Binary Superposed Quantum Decision Diagrams

David Rosenbaum
Portland State University, Department of Computer Science
Email: drosenba@cs.pdx.edu

Abstract

Binary Superposed Decision Diagrams (BSQDDs) are a new type of quantum decision diagram that can be used for representing arbitrary quantum superpositions. One major advantage of BSQDDs is that they are dependent on the types of gates used in synthesis and a BSQDD can be used to efficiently generate a quantum array that will initialize the quantum superposition that the BSQDD represents. Transformation rules for BSQDDs allow BSQDDs to be reduced into simpler BSQDDs that represent the same quantum superposition. Canonical forms exist for a broad class of BSQDDs. This allows BSQDDs to be used for synthesizing quantum arrays that are capable of initializing arbitrary quantum superpositions.

1 Introduction

1.1 Initialization Algorithms

Initializing a quantum superposition from a basis state is an important problem in quantum computing with applications in Grover's algorithm [5, 2] and quantum neural networks [12, 4]. Several initialization algorithms have been created to solve this problem. The Ventura-Martinez algorithm [11] requires $\Theta(mn)$ two qubit gates as well as $n+1$ ancilla qubits where m is the number of terms in the desired quantum superposition and n is the number of qubits in the desired quantum superposition. Another initialization algorithm that is based on a different idea is the Long-Sun algorithm [6] which requires no ancilla qubits but uses $\Theta(n^2 2^n)$ two qubit gates. The SQUID algorithm [8] is an improvement over the Ventura-Martinez algorithm [11] and uses $O(pn)$ two qubit gates and requires $n+2$ ancilla qubits where p is the number of disjoint phase groups in the phase map of the desired superposition. The ESQUID algorithm [9] is an extension of the SQUID algorithm [8] and uses $O(bn)$ two qubit gates and requires $n+2$ ancilla qubits where b is the number of disjoint generalized phase groups in the phase map of the desired superposition. BSQDDs do not require the ancilla qubits or the special initialization operators used in the Ventura-Martinez [11], SQUID [8] and ESQUID [9] algorithms and can be used to find quantum arrays that are more efficient than those generated by the Ventura-Martinez [11], Long-Sun [6], SQUID [8] and ESQUID [9] algorithms.

1.2 Quantum Decision Diagrams

Quantum decision diagrams called Quantum Information Decision Diagrams (QuIDDs) were first created by Viamontes, Rajagopalan, Markov and Hayes [14, 13] for representing quantum operators and states. Miller and Thornton [7] developed improved decision diagrams called Quantum Multivalued Decision Diagrams (QMDDs) for representing binary and multivalued quantum operators. Another set of quantum decision diagrams called Quantum Decision Diagrams (QDDs) was developed by Abdollahi and Pedram [1] for representing and synthesizing quantum operators. The purpose of BSQDDs is to provide a representation for quantum superpositions that can be used to synthesize a quantum array which will initialize the desired quantum superposition. This is done using only gates that are available for synthesis in a way that allows the generated quantum array to be synthesized directly from the resulting BSQDD. The generated quantum array can then be applied to the starting state in order to initialize the desired quantum superposition. The starting state can be any basis state.

1.3 Advantages of BSQDDs

The main purpose of BSQDDs is to synthesize quantum arrays for initialization. This is different from other quantum decision diagrams such as QuIDDs [14] and QMDDs [7] which focus on providing efficient representations of quantum operators and states rather than synthesizing quantum arrays for initialization. BSQDDs also differ from QDDs [1] which are used for synthesizing operators rather than states. For these reasons, BSQDDs are mainly comparable to quantum initialization algorithms since other quantum decision diagrams are not applicable to the problem of synthesizing quantum arrays for initializing desired quantum superpositions. BSQDDs have several important advantages over existing methods for synthesizing quantum arrays for initializing quantum superpositions. Some quantum superpositions can be initialized using only a linear number of one and two qubit operations with quantum arrays generated using BSQDDs while the Ventura-Martinez [11], SQUID [8] and Long-Sun [6] algorithms all require an exponential number of one and two qubit operations as is shown in section 11. This shows that BSQDDs can be used to achieve an exponential reduction in the number of required gates over existing methods other than the ESQUID algorithm [9] for initializing some classes of quantum superpositions. However, the ESQUID algorithm [9] requires the quantum superposition to be represented using generalized phase groups; this is a significant drawback because finding a sequence of generalized phase groups that will result in an efficient quantum array is a difficult problem that is not solved by the ESQUID algorithm [9]. The ESQUID algorithm [9] also still requires more one and two qubit operations than quantum arrays generated using BSQDDs for a class of quantum superpositions even though the difference in complexity is not exponential. Additionally, the ESQUID algorithm is only capable of initializing a narrow class of quantum superpositions while BSQDDs can be used for any quantum superposition given an appropriate set of gates. Unlike initialization algorithms such as the Ventura-Martinez [11], SQUID [8] and ESQUID [9] algorithms, BSQDDs do not require ancilla qubits for bookkeeping and therefore use less qubits. Another disadvantage of the Ventura-Martinez [11], SQUID [8] and ESQUID [9] algorithms is that they require special initialization operators in order to initialize the desired quantum superposition. Although these operators are unitary, it is unclear how they can be implemented efficiently using controlled single qubit gates. This means that it is not clear how a quantum array generated by the Ventura-Martinez [11], SQUID [8] or ESQUID [9] algorithm could actually be implemented on a quantum computer. BSQDDs do not suffer from this drawback and use only controlled single qubit gates from the set of gates available for synthesis. Although the Long-Sun algorithm [6] also does not require a special training operator and uses only controlled single qubit gates, it requires $\Theta(n^2 2^n)$ one and two qubit gates. BSQDDs are also capable of initializing any quantum superposition unlike initialization algorithms which can only initialize certain classes of quantum superpositions.

2 Creating the Starting State

Because BSQDDs require the starting state to be a basis state, it is necessary to run a special initialization algorithm before applying the quantum array that is generated by the BSQDD in order to create the starting state. This requires a different type of initialization algorithm than those discussed in section 1.1 as all of the algorithms in section 1.1 require the starting state to be $|0^n\rangle$. One algorithm that can be used for this task is the Schulman-Vazirani heat engine [10] which is capable of transforming the initial mixed state into the state $|0^n\rangle$. From now on, it will be assumed that the starting state can be created and the focus will be on properties and examples of BSQDDs.

3 The BSQDD

The idea behind BSQDDs is to represent a quantum superposition as a decision diagram where each node corresponds to a gate. The gate that corresponds to the node on each branch of the BSQDD is controlled by the path that was used to reach it from the root of the decision diagram. Thus, each branch of the BSQDD represents a different part of the desired quantum superposition. This idea is inspired by the observation that the quantum array synthesized by the Long-Sun [6] algorithm is similar to a binary tree and also by the idea of Binary Decision Diagrams [3].

4 A Simple BSQDD

Given a sufficient set of gates, a BSQDD can represent any quantum superposition as will be proven later in theorem 12.1. This section will illustrate the general concepts behind BSQDDs by finding a quantum array for initializing the state

$$|\psi\rangle = |x_1x_2x_3x_4\rangle = \frac{1}{2}|0101\rangle + \frac{1}{2}|0110\rangle + \frac{1}{2}|1001\rangle + \frac{1}{2}|1010\rangle \tag{1}$$

4.1 Finding the BSQDD

Using Hadamard gates, Feynman gates and inverters, this quantum superposition can be represented by the BSQDD shown in figure 1 for the order of variables (x_1, x_2, x_3, x_4) with respect to the starting state $|0000\rangle$. In figure 1, the quantum superpositions $\left|\psi^0\right\rangle$, $\left|\psi^1\right\rangle$, $\left|\psi^{01}\right\rangle$, $\left|\psi^{10}\right\rangle$, $\left|\psi^{010}\right\rangle$, $\left|\psi^{011}\right\rangle$, $\left|\psi^{100}\right\rangle$ and $\left|\psi^{101}\right\rangle$ next to the nodes are the quantum states that those nodes represent on their respective paths from the root node of the BSQDD where $\left|\psi^0\right\rangle = \frac{1}{2}|0101\rangle + \frac{1}{2}|0110\rangle$, $\left|\psi^1\right\rangle = \frac{1}{2}|1001\rangle + \frac{1}{2}|1010\rangle$, $\left|\psi^{01}\right\rangle = \frac{1}{2}|0101\rangle + \frac{1}{2}|0110\rangle$, $\left|\psi^{10}\right\rangle = \frac{1}{2}|1001\rangle + \frac{1}{2}|1010\rangle$, $\left|\psi^{010}\right\rangle = \frac{1}{2}|0101\rangle$, $\left|\psi^{011}\right\rangle = \frac{1}{2}|0110\rangle$, $\left|\psi^{100}\right\rangle = \frac{1}{2}|1001\rangle$ and $\left|\psi^{101}\right\rangle = \frac{1}{2}|1010\rangle$. The superscripts in each of the these quantum states indicates the path from the root node a_1 of the BSQDD to the node that represents the quantum state. For example, the quantum superposition $\left|\psi^{10}\right\rangle$ is represented by the node a_5 which can be reached from the root node a_1 by following the edge labeled by $|1\rangle$ to the node a_3 and then following the edge labeled with $|0\rangle$ to the node a_5. The reasoning behind these superscripts should become clear in the rest of this example. The BSQDD in figure 1 can be found from the quantum superposition in equation (1). Because the order of variables is (x_1, x_2, x_3, x_4), the qubit $|x_1\rangle$ is initialized first. Note that the qubit $|x_1\rangle$ is equal to $|0\rangle$ in half of the terms in equation (1) and is $|1\rangle$ in half of the terms in equation (1). Thus, the gate that corresponds to the first node a_1 is a Hadamard gate. The gate that corresponds to each node is controlled by the path used to reach it from the root node of the BSQDD. Thus, the gate that corresponds to the node a_2 is controlled by $\overline{x}_1$ and the gate that corresponds to the node a_3 is controlled by x_1. Because $|x_2\rangle = |1\rangle$ in the quantum superposition $\left|\psi^0\right\rangle$ represented by the BSQDD rooted at the node a_2, an inverter is used as the gate for the node a_2 because $|x_2\rangle = |0\rangle$ in the starting state. Note that the states represented by nodes other than a_1 are not normalized. This is because these states exist only as parts of the quantum superposition $|\psi\rangle$ and will not be initialized themselves. For the quantum superposition $\left|\psi^1\right\rangle$ represented by the BSQDD rooted at the node a_3, $|x_2\rangle = |0\rangle$ so the identity matrix is the operation that corresponds to the node a_3. Now consider the quantum superposition $\left|\psi^{01}\right\rangle$ represented by the node a_4. Because $|x_3\rangle = |0\rangle$ for half of the terms in $\left|\psi^{01}\right\rangle$ and $|x_3\rangle = |1\rangle$ for half of the terms in $\left|\psi^{01}\right\rangle$, the operation that corresponds to a_4 is a Hadamard gate. For the state $\left|\psi^{010}\right\rangle$ represented by the node a_6, $|x_4\rangle = |1\rangle$. Because $x_4 = |0\rangle$ in the starting state, the operation that corresponds to the node a_6 is an inverter. Consider the state $\left|\psi^{011}\right\rangle$ represented by the node a_7. Since $|x_4\rangle = |0\rangle$ in $\left|\psi^{011}\right\rangle$ and $x_4 = |0\rangle$ in the starting state the operation that corresponds to the node a_7 is the identity matrix. Using the similar reasoning, the gates for the nodes a_5, a_8 and a_9 are obtained as shown in figure 1.

