}) \neq 0$.
- *Fully inseparable states.* These can only be written as $|\psi\rangle_{q_1,q_2,q_3}$, i.e., as an entangled three-qubit state. States belonging to this case might have $E_{|\psi\rangle}(q_i, q_j) = 0$

for some pairs of qubits q_i and q_j. However, the bipartite entanglement $E_{|\psi\rangle}(q_i, \{q_j, q_k\})$ always differs from zero for all i, j, k.

Thus, full entanglement of a multipartite system does not imply the full entanglement of its subsystems. For instance, consider the well-known fully inseparable (or fully entangled) GHZ_3 state $|\psi\rangle_{q_1,q_2,q_3} = 1/\sqrt{2}(|000\rangle + |111\rangle)_{q_1,q_2,q_3}$. As shown in [2], for this state we have $E(q_i, q_j) = 0$ for all $i, j \in \{1, 2, 3\}$, i.e. any two qubits taken in isolation form a separable subsystem, while for the other well-known fully inseparable state $W_3 = 1/\sqrt{3}(|100\rangle + |010\rangle + |001\rangle)_{q_1,q_2,q_3}$, each pair of qubits is entangled as $E(q_i, q_j) \neq 0$ for all $i, j \in \{1, 2, 3\}$. Moreover, the multipartite entanglement is not transitive within the multipartite system. This means that for a system of three variables q_1, q_2 and q_3, if q_1 and q_2 are entangled and q_2 and q_3 are entangled, it is not always the case that q_1 and q_3 are entangled. As an example consider the state $1/2(|000\rangle + |001\rangle + |011\rangle + |111\rangle)_{q_1,q_2,q_3}$. For this state we have $E(q_1, q_2) > 0$, $E(q_2, q_3) > 0$ but $E(q_1, q_3) = 0$.

3.1 Checking Separabilty

A criterion to check the full separability of a pure n-multipartite state $|\psi\rangle_{q_1,\ldots,q_n}$, i.e. checking that $|\psi\rangle_{q_1,\ldots,q_n} = |\psi\rangle_{q_1} \otimes |\psi\rangle_{q_2} \otimes \ldots \otimes |\psi\rangle_{q_n}$, is to compute reduced density matrices of the elementary subsystems and see whether they are pure. In fact, since tracing out a part of a quantum system means measuring and discarding that part, the partial trace will produce different results if the one we discard is entangled with the rest. For example, consider systems A and B in the two-qubit state $|\psi\rangle = |1\rangle_A \otimes 1/\sqrt{2}(|0\rangle + |1\rangle)_B$, where A and B are separable. The density operator of the system is

$$\rho = |\psi\rangle\langle\psi| = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & .5 & .5 \\ 0 & 0 & .5 & .5 \end{bmatrix}.$$

Applying the partial trace operators, we obtain

$$\mathrm{Tr}_A(\rho) = \begin{bmatrix} .5 & .5 \\ .5 & .5 \end{bmatrix} \quad \mathrm{Tr}_B(\rho) = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

Since the two systems are separable, computing $\mathrm{Tr}_A(\rho)$ and $\mathrm{Tr}_B(\rho)$ gives the state of B and A respectively.

Consider now an entangled state like $|\psi\rangle = 1/\sqrt{2}(|00\rangle + |11\rangle)_{AB}$, characterised by the following density operator:

$$\rho = |\psi\rangle\langle\psi| = \begin{bmatrix} .5 & 0 & 0 & .5 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ .5 & 0 & 0 & .5 \end{bmatrix}.$$

Applying the partial trace operators, we obtain

$$\mathrm{Tr}_A(|\psi\rangle\langle\psi|) = \mathrm{Tr}_B(|\psi\rangle\langle\psi|) = \begin{bmatrix} .5 & 0 \\ 0 & .5 \end{bmatrix}.$$

Deleting one qubit alters the state of the other, causing it to collapse to $|0\rangle$ or $|1\rangle$ with equal probability. The resulting density operator is, therefore, a mixed state[3]. Thus, we can use these properties to verify if two or more subsystems are separable. In particular, given ρ_{AB}, A is separable from B if and only if $\mathrm{Tr}_A(\rho_{AB})$ (or $\mathrm{Tr}_B(\rho_{AB})$) is a pure state.