4.2 Reducing the BSQDD

The BSQDD in figure 1 will now be reduced. Reducing BSQDDs is important because the number of nodes in a BSQDD is an upper bound on the number of gates that will be required in the quantum array that is generated from the BSQDD. Observe that since $|x_3\rangle = |0\rangle$ in the quantum superposition the node a_6 is applied to, the control $\overline{x}_3$ can be added to this inverter without affecting the quantum superposition that will be initialized. Since the gate that corresponds to the node a_7 is the identity matrix and

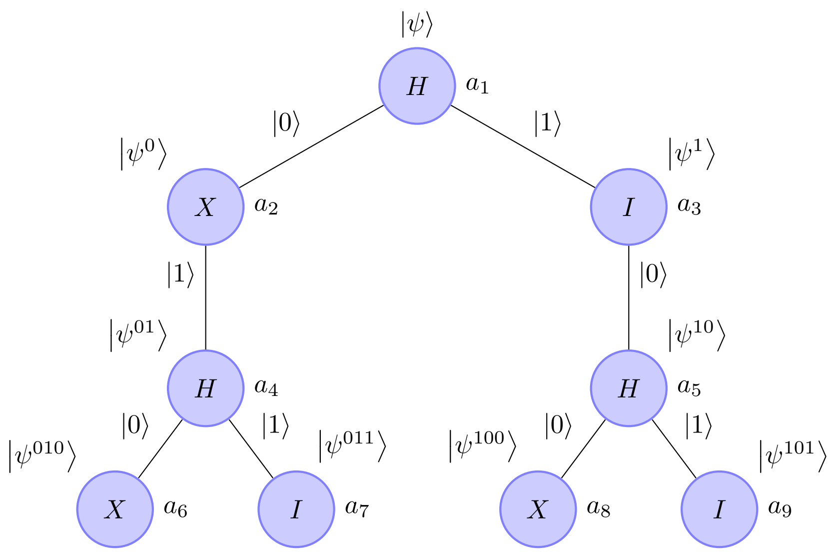


Figure 1: A simple unsimplified BSQDD

$|x_3\rangle = |1\rangle$ in the superposition the node a_6 is applied to, this identity matrix can be replaced by an inverter controlled by $\overline{x}_3$. Similarly, the gates that correspond to the nodes a_8 and a_9 can be replaced by the inverters controlled by $\overline{x}_3$. This results in the BSQDD shown in figure 2. Because the nodes a_6, a_7, a_8 and a_9 are now the same, they can be merged as shown in figure 3(a). Note that the node a_6 in figure 3(a) no longer has the state it represents shown. This is because the node a_6 now represents a different state on each of the four paths from the root node to the node a_6. The node a_6 represents $|\psi^{010}\rangle = \frac{1}{2}|0101\rangle$ on the path $(\overline{x}_1, x_2, \overline{x}_3)$, $|\psi^{011}\rangle = \frac{1}{2}|0110\rangle$ on the path $(\overline{x}_1, x_2, x_3)$, $|\psi^{100}\rangle = \frac{1}{2}|1001\rangle$ on the path $(x_1, \overline{x}_2, \overline{x}_3)$ and $|\psi^{101}\rangle = \frac{1}{2}|1010\rangle$ on the path $(x_1, \overline{x}_2, x_3)$. Each of the above tuples of literals denotes the path from the root node where all of the literals in the tuple are equal to 1. Note that summing the states represented by the node a_6 results in $|\psi\rangle$ which is the quantum superposition represented by the BSQDD. This is a general property of BSQDDs and will be proven later in theorem 7.3. The nodes a_4 and a_5 are also now the same so they can also be merged as shown in figure 3(b). The paths to the node a_5 from the root in figure 3(b) are the same as for the node a_6 in figure 3(a) and these nodes also represent the same states. The node a_4 in figure 3(b) represents $|\psi^{01}\rangle = \frac{1}{2}|0101\rangle + \frac{1}{2}|0110\rangle$ on the path $(\overline{x}_1, x_2)$ and $|\psi^{10}\rangle = \frac{1}{2}|1001\rangle + \frac{1}{2}|1010\rangle$ on the path $(x_1, \overline{x}_2)$. The gate for the node a_2 can be replaced by $X_{\overline{x}_1}$ because $|x_1\rangle = |0\rangle$ in the part of the quantum superposition the operation of the node a_2 is applied to. Similarly, the identity operation of the node a_3 can be replaced by $X_{\overline{x}_1}$ because $|x_1\rangle = |1\rangle$ in the part of the quantum superposition the operation of the node a_3 is applied to. Nodes a_2 and a_3 can then be merged which results in the final BSQDD shown in figure 4(a). Note that in this final BSQDD, the edge from the node a_2 to the node a_3 does not have a $|0\rangle$ or a $|1\rangle$ next to it as all the other

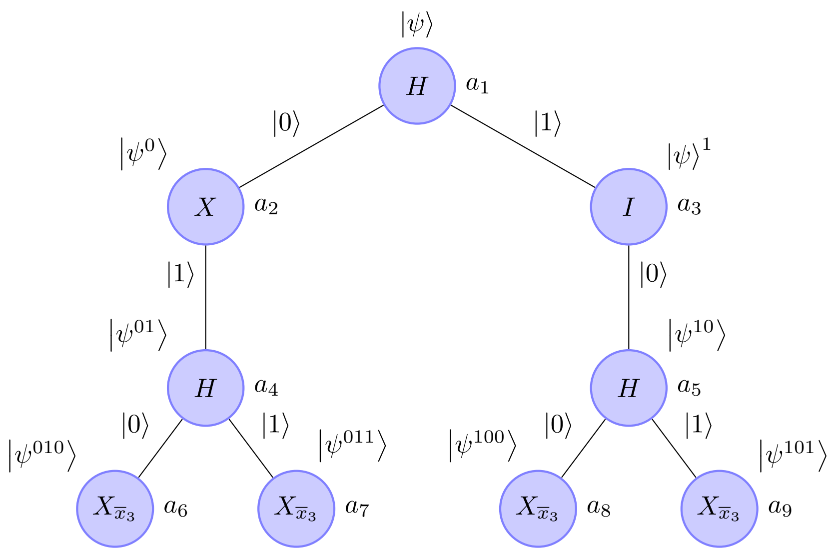
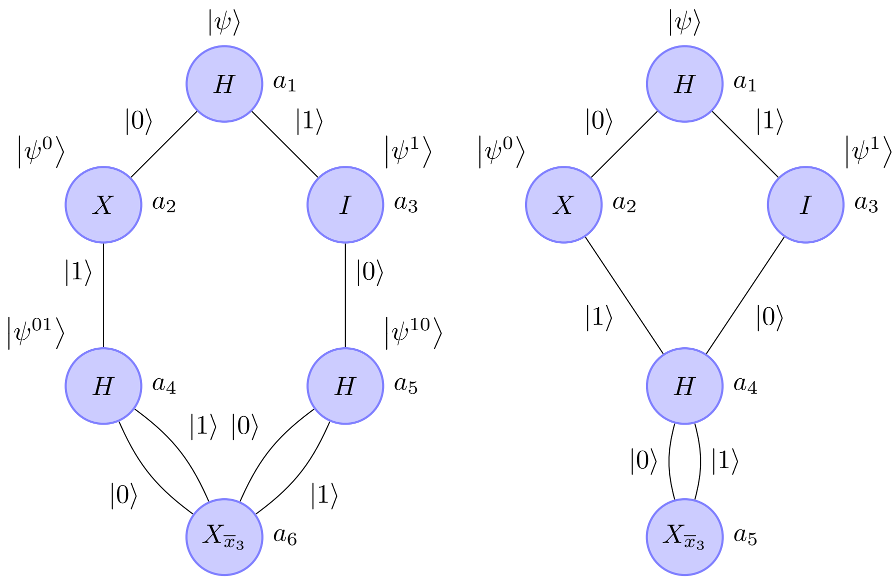


Figure 2: Replacing the gates for a_6, a_7, a_8 and a_9 with inverters controlled by $\overline{x}_3$

edges do; this is because this edge indicates a part of the quantum superposition where $|x_2\rangle = |0\rangle$ and also a different part of the quantum superposition where $|x_2\rangle = |1\rangle$ depending on which path from the root node is taken. The states represented by the nodes a_3 and a_4 in figure 4(a) are the same as the states represented by the nodes a_4 and a_5 in figure 3(b). The node a_2 represents the state $\frac{1}{2}|0101\rangle + \frac{1}{2}|0110\rangle$ on the path $(\overline{x}_1)$ and $\frac{1}{2}|1001\rangle + \frac{1}{2}|1010\rangle$ on the path (x_1).