For a set of variables, we can formulate a similar criterion as follows: given a set Q of quantum variables and a state $|\psi\rangle_Q$, a set of variables $e \subseteq Q$ is separable, i.e. $|\psi\rangle_Q = |\psi\rangle_{Q\setminus e} \otimes |\psi\rangle_e$, if and only if $\mathrm{Tr}_e(|\psi\rangle\langle\psi|)$ or $\mathrm{Tr}_{Q\setminus e}(|\psi\rangle\langle\psi|)$ is a pure state.

The partial trace underlines the most interesting feature of separability, that is, if two particles are separable (and thus not entangled), then we know that we can measure one of them without altering the other.

4 Non-separability Domain

We now give the formal definition of the separability of two variables in a multi-variable state. Let $Q = \{q_i\}_i$ be a set of quantum variables and $\mathcal{H}_Q = \bigotimes_i \mathcal{H}_{q_i}$ the Hilbert space of all the variables values.

Definition 2 (Separability on Variables)**.** Let Q_ψ be the set of variables in a state $|\psi\rangle$. Two variables $q_1, q_2 \in Q_\psi$ are separable if the state $|\psi\rangle$ can be written as $|\psi\rangle = |\phi_1\rangle_{Q_1} \otimes |\phi_2\rangle_{Q_2}$, where $Q_1, Q_2 \subset Q_\psi$, $q_1 \in Q_1$ and $q_2 \in Q_2$. Otherwise, we say that q_1, q_2 are *non-separable*.

We note that the (non-)separability can also be defined in terms of partial trace by saying that q_1, q_2 are (non-)separable if and only if there (does not) exist two sets $Q_1, Q_2 \subset Q_\psi$ with $q_1 \in Q_1$ and $q_2 \in Q_2$, such that $\mathrm{Tr}_{Q_1}(|\psi\rangle\langle\psi|)$ and $\mathrm{Tr}_{Q_2}(|\psi\rangle\langle\psi|)$ give pure states.

Proposition 3. *Given a set of variables Q in a state $|\psi\rangle_Q$ and three variables q_1, q_2 and q_3 in Q, if q_1 and q_2 are non-separable and q_2 and q_3 are non-separable, then q_1 and q_3 are non-separable.*

Proof. Let $|\psi\rangle_Q = |\phi_1\rangle_{Q_1} \otimes |\phi_2\rangle_{Q_2}$. Without loss of generality, we can assume that $q_1 \in Q_1$. Since q_1 and q_2 are non-separable q_2 must be in Q_1. But, by hypothesis also q_2 and q_3 are non-separable, so q_3 must also be in Q_1. This means that q_1 and q_3 must be in the same set (in this case, Q_1), and so they are non-separable. □

Let V_Q be the set of all vectors $|\psi\rangle \in \mathcal{H}_Q$. We can extend the definition of the non-separability property as a relation on the powerset $\wp(V_Q)$ of V_Q as follows.

Definition 4 (Non-separability on $\wp(V_Q)$)**.** Given a set Q of variables and a set of states $v \in \wp(V_Q)$, two variables $q_1, q_2 \in Q$ are non-separable in v if they are non-separable in at least one state $|\psi\rangle_Q \in v$.

[3]We remark once more that having $|0\rangle$ and $|1\rangle$ with equal probability is different from having a uniform superposition of $|0\rangle$ and $|1\rangle$: in the former case we will have a classical probabilistic distribution on states while in the latter a quantum superposition.