4.3 Converting the BSQDD to a Quantum Array

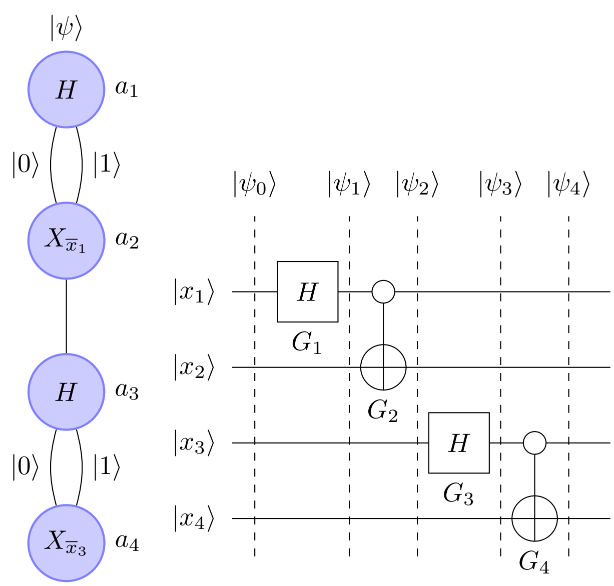
Now that the BSQDD has been reduced, it needs to be converted to a quantum array so that the desired superposition in equation (1) can be initialized. The quantum array in figure 4(b) generated by the final BSQDD in figure 4(a) can be obtained by adding the gates for the nodes in each layer of the BSQDD starting with the first layer. New gates are always placed to the right of gates that have already been placed in the quantum array. The first gate to be added is the Hadamard gate that corresponds to the node a_1 in figure 4(a). Because a_1 is the root node, no controls are needed for the gate that corresponds to this node. This results in the gate G_1 in figure 4(b). Now consider the node a_2. Since all paths from the root node to the second layer end at this node, no controls are required due to the paths to a_2 from the root node. However, the gate for this node is controlled by $\overline{x}_1$ so the inverter for this node must be controlled by $|0\rangle$ on $|x_1\rangle$. This causes the gate G_2 to be added to the quantum array. The next node is a_3. Because all paths from the root node to the third layer all end at the node a_3, no controls are required. The gate that corresponds to the node a_3 is G_3. The last node is a_4. All paths from the root node to the fourth layer terminate at the node a_4 so no



(a) Merging a_6, a_7, a_8 and a_9

(b) Merging a_4 and a_5

Figure 3: Merging nodes



(a) The final BSQDD

(b) The generated quantum array

Figure 4: The final BSQDD and the quantum array it generates

controls are needed. However, the gate for the node a_4 still needs to be controlled by $\overline{x}_3$ because the gate for the node a_4 is controlled by $\overline{x}_3$. This results in the gate G_4 being added to the quantum array. It is now necessary to apply the quantum array in figure 4(b) to the state $|0000\rangle$ to confirm that it initializes the superposition from equation (1) represented by the BSQDDs in figures 1, 2, 3(a), 3(b) and 4(a). The starting state is $|\psi_0\rangle = |0000\rangle$. Applying the Hadamard gate denoted by G_1 in figure 4(b) results in the state $|\psi_1\rangle = \frac{1}{\sqrt{2}}|0000\rangle + \frac{1}{\sqrt{2}}|1000\rangle$. The G_2 gate is then applied which changes the state to $|\psi_2\rangle = \frac{1}{\sqrt{2}}|0100\rangle + \frac{1}{\sqrt{2}}|1000\rangle$. The state $|\psi_3\rangle = \frac{1}{2}|0100\rangle + \frac{1}{2}|0110\rangle + \frac{1}{2}|1000\rangle + \frac{1}{2}|1010\rangle$ results after applying the G_3 Hadamard gate. After applying the final G_4 gate, the state is $|\psi_4\rangle = \frac{1}{2}|0101\rangle + \frac{1}{2}|0110\rangle + \frac{1}{2}|1001\rangle + \frac{1}{2}|1010\rangle$. Observe that $|\psi_4\rangle = |\psi\rangle$ where $|\psi\rangle$ is as defined in equation (1). Thus, BSQDDs can be used to find efficient quantum arrays for initializing quantum superpositions.

5 Formalizing BSQDDs

A formalization of BSQDDs will now be presented.

Definition 5.1. *A node in a BSQDD is denoted by $a = (G, f(y_1, \ldots, y_{j-1}), t)$ where G is the single qubit gate that corresponds to the node a, $f(y_1, \ldots, y_{j-1})$ is a boolean function called the control function of the node a and t is a tuple denoting the children of the node a. If $t = ()$ where $()$ denotes the empty tuple, then a has no children and is therefore a leaf node. Otherwise, if $g_{00} = 0$ or $g_{10} = 0$ where $G|0\rangle = g_{00}|0\rangle + g_{10}|1\rangle$ then t contains only one element; if neither of the first two conditions is satisfied, t is an ordered pair where the first element of t is the left child and the second element of t is the right child. The edge to the left child is called the $|0\rangle$ edge and the edge to the right child is called the $|1\rangle$ edge. Note that since G is unitary, $g_{00} = 0$ or $g_{10} = 0$ if and only if $g_{01} = 0$ or $g_{11} = 0$ where $G|1\rangle = g_{01}|0\rangle + g_{11}|1\rangle$ so it is not necessary to consider the case where $g_{01} = 0$ or $g_{11} = 0$ separately.*

For the BSQDD in figure 4(a), $a_1 = (H, f_1() = 1, (a_2, a_2))$, $a_2 = (X, f_2(x_1) = \overline{x}_1, (a_3))$, $a_3 = (H, f_3(x_1, x_2) = 1, (a_4, a_4))$ and $a_4 = (X, f_4(x_1, x_2, x_3) = \overline{x}_3, ())$. Note that because the control function for the root node $f_1()$ takes no arguments, it is always a constant.

Definition 5.2. *A layer of a BSQDD is denoted by $L = (C, |y\rangle)$ where C is a set nodes as defined in definition 5.1. Each node in the set C is said to be in the layer L. The qubit $|y\rangle$ is called the qubit operated on by the layer L. Each node in the set C is also said to operate on the qubit $|y\rangle$.*

In the BSQDD in figure 1, the first layer is $L_1 = (\{a_1\}, |x_1\rangle)$, the second layer is $L_2 = (\{a_2, a_3\}, |x_2\rangle)$, the third layer is $L_3 = (\{a_4, a_5\}, |x_3\rangle)$ and the fourth layer is $L_4 = (\{a_6, a_7, a_8, a_9\}, |x_4\rangle)$. Note that in this case all the nodes that operate on a qubit are in the same layer; this is not true in general as two or more layers may operate on the same qubit if the BSQDD has repeated variables. An example of repeated variables will be shown later in section 9. However, the nodes within any given layer always operate on the same qubit.

Definition 5.3. *A BSQDD is a 5-tuple* $B = (A, (L_1, \dots, L_m), \{x_1, \dots, x_n\}, (x_{i_1}, \dots, x_{i_m}), F)$ *where* A *is a non-empty set of nodes,* $\{x_1, \dots, x_n\}$ *is the set of variables that the nodes operate on, the* j^{th} *layer of the BSQDD is* L_j*, the order of variables is* $(x_{i_1}, \dots, x_{i_m})$ *and the gate that corresponds to each node is selected from the set of gates* F*. The qubit operated on by the layer* L_j *must be* $\left|x_{i_j}\right\rangle$ *and the children of nodes in the layer* L_j *must be in the* $j+1^{\mathrm{th}}$ *layer for* $j = 1, \dots, m-1$*. Also, the tuple denoting the children of any node in the layer* L_m *must be* $()$*. Every variable* x_k *must occur at least once in the order of variables. Every node in the BSQDD except the root node must be a child of some other node in the BSQDD. If the control function of any node in the* j^{th} *layer is* $f(y_1, \dots, y_{j-1})$ *then* $y_k \equiv x_{i_k}$ *for* $k = 1, \dots, j-1$*. Also, if* $x_{i_j} \equiv x_{i_k}$ *for some* $1 \leq k \leq j-1$ *then* $f(x_{i_1}, \dots, x_{i_{k-1}}, 0, x_{i_{k+1}}, \dots, x_{i_{j-1}}) = f(x_{i_1}, \dots, x_{i_{k-1}}, 1, x_{i_{k+1}}, \dots, x_{i_{j-1}})$ *must hold. This means that the output of the control function of a node cannot depend on the variable it operates on. Furthermore, if* $x_{i_k} \equiv x_{i_\ell}$ *for some* $1 \leq k < \ell \leq j-1$ *then* $f(x_{i_1}, \dots, x_{i_{k-1}}, 0, x_{i_{k+1}}, \dots, x_{i_{j-1}}) = f(x_{i_1}, \dots, x_{i_{k-1}}, 1, x_{i_{k+1}}, \dots, x_{i_{j-1}})$ *which means that a control function can only depend on the most recent repetition of a variable. In order to state the final constraint paths must be defined. A path from the root of a BSQDD to a node* $a = (G, f(x_{i_1}, \dots, x_{i_{j-1}}), t)$ *in the* j^{th} *layer is denoted by the tuple* $v = (v_{i_1}, \dots, v_{i_{j-1}})$ *where each* $v_{i_k} \equiv \overline{x}_{i_k}$ *if* $x_{i_k} = 0$ *on the path from the root and* $v_{i_k} \equiv x_{i_k}$ *if* $x_{i_k} = 1$ *on the path from the root. The path from the root node to itself contains no branches and is denoted by* $()$ *where* $()$ *represents the empty tuple. If* $x_{i_j} \equiv x_{i_k}$ *for some* $k \leq j-1$ *and* $v = (v_{i_1}, \dots, v_{i_{j-1}})$ *and* $\hat{v} = (\hat{v}_{i_1}, \dots, \hat{v}_{i_{j-1}})$ *are paths to the* j^{th} *layer with* $v_{i_\ell} \equiv \hat{v}_{i_\ell}$ *for* $\ell < j$ *and* $\ell \neq k$ *then* $v_{i_k} \equiv \hat{v}_{i_k}$ *must hold. Leaf nodes may exist only in the* m^{th} *layer. Nodes in the set* A *are said to be in the BSQDD* B*.*

Several examples of BSQDDs have been shown in figures 1, 2, 3(a), 3(b) and 4(a) although repeated variables were not used in any of them. A more complicated example will be shown later in section 9 that illustrates the use of repeated variables. Note that it is possible for there to be more than one path from the root node in a BSQDD to another node in a BSQDD. For example, in figure 4(a), the possible paths from the root node a_1 to the node a_3 are $(\overline{x}_1, x_2)$ and $(x_1, \overline{x}_2)$.

Definition 5.4. *The path function* $p(x_{i_1}, \dots, x_{i_{j-1}})$ *of a node* a *in the* j^{th} *layer of a BSQDD* $B = (A, (L_1, \dots, L_m), \{x_1, \dots, x_n\}, (x_{i_1}, \dots, x_{i_m}), F)$ *is the boolean function that outputs* 1 *when the input variables correspond to a path from the root node to the node* a *for some starting state and outputs a* 0 *for all inputs that correspond to paths to other nodes.*

The path function is essentially a way of describing all paths that end at a particular node. For example, the path function for the node a_4 in the BSQDD in figure 4(a) would be $p_4(x_1, x_2, x_3) = 1$ because all paths from the root node to the fourth layer terminate at the node a_4.

Definition 5.5. *The initial state of a node* $a = (G, f(x_{i_1}, \dots, x_{i_{j-1}}), t)$ *in the* j^{th} *layer of a BSQDD* $B = (A, (L_1, \dots, L_m), \{x_1, \dots, x_n\}, (x_{i_1}, \dots, x_{i_m}), F)$ *on a path* $v = (v_{i_1}, \dots, v_{i_{j-1}})$ *is denoted by* $\left|\hat{\psi}_v\right\rangle$*. If* $v = ()$ *then* v *is the empty path so* a *is the root node and the initial state is* $\left|\hat{\psi}_{()}\right\rangle = (I_{2^{i_1-1}} \otimes G \otimes I_{2^{n-i_1}}) \left|\psi_0\right\rangle$ *where* $\left|\psi_0\right\rangle$ *is* *the starting state which must be a basis state. Otherwise if $v \neq ()$, the initial state is $\left|\hat{\psi}_v\right\rangle = (I_{2^{i_j-1}} \otimes G \otimes I_{2^{n-i_j}})_{f(x_{i_1},\ldots,x_{i_{j-1}})} \left|\hat{\psi}^{v_{i_{j-1}}}_{(v_{i_1},\ldots,v_{i_{j-2}})}\right\rangle$ where the operator that results from the expression $(I_{2^{i_j-1}} \otimes G \otimes I_{2^{n-i_j}})$ is controlled by the boolean function $f(x_{i_1},\ldots,x_{i_{j-1}})$ and the state $\left|\hat{\psi}^{v_{i_{j-1}}}_{(v_{i_1},\ldots,v_{i_{j-2}})}\right\rangle$ is obtained by taking the sum of all terms in $\left|\hat{\psi}_{(v_{i_1},\ldots,v_{i_{j-2}})}\right\rangle$ where $v_{i_{j-1}} = 1$.*

The reason why this is called the initial state of a node a on a path v is because it is the state that the child nodes of a will operate on. The basic idea is that the initial state of a node is equal to the operator for node controlled by control function $f(x_{i_1},\ldots,x_{i_{j-1}})$ applied to the sum of the terms in the initial state of the parent node on the path v. As an example, consider the initial state of the node a_2 on the path $v = (\overline{x}_1)$ for the BSQDD in figure 4(a). First, it is necessary to find the initial state of the root node which is $\left|\hat{\psi}_{()}\right\rangle = (H \otimes I_8)\left|0000\right\rangle$ so $\left|\hat{\psi}_{()}\right\rangle = \frac{1}{\sqrt{2}}\left|0000\right\rangle + \frac{1}{\sqrt{2}}\left|1000\right\rangle$. Now $\left|\hat{\psi}^{\overline{x}_1}_{()}\right\rangle = \frac{1}{\sqrt{2}}\left|0000\right\rangle$ since $\overline{x}_1 = 0$ for the term $\frac{1}{\sqrt{2}}\left|1000\right\rangle$. Therefore, the initial state of a_2 on the path v is $\left|\hat{\psi}_{(\overline{x}_1)}\right\rangle = (I_2 \otimes X \otimes I_4)_{\overline{x}_1} \frac{1}{\sqrt{2}}\left|0000\right\rangle$ which is equal to $\frac{1}{\sqrt{2}}\left|0100\right\rangle$.

Definition 5.6. *The state represented by a BSQDD with respect to the starting state $\left|\psi_0\right\rangle$ is the sum of the initial states of the leaf nodes over all paths from the root node to each leaf node.*

As an example, consider the BSQDD in figure 4(a). Note that the state that was being represented in equation (1) is the sum of the initial states of the leaf nodes since the initial states of the leaf node a_4 are $\frac{1}{2}\left|0101\right\rangle$, $\frac{1}{2}\left|0110\right\rangle$, $\frac{1}{2}\left|1001\right\rangle$ and $\frac{1}{2}\left|1010\right\rangle$ on the paths $(\overline{x}_1, x_2, \overline{x}_3)$, $(\overline{x}_1, x_2, x_3)$, $(x_1, \overline{x}_2, \overline{x}_3)$ and $(x_1, \overline{x}_2, x_3)$ respectively. An algorithm for constructing a BSQDD that represents a desired quantum superposition will be shown later in section 10.

6 Equivalence Relations for BSQDDs

Definition 6.1. *The nodes a and $\hat{a}$ are equal, denoted $a = \hat{a}$ if the tuples that correspond to the nodes a and $\hat{a}$ are equal.*

Definition 6.2. *The layers L and $\hat{L}$ are equal, denoted $L = \hat{L}$ if the tuples that correspond to the layers L and $\hat{L}$ are equal.*

Definition 6.3. *The BSQDDs B and $\hat{B}$ are equal, denoted $B = \hat{B}$ if the tuples that correspond to the BSQDDs B and $\hat{B}$ are equal.*

Definition 6.4. *The BSQDDs B and $\hat{B}$ are equivalent, denoted $B \approx \hat{B}$ if the quantum superpositions they represent as defined in definition 5.6 are equal with respect to each possible starting state, they operate on the same set of variables, have the same order of variables and have the same set of gates.*

An example of BSQDDs that are equivalent but not equal can be seen in the example from section 4. Consider the BSQDDs in figures 1, 2, 3(a), 3(b) and 4(a). None of these BSQDDs are equal because their sets of nodes are not equal. However, all of these BSQDDs represent the quantum superposition from equation (1) so they are equivalent. Hence, these BSQDDs are all equivalent but are not equal.

Theorem 6.5. *Equality and equivalence of BSQDDs as defined in definitions 6.3 and 6.4 are equivalence relations.*

Proof. By definition 5.3, BSQDDs are tuples. Because equality of tuples is an equivalence relation, equality of BSQDDs is an equivalence relation. By definition 6.4, two BSQDDs are equivalent if the they represent the same quantum superposition, operate on the same set of variables, have the same order of variables and have the same set of gates. Because all of these relations are equality relations, equivalence of BSQDDs is an equivalence relation. □

7 Generating Quantum Arrays Using BSQDDs

This section will prove a general theorem that relates the state at different points in the quantum array that is generated by a BSQDD to the initial states of the BSQDD. This will then be used to derive a theorem that shows that the quantum array generated by a BSQDD initializes the state that the BSQDD represents.

Definition 7.1. *The quantum array that is generated by a BSQDD B where $B = (A, (L_1, \ldots, L_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_m}), F)$ is created by adding the gates from the nodes in each layer to the quantum array. The layers are added in the order of their indexes from smallest to largest. Each new gate is placed to the right of all previous gates and operates on the qubit that its layer operates on in the BSQDD and is controlled by $p(x_{i_1}, \ldots, x_{i_{j-1}})f(x_{i_1}, \ldots, x_{i_{j-1}})$ where $a = (G, f(x_{i_1}, \ldots, x_{i_{j-1}}), t)$ is the node that is currently being added and $p(x_{i_1}, \ldots, x_{i_{j-1}})$ is the path function of the node a from definition 5.4.*

For an example of quantum array that is generated by a BSQDD, see section 4. The idea in definition 7.1 can be implemented using algorithm 1. The algorithm includes the optimization that if all nodes in a layer have the same operation and the product of the path function and control function of each node is equal to the path function, then the operation can be applied to the qubit operated on by the layer and no controls are needed. Note that since the algorithm iterates over all the nodes in the BSQDD at most two times, it is in the complexity class $\Theta(|A|)$.

Theorem 7.2. *The state of the quantum array that is generated from a BSQDD after the gates in the quantum array that correspond to the nodes in layers $1, \ldots, j$ have been applied to the starting state is the sum of the initial states of the nodes in the j^{th} layer over all paths to each node in the j^{th} layer.*

Proof. Let $B = (A, (L_1, \ldots, L_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_m}), F)$ be a BSQDD with m layers and the order of variables $(x_{i_1}, \ldots, x_{i_m})$. The theorem will be proven by