Since the non-separability with respect to a single value is transitive, so is the non-separability with respect to a set of values. The non-separability relation is trivially symmetric, and we can easily assume that a state is non-separable from itself, i.e. that the non-separability is reflexive. It is, therefore, an equivalence relation.

We now introduce our abstract domain for the analysis of entanglement. To this purpose, we will define an abstraction of the non-separability relation. The fact that this is an equivalence relation guarantees that our abstraction is supported by a Galois insertion [7, 15]. Moreover, it can be represented by the set of its equivalence classes, which determine a partition of the set of variables Q. We recall that $\pi^Q \subset \wp(Q)$ is a partition of Q, iff $\forall\, p_1, p_2 \in \pi^Q, p_1 \cap p_2 = \varnothing$, meaning that all sets in π^Q are disjoint from each other, and $\cup_{p_i \in Q} p_i = Q$. For instance, given three variables a, b, c in the state $(|00\rangle + |11\rangle)_{a,b} \otimes |0\rangle_c$, the non-separability relation is represented by the partition $(\{a, b\}, \{c\})$.

4.1 Abstract Domain

As already mentioned, given a set of variables Q, the non-separability relation determines a partition, π^Q, of Q. We then define our abstract domain as the set, $\Pi^Q \subset \wp(\wp(Q))$, of all partitions of Q. An order relation on Π^Q can be defined as follows.

Definition 5 ($\Pi^Q, \sqsubseteq$)**.** Given $\pi_1^Q, \pi_2^Q \in \Pi^Q$, $\pi_1^Q \sqsubseteq \pi_2^Q$ iff $\forall p_1 \in \pi_1^Q, \exists\, p_2 \in \pi_2^Q$ such that $p_1 \subseteq p_2$.

We call $\sqcup$ and $\sqcap$ the least upper bound (LUB) and the greater lower bound (GLB) induced by $\sqsubseteq$.
For instance, $(\{a\}, \{b\}, \{c\}) \sqsubset (\{a, b\}, \{c\})$, $(\{a, b\}, \{c\}) \sqcup (\{a\}, \{b, c\}) = (\{a, b, c\})$ and $(\{a, b\}, \{c\}) \sqcap (\{a\}, \{b, c\}) = (\{a\}, \{b\}, \{c\})$.

We can now define a pair of functions α_π, γ_π between the concrete domain and the abstract domain that form a Galois Insertion[7, 15].

4.2 Abstraction and Concretization

We need to define the concretisation function to give real meaning to elements in the abstract domain. Let $Q = \{q_i\}_i$ be the set of variables, we call $\mathcal{H}_Q = \bigotimes_i \mathcal{H}_{q_i}$ the Hilbert space of all variables. Let V_Q be the set of all vectors $|\psi\rangle \in \mathcal{H}_Q$, we define the concretization function $\gamma_\pi : \Pi^Q \to \wp(V_Q)$ as:

$$\gamma_\pi(\pi^Q) = \left\{ |\psi\rangle_Q \,\middle|\, |\psi\rangle_Q = \bigotimes |\phi_i\rangle_{p_i}, \forall p_i \in \pi^Q \right\},$$

i.e. the set of all states we can separate according to the partition π^Q. For instance, if $Q = \{q_1, q_2, q_3\}$ and $\pi^Q = (\{q_1, q_2\}\{q_3\})$, $\gamma_\pi(\pi^Q) = \{|\psi\rangle \,|\, |\psi\rangle = |\phi_1\rangle_{q_1,q_2} \otimes |\phi_2\rangle_{q_2}\}$, i.e., all states in which we can separe q_1 and q_2 from q_3. We can write the concretisation function also in terms of partial trace, in particular,

$$\gamma_\pi(\pi^Q) = \left\{ |\psi\rangle \,\middle|\, \forall p_i \in \pi^Q, \mathrm{Tr}_{p_i}(|\psi\rangle\langle\psi|) \text{ is pure} \right\}.$$

Using γ_π we can define the abstraction function $\alpha_\pi : \wp(V_Q) \to \Pi^Q$.