Algorithm 1 The algorithm for generating a quantum array from a BSQDD

Let $B = (A, (L_1, \ldots, L_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_m}), F)$ be a BSQDD
for all $j = 1, \ldots, m$ **do**
  Let $f_a(x_{i_1}, \ldots, x_{i_{j-1}})$ denote the control function of the node a in the j^{th} layer of the BSQDD B according to definitions 5.1 and 5.3
  Let $p_a(x_{i_1}, \ldots, x_{i_{j-1}})$ denote the path function of the node a in the j^{th} layer of the BSQDD B according to definition 5.4
  if every node a in the j^{th} layer has the same operation U and $p_a(x_{i_1}, \ldots, x_{i_{j-1}}) = p_a(x_{i_1}, \ldots, x_{i_{j-1}}) f_a(x_{i_1}, \ldots, x_{i_{j-1}})$ for all nodes a in the j^{th} layer **then**
    Apply the operation U to the qubit $\left|x_{i_j}\right\rangle$ without using any controls
  else
    for all nodes a in the layer L_j **do**
      Let the operation of a be U_a, let $f_a(x_{i_1}, \ldots, x_{i_{j-1}})$ be the control function of the node a and let $p_a(x_{i_1}, \ldots, x_{i_{j-1}})$ be the path function of the node a
      Apply the operation U_a to the qubit $\left|x_{i_j}\right\rangle$ and control by $p_a(x_{i_1}, \ldots, x_{i_{j-1}}) f_a(x_{i_1}, \ldots, x_{i_{j-1}})$
    end for
  end if
end for

induction. For the basis case $j = 1$, the initial state is the gate that corresponds to the root node applied to the starting state $|\psi_0\rangle$ by definition 5.5. Because the quantum state before any of the gates in the quantum array are applied is also $|\psi_0\rangle$, applying only the gate that corresponds to the root node will result in the initial state of the root node. This proves the basis case. For the inductive case, assume that the state of the quantum array after the gates that correspond to the nodes in the layers $1, \ldots, j$ are applied is the sum of the initial states of the nodes in the j^{th} layer of the BSQDD B. Let V_j be the set of all paths to nodes in the j^{th} layer from the root and let $|\psi_j\rangle$ denote the state of the quantum array after the gates that correspond to the nodes in the layers $1, \ldots, j$ are applied. Then by the inductive hypothesis

$$|\psi_j\rangle = \sum_{v \in V_j} \left|\hat{\psi}_v\right\rangle \tag{2}$$

Let P_j be the set of all path functions as defined in definition 5.4 for the nodes in the j^{th} layer. Because different nodes in the j^{th} layer are in different locations, their path functions are unique within the j^{th} layer. Therefore, the node in the j^{th} layer with the path function $p \in P_j$ denoted by $a_p = (G_p, f_p(x_{i_1}, \ldots, x_{i_{j-1}}), t_p)$ is unique. This allows nodes to be indexed by their path functions. Applying the gates in the quantum array that correspond to the gates in the $j+1^{\mathrm{th}}$ layer of the BSQDD B to $|\psi_j\rangle$ results in $|\psi_{j+1}\rangle = \left[\prod_{p \in P_{j+1}} (I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{p(x_{i_1}, \ldots, x_{i_j}) f_p(x_{i_1}, \ldots, x_{i_j})}\right] |\psi_j\rangle$ by definition 7.1 where the subscript $p(x_{i_1}, \ldots, x_{i_j}) f_p(x_{i_1}, \ldots, x_{i_j})$ denotes the function that controls $I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}}$. Substituting $\sum_{v \in V_j} \left|\hat{\psi}_v\right\rangle$ for $|\psi_j\rangle$ according to equation (2) shows that

$$|\psi_{j+1}\rangle = \left[\prod_{p\in P_{j+1}} (I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{p(x_{i_1},\ldots,x_{i_j})f_p(x_{i_1},\ldots,x_{i_j})}\right] \sum_{v\in V_j} \left|\hat{\psi}_v\right\rangle \tag{3}$$

The summation can now be distributed over the product. Doing this results in

$$|\psi_{j+1}\rangle = \sum_{v\in V_j} \prod_{p\in P_{j+1}} \left[(I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{p(x_{i_1},\ldots,x_{i_j})f_p(x_{i_1},\ldots,x_{i_j})}\right] \left|\hat{\psi}_v\right\rangle \tag{4}$$

Let

$$|\alpha_v\rangle = \prod_{p\in P_{j+1}} \left[(I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{p(x_{i_1},\ldots,x_{i_j})f_p(x_{i_1},\ldots,x_{i_j})}\right] \left|\hat{\psi}_v\right\rangle \tag{5}$$

Then

$$|\psi_{j+1}\rangle = \sum_{v\in V_j} |\alpha_v\rangle \tag{6}$$

It is now necessary to consider three cases. First assume that the node a_v that the path $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ terminates at in equation (5) has only one child node. In this case, only the operation of the child node of the node a_v will be applied to $\left|\hat{\psi}_v\right\rangle$ in equation (4) because the path function $p(x_{i_1}, \ldots, x_{i_j})$ of the child node of a_v is the only path function in the $j + 1^{\text{th}}$ layer that is equal to 1 in the path v by definition 5.4. Thus, $|\alpha_v\rangle = (I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{p(x_{i_1},\ldots,x_{i_j})f_p(x_{i_1},\ldots,x_{i_j})} \left|\hat{\psi}_v\right\rangle$. Let $\hat{v} = (\hat{v}_{i_1}, \ldots, \hat{v}_{i_j})$ be the path to the child node of the node a_v such that $\hat{v}_{i_k} \equiv v_{i_k}$ for $k = 1 \ldots j-1$. Then since the node a_v has only one child node, $\left|\hat{\psi}_v\right\rangle = \left|\hat{\psi}_v^{\hat{v}_{i_j}}\right\rangle$ by applying definition 5.5. Therefore, $|\alpha_v\rangle = (I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{p(x_{i_1},\ldots,x_{i_j})f_p(x_{i_1},\ldots,x_{i_j})} \left|\hat{\psi}_v^{\hat{v}_{i_j}}\right\rangle$. Now $p(x_{i_1}, \ldots, x_{i_j}) = 1$ for $\left|\hat{\psi}_v^{\hat{v}_{i_j}}\right\rangle$ by definition 5.4, so the path function can be removed which results in $|\alpha_v\rangle = (I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{f_p(x_{i_1},\ldots,x_{i_j})} \left|\hat{\psi}_v^{\hat{v}_{i_j}}\right\rangle$. Thus by definition 5.5,

$$|\alpha_v\rangle = \left|\hat{\psi}_{\hat{v}}\right\rangle \tag{7}$$

For the second case assume that the node a_v that the path $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ terminates at in equation (5) has two equal child nodes. In this case, only the operation of the child node of the node a_v will be applied to $\left|\hat{\psi}_v\right\rangle$ in equation (4) because the path function $p(x_{i_1}, \ldots, x_{i_j})$ of the child node of a_v is the only path function in the $j + 1^{\text{th}}$ layer that is equal to 1 in the path v by definition 5.4. Thus, $|\alpha_v\rangle = (I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{p(x_{i_1},\ldots,x_{i_j})f_p(x_{i_1},\ldots,x_{i_j})} \left|\hat{\psi}_v\right\rangle$. Since $\left|\hat{\psi}_v\right\rangle = \left|\hat{\psi}_v^{\overline{x}_{i_j}}\right\rangle + \left|\hat{\psi}_v^{x_{i_j}}\right\rangle$ from definition 5.5, $|\alpha_v\rangle = (I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{p(x_{i_1},\ldots,x_{i_j})f_{p(x_{i_1},\ldots,x_{i_j})}} \left(\left|\hat{\psi}_v^{\overline{x}_{i_j}}\right\rangle + \left|\hat{\psi}_v^{x_{i_j}}\right\rangle\right)$. By definition 5.4, $p(x_{i_1}, \ldots, x_{i_j}) = 1$ for both $\left|\hat{\psi}_v^{\overline{x}_{i_j}}\right\rangle$ and $\left|\hat{\psi}_v^{x_{i_j}}\right\rangle$. Therefore by definition 5.5,

$$|\alpha_v\rangle = \left|\hat{\psi}_{(v_{i_1},\ldots,v_{i_{j-1}},\overline{x}_{i_j})}\right\rangle + \left|\hat{\psi}_{(v_{i_1},\ldots,v_{i_{j-1}},x_{i_j})}\right\rangle \tag{8}$$

For the final case, suppose that the node a_v has two unique children. In this case, only the path functions of the child nodes of a_v can be equal to 1 on the path v by definition 5.4. This allows all operations in the product in equation (5) to be removed except the operations of the nodes that the paths $(v_{i_1}, \ldots, v_{i_{j-1}}, \overline{x}_{i_j})$ and $(v_{i_1}, \ldots, v_{i_{j-1}}, x_{i_j})$ terminate at. Thus,

$$\begin{aligned} |\alpha_v\rangle =&(I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{p(x_{i_1},\ldots,x_{i_j})f_p(x_{i_1},\ldots,x_{i_j})} \\ &\cdot (I_{2^{i_{j+1}-1}} \otimes G_{p'} \otimes I_{2^{n-i_{j+1}}})_{p'(x_{i_1},\ldots,x_{i_j})f_{p'}(x_{i_1},\ldots,x_{i_j})} \left|\hat{\psi}_v\right\rangle \end{aligned} \tag{9}$$

where $p(x_{i_1}, \ldots, x_{i_j})$ is the path function of the node that the path $(v_{i_1}, \ldots, v_{i_{j-1}}, \overline{x}_{i_j})$ terminates at and $p'(x_{i_1}, \ldots, x_{i_j})$ is the path function of the node at which the path $(v_{i_1}, \ldots, v_{i_{j-1}}, x_{i_j})$ terminates. Now $\left|\hat{\psi}_v\right\rangle = \left|\hat{\psi}_v^{\overline{x}_{i_j}}\right\rangle + \left|\hat{\psi}_v^{x_{i_j}}\right\rangle$ from definition 5.5 so

$$\begin{aligned} |\alpha_v\rangle =&(I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{p(x_{i_1},\ldots,x_{i_j})f_{p(x_{i_1},\ldots,x_{i_j})}} \\ &\cdot (I_{2^{i_{j+1}-1}} \otimes G_{p'} \otimes I_{2^{n-i_{j+1}}})_{p'(x_{i_1},\ldots,x_{i_j})f_{p'}(x_{i_1},\ldots,x_{i_j})} \left(\left|\hat{\psi}_v^{\overline{x}_{i_j}}\right\rangle + \left|\hat{\psi}_v^{x_{i_j}}\right\rangle\right) \end{aligned} \tag{10}$$

Now $I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}}$ will only be applied to $\left|\hat{\psi}_v^{\overline{x}_{i_j}}\right\rangle$ because the path function $p(x_{i_1}, \ldots, x_{i_j})$ will be 0 for $\left|\hat{\psi}_v^{x_{i_j}}\right\rangle$ by definition 5.4. Similarly, $I_{2^{i_{j+1}-1}} \otimes G_{p'} \otimes I_{2^{n-i_{j+1}}}$ will only be applied to $\left|\hat{\psi}_v^{x_{i_j}}\right\rangle$. Therefore, distributing the sum over the product results in

$$\begin{aligned} |\alpha_v\rangle =&(I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{p(x_{i_1},\ldots,x_{i_j})f_p(x_{i_1},\ldots,x_{i_j})} \left|\hat{\psi}_v^{\overline{x}_{i_j}}\right\rangle \\ &+ (I_{2^{i_{j+1}-1}} \otimes G_{p'} \otimes I_{2^{n-i_{j+1}}})_{p'(x_{i_1},\ldots,x_{i_j})f_{p'}(x_{i_1},\ldots,x_{i_j})} \left|\hat{\psi}_v^{x_{i_j}}\right\rangle \end{aligned} \tag{11}$$

Because $p(x_{i_1}, \ldots, x_{i_j}) = 1$ for $\left|\hat{\psi}_v^{\overline{x}_{i_j}}\right\rangle$ and $p'(x_{i_1}, \ldots, x_{i_j}) = 1$ for $\left|\hat{\psi}_v^{x_{i_j}}\right\rangle$ by definition 5.4 these path functions can be removed. Hence,

$$\begin{aligned} |\alpha_v\rangle =&(I_{2^{i_{j+1}-1}} \otimes G_p \otimes I_{2^{n-i_{j+1}}})_{f_p(x_{i_1},\ldots,x_{i_j})} \left|\hat{\psi}_v^{\overline{x}_{i_j}}\right\rangle \\ &+ (I_{2^{i_{j+1}-1}} \otimes G_{p'} \otimes I_{2^{n-i_{j+1}}})_{f_{p'}(x_{i_1},\ldots,x_{i_j})} \left|\hat{\psi}_v^{x_{i_j}}\right\rangle \end{aligned} \tag{12}$$

Thus, by definition 5.5,

$$|\alpha_v\rangle = \left|\hat{\psi}_{(v_{i_1},\ldots,v_{i_{j-1}},\overline{x}_{i_j})}\right\rangle + \left|\hat{\psi}_{(v_{i_1},\ldots,v_{i_{j-1}},x_{i_j})}\right\rangle \tag{13}$$

Therefore, by equations (7), (8) and (13), $|\alpha_v\rangle = \sum_{\hat{v}\in V_{j+1}^v} \left|\hat{\psi}_{\hat{v}}\right\rangle$ where V_{j+1}^v denotes the set of all paths $\hat{v} = (\hat{v}_{i_1}, \ldots, \hat{v}_{i_j})$ to the $j + 1^{\text{th}}$ layer where $\hat{v}_{i_k} \equiv v_{i_k}$ for $k =$

$1, \ldots, j-1$. By equation (6), $|\psi_{j+1}\rangle = \sum_{v \in V_j} |\alpha_v\rangle$. Now every path to the $j+1^{\text{th}}$ layer must pass through a node in the j^{th} layer. Therefore,

$$|\psi_{j+1}\rangle = \sum_{v \in V_{j+1}} \left|\hat{\psi}_v\right\rangle \tag{14}$$

Thus, the inductive case holds so by the principle of mathematical induction, the state of the quantum array after the gates that correspond to the nodes in the layers $1, \ldots, j$ of the BSQDD B have been applied is the sum of the initial states of the nodes in the j^{th} layer over all paths to each node in the j^{th} layer. □

Theorem 7.3. *The state initialized by the quantum array generated from a BSQDD B from the starting state $|\psi_0\rangle$ is the quantum superposition represented by the BSQDD B with respect to the starting state $|\psi_0\rangle$.*

Proof. Assume that the BSQDD B has m layers. By definition 5.3, the leaf nodes are in the m^{th} layer so it follows that the quantum superposition represented by the BSQDD B is the sum of the initial states of the nodes in the m^{th} layer over all paths to each node in the m^{th} layer by definition 5.6. By theorem 7.2, this is the state of the quantum array after the gates that correspond to the nodes in layers $1, \ldots, m$ have been applied. Since this is the state of the quantum array after all gates have been applied, the quantum array initializes the quantum superposition represented by the BSQDD when applied to the starting state $|\psi_0\rangle$. □

This theorem is important because it shows that BSQDDs can be used to find quantum arrays for initializing quantum superpositions. All that needs to be done is to represent the desired quantum superposition using a BSQDD and then use the BSQDD to generate a quantum array. However, this quantum array is sometimes inefficient so it is usually necessary to reduce the BSQDD using transformation rules before using it to generate a quantum array. These transformation rules will be presented now.

8 Transformation Rules

In this section, two transformation rules that can be used to manipulate and reduce BSQDDs will be derived. First, the transformation rule which allows equal nodes to be merged will be shown.

Transformation Rule 8.1. *If $a = \hat{a}$ for two distinct nodes $a = (G, f(x_{i_1}, \ldots, x_{i_{j-1}}), t)$ and $\hat{a} = (\hat{G}, \hat{f}(x_{i_1}, \ldots, x_{i_{j-1}}), \hat{t})$ in the j^{th} layer of a BSQDD, then merging the two nodes into one new node results in an equivalent BSQDD. Performing the inverse operation by splitting a node $\tilde{a} = (\tilde{G}, \tilde{f}(x_{i_1}, \ldots, x_{i_{j-1}}), \tilde{t})$ into two nodes a and $\hat{a}$ where $a = \hat{a} = \tilde{a}$ where the node $\tilde{a}$ has at least two parents also results in an equivalent BSQDD.*

Proof. Let $B = (A, (L_1, \ldots, L_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_m}), F)$ be a BSQDD and let $a = \hat{a}$ where $a = (G, f(x_{i_1}, \ldots, x_{i_{j-1}}), t)$ and $\hat{a} = (\hat{G}, \hat{f}(x_{i_1}, \ldots, x_{i_{j-1}}), \hat{t})$ are two nodes in the j^{th} layer of the BSQDD B. Let $\tilde{B}$ be a BSQDD where $\tilde{B} =$

$(\tilde{A}, (\tilde{L}_1, \ldots, \tilde{L}_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_m}), F)$, $\tilde{A}$ is obtained from A by merging the nodes a and $\hat{a}$ into a new node $\tilde{a}$ with $a = \hat{a} = \tilde{a}$ and replacing a and $\hat{a}$ by $\tilde{a}$ in the tuple t for each $(G, f(x_{i_1}, \ldots, x_{i_{j-2}}), t) \in A$. It will now be proven that the sum of initial states in the k^{th} layer of the BSQDD B is the same as the sum of the initial states in the k^{th} layer of the BSQDD $\tilde{B}$. Consider a path $v = (v_{i_1}, \ldots, v_{i_{k-1}})$ to a node $a_v = (G_v, f_v(x_{i_1}, \ldots, x_{i_{k-1}}), t_v)$ in the k^{th} layer of the BSQDD B. Let the node that the path v terminates at in the BSQDD $\tilde{B}$ be denoted by $\tilde{a}_v$. First suppose that $k < j$. In this case, the equation for the initial state of node a_v on the path v will be the same as the initial state of node $\tilde{a}_v$ in the k^{th} layer of the BSQDD $\tilde{B}$ on the path v due to definition 5.5. Therefore, since a_v is an arbitrary node in the k^{th} layer of the BSQDD B, the sum of the initial states in the k^{th} layers of the BSQDDs B and $\tilde{B}$ will be the same when $k < j$. Now assume that $k = j$. If $a_v \not\equiv a$ and $a_v \not\equiv \hat{a}$ then the initial state of the node a_v on the path v in the BSQDD B is equal to the initial state of the node $\tilde{a}_v$ on the path v in the BSQDD $\tilde{B}$ because of definition 5.5. Suppose that $a_v \equiv a$ or $a_v \equiv \hat{a}$. In this case, the initial state of the node a_v on the path v in the BSQDD B is $\left|\hat{\psi}_{v,B}\right\rangle = \left(I_{2^{i_j-1}} \otimes G \otimes I_{2^{n-i_j}}\right)_{f(x_{i_1}, \ldots, x_{i_{j-1}})} \left|\hat{\psi}^{v_{i_{j-1}}}_{(v_{i_1}, \ldots, v_{i_{j-2}}),B}\right\rangle$ where the subscript B has been added to the initial state to indicate that it is for the BSQDD B. Similarly, the initial state of the node $\tilde{a}_v$ on the path v in the BSQDD $\tilde{B}$ is $\left|\hat{\psi}_{v,\tilde{B}}\right\rangle = \left(I_{2^{i_j-1}} \otimes G \otimes I_{2^{n-i_j}}\right)_{f(x_{i_1}, \ldots, x_{i_{j-1}})} \left|\hat{\psi}^{v_{i_{j-1}}}_{(v_{i_1}, \ldots, v_{i_{j-2}}),\tilde{B}}\right\rangle$. Note that $v \neq ()$ since it is not possible for any node to be equal to the root node except for the root node itself. Hence, no node can be merged with the root node so it is not necessary to consider the case where $v = ()$. Since the initial states of the $j - 1^{\text{th}}$ layer are the same in the BSQDDs B and $\tilde{B}$, $\left|\hat{\psi}_{(v_{i_1}, \ldots, v_{i_{j-2}}),B}\right\rangle = \left|\hat{\psi}_{(v_{i_1}, \ldots, v_{i_{j-2}}),\tilde{B}}\right\rangle$ so $\left|\hat{\psi}^{v_{i_{j-1}}}_{(v_{i_1}, \ldots, v_{i_{j-2}}),B}\right\rangle = \left|\hat{\psi}^{v_{i_{j-1}}}_{(v_{i_1}, \ldots, v_{i_{j-2}}),\tilde{B}}\right\rangle$ which implies that $\left|\hat{\psi}_{v,B}\right\rangle = \left|\hat{\psi}_{v,\tilde{B}}\right\rangle$ by definition 5.5. Because the union of the set of paths to a and the set of paths to $\hat{a}$ is equal to the set of paths to $\tilde{a}$, the sum of the initial states of the nodes a and $\hat{a}$ is equal to the sum of the initial states of the node $\tilde{a}$. Thus, the sum of the initial states of the nodes in the $\jmath^{\text{th}}$ layer of the BSQDD B is equal to the sum of the initial states in the j^{th} layer of the BSQDD $\tilde{B}$. Consider the case where $k > j$. It will be proven by induction that the initial state of a node in the k^{th} layer of the BSQDD B on a given path is equal to the initial state of the corresponding node in the k^{th} layer of the BSQDD $\tilde{B}$ on the same path. Consider the basis case where $k = j + 1$. If the path v does not pass through the node a or the node $\hat{a}$ in the BSQDD B, then the initial state of the node a_v on the path v in the BSQDD B will be equal to the initial state of the node $\tilde{a}_v$ in the BSQDD $\tilde{B}$ by definition 5.5. Suppose that the path v passes through the node a or the node $\hat{a}$ in the BSQDD B. Then the path v passes through the node $\tilde{a}$ in the BSQDD $\tilde{B}$. Let $\hat{v} = (v_{i_1}, \ldots, v_{i_{j-1}})$ and let $a_{\hat{v}}$ and $\tilde{a}_{\hat{v}}$ be the nodes that the path $\hat{v}$ terminates at in the BSQDDs B and $\tilde{B}$ respectively. Because the initial state of the node $\tilde{a}$ on the path $\hat{v}$ in the BSQDD $\tilde{B}$ is equal to the initial state of the node $a_{\hat{v}}$ on the path $\hat{v}$ in the BSQDD B, $\left|\hat{\psi}_{\hat{v},B}\right\rangle = \left|\hat{\psi}_{\hat{v},\tilde{B}}\right\rangle$ and therefore $\left|\hat{\psi}^{v_{i_j}}_{\hat{v},B}\right\rangle = \left|\hat{\psi}^{v_{i_j}}_{\hat{v},\tilde{B}}\right\rangle$ which implies that $\left|\hat{\psi}_{v,B}\right\rangle = \left|\hat{\psi}_{v,\tilde{B}}\right\rangle$ by definition 5.5.