Definition 6. Let $v \subseteq V_Q$ be a set of states in $\mathcal{H}_Q$, we define

$$\alpha_\pi(v) = \bigsqcap \left\{ a \in \Pi^Q \,\middle|\, v \subseteq \gamma_\pi(a) \right\}$$

In other words, given a set of states, we take the abstract state that best approximates the concrete state.

5 Improving the Abstract Domain

Now that we are able to effectively approximate the non-separability of variables, we also want to analyse the different relations that can exist between them. For instance, let us consider the set of variables a, b, c in the state $|\psi\rangle_{a,b,c} = ((|00\rangle + |11\rangle)\,|0\rangle + (|00\rangle - |11\rangle)\,|1\rangle)_{a,b,c}$. On an intuitive level, it can be seen that the three variables are not related in the same way. In fact, a and b are more closely related to each other than either a with c or b with c: if we measure a, b collapses to a base state (0 or 1) and vice versa, while if we measure c, a and b remain in a superposition state. When two variables are related as a and b in this example, we say that they are *on the same level.*

Definition 7. Given two variables a and b in a state $|\psi\rangle$, we say that two entangled variables are *on the same level* if, by measuring one of them, the other also collapses to a base state.

A direct consequence of being on the same level is that if we apply a controlled not (cx) between two same-level variables, we will always 'disentangle' the target variable. For instance, if we apply $\mathsf{cx}(a, b)$, where a is the controller and b is the target, to the state $|\psi\rangle_{a,b,c}$, we obtain:

$$\begin{aligned}\mathsf{cx}(a,b)(|\psi\rangle_{a,b,c}) &= ((|00\rangle + |10\rangle)\,|0\rangle + (|00\rangle - |10\rangle)\,|1\rangle)_{a,b,c} \\ &= ((|0\rangle + |1\rangle)\,|0\rangle + (|0\rangle - |1\rangle)\,|1\rangle)_{a,c} \otimes |0\rangle_b\,. \end{aligned} \tag{3}$$

That is, we have separated b from the other variables. Instead if we apply $\mathsf{cx}(c, a)$ we obtain:

$$\mathsf{cx}(c,a)(|\psi\rangle_{a,b,c}) = ((|00\rangle + |00\rangle)\,|0\rangle + (|10\rangle - |01\rangle)\,|1\rangle)_{a,b,c}. \tag{4}$$

In this case, since c and a are not on the same level, we do not 'disentangle' a.

To represent the entangled states in which this property holds, we need to introduce an improvement in the abstract domain we previously defined.

Intuitively, given as an example the four variables a, b, c, d in the state

$$((|00\rangle + |11\rangle)\,|0\rangle + (|00\rangle - |11\rangle)\,|1\rangle)_{a,b,c} \otimes |1\rangle_d\,,$$

we can build the partition $(\{a, b, c\}\{d\})$ that represents the non-separable variables and then split it into another partition $(\{a, b\}\{c\}, \{d\})$ that identifies, for each non-separable set of variables, which ones are on the same level. To have a compact representation of both the partitionings, we use

a list of numbered sets $[(\{a,b\},0),(\{c\},0),(\{d\},1)]$. Here, the sets $(\{a,b\}\{c\}\{d\})$ indicates which variables are on the same level while joining the sets marked the same number, we obtain $(\{a,b,c\}\{d\})$, i.e. the partition representing the non-separable variables. More formally,

Definition 8. Given a set of quantum variables Q, we define the abstract state $\mathcal{E}^Q$ as a set of tuple, as follows:

$$\mathcal{E}^Q = \left\{ (e_i, k_i) \,\middle|\, \{e_i\}_i \in \Pi^Q \text{ and } k_i \in \mathbb{N} \right\}.$$