Now consider the inductive case where the initial state of any node in the k^{th} layer of the BSQDD B on a given path is equal to the initial state of the corresponding node in the k^{th} layer of the BSQDD $\tilde{B}$ on the same path. From definition 5.5, the initial state of a node $a_v = (G_v, f_v(x_{i_1}, \ldots, x_{i_k}), t_v)$ on the path v in $k+1^{\text{th}}$ layer of the BSQDD B is $\left|\hat{\psi}_{v,B}\right\rangle = \left(I_{2^{i_{k+1}-1}} \otimes G_v \otimes I_{2^{n-i_{k+1}}}\right)_{f_v(x_{i_1},\ldots,x_{i_k})} \left|\hat{\psi}^{v_{i_k}}_{(v_{i_1},\ldots,v_{i_{k-1}}),B}\right\rangle$ and the initial state of the node $\tilde{a}_v$ on the path v in the BSQDD $\tilde{B}$ is $\left|\hat{\psi}_{v,\tilde{B}}\right\rangle = \left(I_{2^{i_{k+1}-1}} \otimes G_v \otimes I_{2^{n-i_{k+1}}}\right)_{f_v(x_{i_1},\ldots,x_{i_k})} \left|\hat{\psi}^{v_{i_k}}_{(v_{i_1},\ldots,v_{i_{k-1}}),\tilde{B}}\right\rangle$. Let $\hat{v} = (v_{i_1}, \ldots, v_{i_{k-1}})$. Since $\left|\hat{\psi}_{\hat{v},B}\right\rangle = \left|\hat{\psi}_{\hat{v},\tilde{B}}\right\rangle$, $\left|\hat{\psi}^{v_{i_k}}_{\hat{v},B}\right\rangle = \left|\hat{\psi}^{v_{i_k}}_{\hat{v},\tilde{B}}\right\rangle$ which implies that $\left|\hat{\psi}_{v,B}\right\rangle = \left|\hat{\psi}_{v,\tilde{B}}\right\rangle$ by definition 5.5. This proves the inductive case. Therefore, by the principle of mathematical induction, the initial state of a node in the k^{th} layer of the BSQDD B is equal to the initial state of the node in the k^{th} layer of the BSQDD $\tilde{B}$. This implies that the sum of the initial states of the nodes in the k^{th} layer of the BSQDD B is equal to the sum of the initial states of the nodes in the k^{th} layer of the BSQDD $\tilde{B}$ when $k > j$. Thus, the quantum superpositions represented by the BSQDDs B and $\tilde{B}$ are equal so $B \approx \tilde{B}$ by definition 6.4. To prove the second part of the transformation rule, observe that B can be obtained from $\tilde{B}$ by splitting the node $\tilde{a}$ to obtain the nodes a and $\hat{a}$ so that the above proof also proves the second part of the transformation rule. □

This transformation rule is very useful for reducing BSQDDs. For examples, see figures 3(a) and 3(b) from the example in section 4. However, some of the transformations used in the example in section 4 are more complicated than the simple merges of equal nodes in the same layer permitted by transformation rule 8.1. This requires another transformation rule.

Transformation Rule 8.2. *Replacing a node $a = (G, f(x_{i_1}, \ldots, x_{i_{j-1}}), t)$ in the j^{th} layer of a BSQDD B with a node $\tilde{a} = (\tilde{G}, \tilde{f}(x_{i_1}, \ldots, x_{i_{j-1}}), t)$ results in an equivalent BSQDD $\tilde{B}$ if the initial state of the node a on a path v in the BSQDD B is equal to the initial state of the node $\tilde{a}$ on the path v in the BSQDD $\tilde{B}$ for all paths v to the node a in the BSQDD B.*

Proof. Let $B = (A, (L_1, \ldots, L_n), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_m}), F)$ be a BSQDD that contains a node $a = (G, f(x_{i_1}, \ldots, x_{i_{j-1}}), t)$ in the j^{th} layer. Let $\tilde{B}$ be the BSQDD obtained from B by replacing the node a with $\tilde{a} = (\tilde{G}, \tilde{f}(x_{i_1}, \ldots, x_{i_{j-1}}), t)$. Then $\tilde{B} = (\tilde{A}, (\tilde{L}_1, \ldots, \tilde{L}_n), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_m}), F)$ where the set of nodes $\tilde{A}$ is obtained from A by replacing the node a with the node $\tilde{a}$ and $\left|\hat{\psi}_{v,B}\right\rangle = \left|\hat{\psi}_{v,\tilde{B}}\right\rangle$ for all paths v to the node a in the BSQDD B. Consider a path $v = (v_{i_1}, \ldots, v_{i_{k-1}})$ to a node $a_v = (G_v, f_v(x_{i_1}, \ldots, x_{i_{k-1}}), t_v)$ in the k^{th} layer of the BSQDD B. Let $\tilde{a}_v$ denote the node that the path v terminates at in the BSQDD $\tilde{B}$. Suppose that $k < j$. Then by definition 5.5, the initial state of the node a_v on the path v will be equal to the initial state of the node $\tilde{a}_v$ on the path v. Now suppose that $k = j$. Then if $a_v \not\equiv a$ then the initial state of the node a_v on the path v in the BSQDDs B will be equal to the initial state of the node $\tilde{a}_v$ on the path v in the BSQDD $\tilde{B}$ by definition 5.5 since the initial states of the corresponding nodes in the $k-1^{\text{th}}$ layers of the BSQDDs B

and $\tilde{B}$ are equal. If $a_v \equiv a$ then the initial state of a_v on the path v in the BSQDD B is equal to the initial state of the node $\tilde{a}$ on the path v by assumption. Suppose that $k > j$. It will be proven by induction that the initial state of node a_v on a path v in the k^{th} layer of the BSQDD B is equal to the initial state of the node $\tilde{a}_v$ on the path v in the BSQDD $\tilde{B}$. Consider the basis case where $k = j + 1$. If the path v does not pass through the node a in the j^{th} layer of the BSQDD B, then the initial state of the node a_v on the path v in the BSQDD B is equal to the initial state of the node $\tilde{a}_v$ in the BSQDD $\tilde{B}$ by definition 5.5. If the path v passes through the node a in the BSQDD B, then the initial state of the node a_v on the path v in the BSQDD B will be $\left|\hat{\psi}_{v,B}\right\rangle = \left(I_{2^{i_{j+1}-1}} \otimes G_v \otimes I_{2^{n-i_{j+1}}}\right)_{f_v(x_{i_1},\ldots,x_{i_j})} \left|\hat{\psi}^{v_{i_j}}_{(v_{i_1},\ldots,v_{i_{j-1}}),B}\right\rangle$ and the initial state of the node $\tilde{a}_v$ on the path v in the BSQDD $\tilde{B}$ will be $\left|\hat{\psi}_{v,\tilde{B}}\right\rangle = \left(I_{2^{i_{j+1}-1}} \otimes G_v \otimes I_{2^{n-i_{j+1}}}\right)_{f_v(x_{i_1},\ldots,x_{i_j})} \left|\hat{\psi}^{v_{i_j}}_{(v_{i_1},\ldots,v_{i_{j-1}}),\tilde{B}}\right\rangle$ in the BSQDD $\tilde{B}$. Since $\left|\hat{\psi}_{(v_{i_1},\ldots,v_{i_{j-1}}),B}\right\rangle = \left|\hat{\psi}_{(v_{i_1},\ldots,v_{i_{j-1}}),\tilde{B}}\right\rangle$ and $\left|\hat{\psi}^{v_{i_j}}_{(v_{i_1},\ldots,v_{i_{j-1}}),B}\right\rangle = \left|\hat{\psi}^{v_{i_j}}_{(v_{i_1},\ldots,v_{i_{j-1}}),\tilde{B}}\right\rangle$, $\left|\hat{\psi}_{v,B}\right\rangle = \left|\hat{\psi}_{v,\tilde{B}}\right\rangle$ so that the basis case is proven. Consider the inductive case where the initial state of any node in the k^{th} layer of the BSQDD B is equal to the initial state of the corresponding node in the BSQDD $\tilde{B}$ on any path that terminates at the node. Let $\hat{v} = (v_{i_1}, \ldots, v_{i_k})$ be a path to the $k + 1^{\text{th}}$ layer that terminates at a node $a_{\hat{v}} = (G_{\hat{v}}, f_{\hat{v}}(x_{i_1}, \ldots, x_{i_k}), t_{\hat{v}})$ in the $k + 1^{\text{th}}$ layer of the BSQDD B. Let $\tilde{a}_{\hat{v}}$ denote the node that the path $\hat{v}$ terminates at in the BSQDD $\tilde{B}$. Then the initial state of the node $a_{\hat{v}}$ on the path $\hat{v}$ is $\left|\hat{\psi}_{\hat{v},B}\right\rangle = \left(I_{2^{i_{k+1}-1}} \otimes G_{\hat{v}} \otimes I_{2^{n-i_{k+1}}}\right)_{f_{\hat{v}}(x_{i_1},\ldots,x_{i_k})} \left|\hat{\psi}^{\hat{v}_{i_k}}_{(\hat{v}_{i_1},\ldots,\hat{v}_{i_{k-1}}),B}\right\rangle$ in the BSQDD B and the initial state of the node $\tilde{a}_v$ on the path $\hat{v}$ in the BSQDD $\tilde{B}$ is $\left|\hat{\psi}_{\hat{v},\tilde{B}}\right\rangle = \left(I_{2^{i_{k+1}-1}} \otimes G_{\hat{v}} \otimes I_{2^{n-i_{k+1}}}\right)_{f_{\hat{v}}(x_{i_1},\ldots,x_{i_k})} \left|\hat{\psi}^{\hat{v}_{i_k}}_{(\hat{v}_{i_1},\ldots,\hat{v}_{i_{k-1}}),\tilde{B}}\right\rangle$. By the inductive hypothesis, $\left|\hat{\psi}_{(\hat{v}_{i_1},\ldots,\hat{v}_{i_{k-1}}),B}\right\rangle = \left|\hat{\psi}_{(\hat{v}_{i_1},\ldots,\hat{v}_{i_{k-1}}),\tilde{B}}\right\rangle$ so that $\left|\hat{\psi}^{\hat{v}_{i_k}}_{(\hat{v}_{i_1},\ldots,\hat{v}_{i_{k-1}}),B}\right\rangle = \left|\hat{\psi}^{\hat{v}_{i_k}}_{(\hat{v}_{i_1},\ldots,\hat{v}_{i_{k-1}}),\tilde{B}}\right\rangle$. Thus, $\left|\hat{\psi}_{\hat{v},B}\right\rangle = \left|\hat{\psi}_{\hat{v},\tilde{B}}\right\rangle$ by definition 5.5 so the inductive case holds. By the principle of mathematical induction, the initial state of a node in the k^{th} layer of the BSQDD B is equal to the initial state of the node in the BSQDD $\tilde{B}$ for any path where $k > j$. Therefore, $B \approx \tilde{B}$ by definition 6.4. □