We call $\mathbb{E}^Q \subset \wp(Q) \times \mathbb{N}$ the abstract domain of all possible $\mathcal{E}^Q$. Given an abstract state $\mathcal{E}^Q = \{(e_i, k_i)\}$, we define $E_{k_i} = \bigcup\{e_i | (e_j, k_i) \in \mathcal{E}^Q\}$ as the union of all e_j (i.e. the sets that compose the tuples in the abstract state) with the same index. For instance, if $\mathcal{E}^{\{a,b,c,d,e\}} = [(\{a,b\},0),(\{c\},0),(\{d,e\},1)]$, $\{e_i\}_i = \{\{a,b\},\{c\}\{d,e\}\}$, $E_0 = \{a,b,c\}$ and $E_1 = \{d,e\}$. We now have all the elements to introduce an order in $\mathbb{E}^Q$.

Definition 9 ($\mathbb{E}^Q, \leqslant$)**.** Given $\mathcal{E}_1^Q, \mathcal{E}_2^Q \in \mathbb{E}^Q$. $\mathcal{E}_1^Q \leqslant_{\mathbb{E}} \mathcal{E}_2^Q$ iff $\forall e_2 \in \mathcal{E}_2^Q$, $\exists\, e_1 \in \mathcal{E}_1^Q$ such that $e_2 \subseteq e_1$ and $\forall E_k \in \mathcal{E}_1^Q$, $\exists\, E_h \in \mathcal{E}_2^Q$ such that $E_k \subseteq E_h$.

We write $\vee$ and $\wedge$ to refer to the least upper bound and the greatest lower bound induced by $\leqslant$.

We note that a most abstract state is a state that overestimates the non-separability (as before) but underestimates the variables on the same level. For instance, $[(\{a,b\},0),(\{c\},1)] \leqslant [(\{a\},0),(\{b\},0),(\{c\},1)] \leqslant [(\{a\},0),(\{b\},0),(\{c\},0)]$, moreover $[(\{a,b\},0),(\{c\},0)] \vee [(\{a\},0),(\{b,c\},0)] = [(\{a\},0),(\{b\},0),(\{c\},0)]$.

We now show that the property of being on the same level (Definition 7) is transitive.

Proposition 10. *If q_1 and q_2 are on the same level and q_2 and q_3 are on the same level, then q_1 and q_3 are on the same level.*

Proof. If q_1 and q_2 are on the same level, then if we measure q_1, then q_2 collapse to a base state, but since q_2 and q_3 are on the same level, then also q_3 will collapse. Thus, q_1 and q_3 are on the same level. □

Being on the same level is also trivially symmetric and reflexive; thus, it is an equivalence relation. The new abstract domain represents a property defined by composing two equivalence relations. In particular, we abstract being non-separable and being non-separable at the same level. This means that we can define a pair of functions $\alpha_l : \wp(V_Q) \to \mathcal{E}^Q$ and $\gamma_l : \mathcal{E}^Q \to \wp(V_Q)$ such that $\langle \mathcal{E}^Q, \alpha_l, \gamma_l, \wp(V_Q)\rangle$ forms a Galois Insertion[7, 15].

5.1 Abstraction and Concretization

We recall that $E_{k_i} = \bigcup\{e_i | (e_j, k_i) \in \mathcal{E}^Q\}$ represent the sets obtained by joining the sets e_j with the same k_i. Let γ_π be the concretisation function defined in the previous section.

Definition 11. We say that $\mathcal{E}^Q \approx |\psi\rangle^Q$ ($|\psi\rangle_Q$ is abstracted by $\mathcal{E}^Q$) if and only if:

- $|\psi\rangle_Q \in \gamma_\pi(\{E_k\})$ where $E_k \in \mathcal{E}^Q$);
- $\forall e_i \in \mathcal{E}^Q$, $\forall q_i, q_j \in e_i$ we have that q_i and q_j are on the same level in $|\psi\rangle_Q$.

In other words, we say that an abstract state $\mathcal{E}^Q$ abstracts a concrete state if and only if the abstract state approximates the set of non-separable variables and all variables in the set e_i are on the same level.

We define the concretization function $\gamma_l : \mathbb{E}^Q \to \wp(V_Q)$ as:

$$\gamma_l(\mathcal{E}^Q) = \left\{ |\psi\rangle_Q \,\middle|\, \mathcal{E}_Q \approx |\psi\rangle_Q \right\}.$$

Then with γ_l we define the abstraction function $\alpha_l : \wp(V_Q) \to \mathcal{E}^Q$.

Definition 12. Let be $v_Q \subseteq V_Q$ a set of states in $\mathcal{H}_Q$, we define

$$\alpha_l(v) = \bigwedge \left\{ a \in \mathcal{E}^Q \,\middle|\, v \subseteq \gamma_l(a) \right\}.$$

6 Using the Domain

The strength of our approach lies in the ability to represent which variables are at the same level within abstract states, improving the precision of entanglement analysis. We show how we use our domain to analyse a quantum program integrating the domain with the labels used by Perdrix in [12]. Perdrix employs a function $B^Q : Q \to \{\mathbf{s}, \mathbf{d}, \top, \bot\}$ that assigns to each variable $q \in Q$ a label $l \in \{\mathbf{s}, \mathbf{d}, \top, \bot\}$. In particular, given $b \in B$, $b(q) = \mathbf{s}$ states that q is in a classical state ($|0\rangle$ and $|1\rangle$) and $b(q) = \mathbf{d}$ indicates that the variable in a uniform superposition ($^1/_{\sqrt{2}}(|0\rangle \pm |1\rangle)$). We compare the analysis of Perdrix that used as domain the pair $\Pi^Q \times B^Q$ with an analysis based on our improved domain, thus using the pair $\mathbb{E}^Q \times B^Q$.

Given $Q = \{p, q\}$, we consider the small quantum program in Figure 1, where we show in black the concrete states, in red the abstract states with the Perdrix domain $\Pi^Q \times B^Q$ and in blue the states in our improved domain $\mathbb{E}^Q \times B^Q$. Since the initial state of the program is $|00\rangle_{q,p}$, we start from abstract states where all the variables are separable and the labelling function b is $\{p, q \to \mathbf{s}\}$. We apply the Hadamard gate h to p, putting p in uniform superposition, so we change its label from **s** to **d**. The first control-not (cx) gate at line **2** entangles p with q. In the Perdrix abstract semantics, the control-not gate (cx(q,p)) makes non-separable two variables only if the controlled (q) is not classic (so its label is not **s**) and if the target (p) is not in uniform superposition (its label is not **d**). In our case, $B(q) = \mathbf{d}$ and $B(p) = \mathbf{s}$ so the abstract cx gate makes p, q non-separable. As we see in the concrete state, if the target (p) is in a classical state, the cx gate also makes q and t two variables at the same level. So, in our domain, the cx gate makes two variables at the same level if the target is labelled as **s**. Moreover, when two variables are entangled, their state is no longer a state representable by the label **s** or **d**, so when the cx gate introduces entanglement, we must change the label of the two variables to $\top$. With the cx

0:	$\{\|00\rangle_{p,q}\}$
	$[\{p\},\{q\}]$ $\{p,q{\rightarrow}\mathbf{s}\}$
	$[(\{p\},0),(\{q\},1)]$ $\{p,q{\rightarrow}\mathbf{s}\}$
1: h(p)	$\{{}^1/_{\sqrt{2}}(\|00\rangle + \|10\rangle)_{p,q}\}$
	$[\{p\},\{q\}]$ $\{p{\rightarrow}\mathbf{d};q,t{\rightarrow}\mathbf{s}\}$
	$[(\{p\},0),(\{q\},1)]$ $\{p{\rightarrow}\mathbf{d};q{\rightarrow}\mathbf{s}\}$
2: cx(p,q)	$\{{}^1/_{\sqrt{2}}(\|00\rangle + \|11\rangle)_{p,q}\}$
	$[\{p,q\}]$ $\{p,q{\rightarrow}\top\}$
	$[(\{p,q\},0)]$ $\{p,q{\rightarrow}\top\}$
3: cx(q,p)	$\{{}^1/_{\sqrt{2}}(\|00\rangle + \|01\rangle)_{p,q}\}$
	$[\{p,q,t\}]$ $\{p,q,t{\rightarrow}\top\}$
	$[(\{p\},1),(\{q\},0)]$ $\{p{\rightarrow}\mathbf{s};q{\rightarrow}\top\}$

Figure 1. A small quantum program with two variables (p, q). On the right, we show the concrete quantum states (in black), the abstract states using the Perdrix domain (in red) and the abstract states in our improved domain (in blue)

gate in line **3** we obtain the final state ${}^1/_{\sqrt{2}}(|00\rangle + |01\rangle)_{p,q} = |0\rangle_p \otimes {}^1/_{\sqrt{2}}(|0\rangle + |1\rangle)_q$, i.e. we separate p from q. At this point in the program, we see the added value of our domain. In fact, with the Perdrix domain, once we have created the state in which the variables are not separable, we no longer have any information on how they are bound, so we can no longer separate them. Instead, with our enriched domain, we know that the variables p, q are at the same level, and therefore we know that the last cx gate separates p and q. Furthermore, by separating p, the last cx gate makes p labelled with **s**. In conclusion, we have shown that with our domain, it is possible to improve precision when the entanglement is nullified.

7 Related Work

An entanglement analysis was introduced in [12] for a simple language which uses abstract semantics based on partitions. However, this approach does not lead to a *best approximation* of a state due to the non-transitivity of entanglement. As we have shown, the entanglement of more than two variables is better described by the notion of non-separability, and we have defined the non-separability relations proving that partitions are a correct abstract domain to capture non-separability. Furthermore, in Section 5, we have shown how to improve this domain.

Other systems have been developed to detect entanglement. All the existing works, apart from Honda's approach [6], model entanglement in terms of non-separability, identifying the group of non-separable variables. Honda's approach [6] is based on an abstract domain that uses density matrices. In this way, it is possible to abstract more information about entanglement, but the space of the abstract states grows exponentially with the program's size. In fact, to obtain a precise abstraction, due to the complex nature of entanglement, we need to represent the abstract states in a quantum way, but this requires a data structure exponentially large. In [13, 14], Rand introduces a type system based on Gottesman's [4] representation of Clifford gates (*H*,*S*,*CX*). This approach proposes a precise analysis of entanglement, although working at the circuit level (i.e. no control flow) and limited to Clifford gates and measurement.

The language Twist [18] includes the verification of the separability of states. However, this approach is based on annotations (that must be inserted manually) and dynamic checking (the scaling of the checking with big programs is limited). Another language which includes an analysis of entanglement is Scaffold[8]. This analysis works at the circuit level, only considering the *CNOT* gate, and is provided by a procedure without any formal definition.

8 Conclusion

We have introduced an abstract domain based on a partition of the set of quantum variables defined via the notion of separability. This domain is suitable for capturing the essential aspects of entanglement. We have also proposed a refinement of this domain by incorporating the concept of 'being on the same level', which captures a specific type of entangled variables with some nice computational properties. As a future work, we aim to build a static analysis to detect separability and entanglement, fully exploiting the information in our abstract domain. Our future analysis will use labels similar to the ones introduced in [12], where they are introduced in support of the analysis to understand when a variable is in a classical state or in a uniform superposition. However, due to the approximation introduced by the representation by partitions, the analysis in [12] fails to track when a gate or a measurement removes entanglement. We believe that combining these labels with our level-based domain makes it possible to improve the analysis. Whenever we apply a control-not gate to two variables of the same level, we will be able to separate them, and in addition, we will also be able to abstract the measurement better. Adding the concept of 'being at the same level' is a first step in trying to represent the entanglement in a better way.

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