These two transformation rules are sufficient for transforming BSQDDs that use the any set of gates where the corresponding elements of the gates have unique amplitudes as will be proven in theorem 10.2.

9 A BSQDD with Repeated Variables

This section will illustrate the use of repeated variables in BSQDDs by showing how to initialize the quantum state

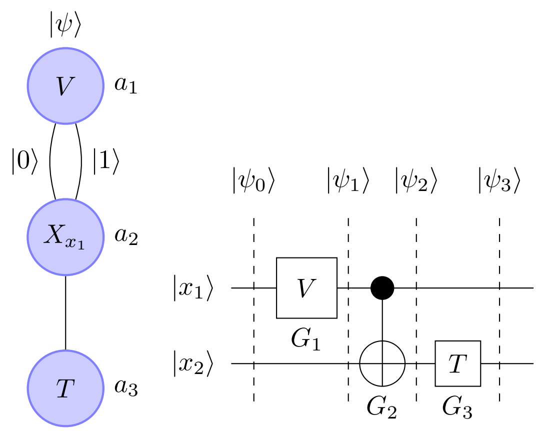
$$|\psi\rangle = \frac{1+i}{2}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle \tag{15}$$

using the set of gates $\{I, T, V, X\}$ and the starting state $|\psi_0\rangle = |00\rangle$ where $T = \left[\begin{smallmatrix} 1 & 0 \\ 0 & \frac{1+i}{\sqrt{2}} \end{smallmatrix}\right]$ and $V = \frac{1}{2}\left[\begin{smallmatrix} 1+i & 1-i \\ 1-i & 1+i \end{smallmatrix}\right]$ is the square root of NOT. The first step for initializing a quantum superposition using these gates is to find a BSQDD that represents the desired quantum superposition $|\psi\rangle$. The desired quantum superposition $|\psi\rangle$ cannot be represented without using repeated variables for this set of gates. To see this, consider the desired quantum superposition $|\psi\rangle$ and assume that the order of variables is (x_1, x_2). Because the first qubit $|x_1\rangle$ is in an entangled state in the desired quantum superposition $|\psi\rangle$, any BSQDD that represents the quantum superposition $|\psi\rangle$ must have V as the operation of the root node because none of the other operations result in a quantum superposition with more than one non-zero term when applied to the state $|0\rangle$. Because the two qubits are entangled, the root node must have either one child node that has an inverter controlled by $|1\rangle$ on the qubit $|x_1\rangle$ as its operation or two child nodes where the child on the path $(\overline{x}_1)$ from the root node has the identity matrix as its operation and the child on the path (x_1) has an inverter as its operation. However, the quantum superposition represented by the resulting BSQDD is $\frac{1+i}{2}|00\rangle + \frac{1-i}{2}|11\rangle$ which is not equal to $|\psi\rangle$ even when the irrelevance of global phase is taken into consideration. Similarly, the desired quantum superposition $|\psi\rangle$ cannot be represented by a BSQDD that uses the set of gates $\{I, T, V, X\}$ and the order of variables (x_2, x_1). However, the desired quantum superposition $|\psi\rangle$ can be represented using the order of variables (x_1, x_2, x_2) by the BSQDD shown in figure 5(a). The quantum array generated by the BSQDD in figure 5(a) is shown in figure 5(b). Because $V|0\rangle = \frac{1+i}{2}|0\rangle + \frac{1-i}{2}|1\rangle$, applying the V gate denoted by G_1 results in the quantum state $|\psi_1\rangle = \frac{1+i}{2}|00\rangle + \frac{1-i}{2}|10\rangle$. After the controlled inverter denoted by G_2 is applied, the quantum state is $|\psi_2\rangle = \frac{1+i}{2}|00\rangle + \frac{1-i}{2}|11\rangle$. Since $\frac{1-i}{2} \cdot \frac{1+i}{\sqrt{2}} = \frac{1}{\sqrt{2}}$, applying the T gate denoted by G_3 results in the quantum state $|\psi_3\rangle = \frac{1+i}{2}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$. Because $|\psi\rangle = |\psi_3\rangle$, the quantum array initializes the desired quantum superposition $|\psi\rangle$. This example shows that repeated variables can be useful for some sets of gates.

10 A Canonical Form for BSQDDs

This section will present a canonical form for BSQDDs that use a set of gates $F \neq \emptyset$ where corresponding elements of gates in the set F have unique amplitudes. The BSQDDs also must not have repeated variables. The set of gates have unique amplitudes if and only if for every $G, \tilde{G} \in F$ none of the corresponding elements of G and $\tilde{G}$ have equal amplitudes unless $G = \tilde{G}$.

Theorem 10.1. *Let $F \neq \emptyset$ be a set of 2×2 unitary matrices such that if $G, \tilde{G} \in F$ where $G = \left[\begin{smallmatrix} g_{00} & g_{01} \\ g_{10} & g_{11} \end{smallmatrix}\right]$, $\tilde{G} = \left[\begin{smallmatrix} \tilde{g}_{00} & \tilde{g}_{01} \\ \tilde{g}_{10} & \tilde{g}_{11} \end{smallmatrix}\right]$ and if $|g_{00}| = |\tilde{g}_{00}|$, $|g_{01}| = |\tilde{g}_{01}|$, $|g_{10}| = |\tilde{g}_{10}|$ or $|g_{11}| = |\tilde{g}_{11}|$ then $G = \tilde{G}$. Let $B = (A, (L_1, \ldots, L_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_n}), F)$ be a BSQDD that has no repeated variables. Then the BSQDD B is in canonical form if for every node $a = (G, f(x_{i_1}, \ldots, x_{i_{j-1}}), t) \in A$, $f(x_{i_1}, \ldots, x_{i_{j-1}}) = 1$ and there are no equal nodes in any layer of the BSQDD B. This form is canonical in the sense that if two BSQDDs B and $\hat{B}$ are in canonical form and $B \approx \hat{B}$, then $B = \hat{B}$.*



(a) A BSQDD that represents $|\psi\rangle$

(b) The quantum array generated by the BSQDD

Figure 5: The BSQDD and quantum array

Proof. Let $B = (A, (L_1, \ldots, L_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_n}), F)$ be a BSQDD in canonical form where $F \neq \emptyset$ is a set of 2×2 unitary matrices such that if $G, \tilde{G} \in F$ where $G = \left[\begin{smallmatrix} g_{00} & g_{01} \\ g_{10} & g_{11} \end{smallmatrix}\right]$, $\tilde{G} = \left[\begin{smallmatrix} \tilde{g}_{00} & \tilde{g}_{01} \\ \tilde{g}_{10} & \tilde{g}_{11} \end{smallmatrix}\right]$ and if $|g_{00}| = |\tilde{g}_{00}|$, $|g_{01}| = |\tilde{g}_{01}|$, $|g_{10}| = |\tilde{g}_{10}|$ or $|g_{11}| = |\tilde{g}_{11}|$ then $G = \tilde{G}$. Let $\tilde{B} = (\tilde{A}, (\tilde{L}_1, \ldots, \tilde{L}_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_n}), F)$ be a BSQDD in canonical form such that $B \approx \tilde{B}$. First observe that for any path $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ to a node in the j^{th} layer of the BSQDD B, there exists a node in the BSQDD $\tilde{B}$ that the path v terminates at. This must be true because otherwise the BSQDDs B and $\tilde{B}$ would not represent the same superposition and therefore would not be equivalent. Also, for any path $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ to a node in the j^{th} layer of the BSQDD $\tilde{B}$, there exists a node in the BSQDD B that the path v terminates at. This implies that the number of nodes in the j^{th} layer of the BSQDD B is equal to the number of nodes in the j^{th} layer of the BSQDD $\tilde{B}$. It will be proven by induction that the initial state of the node a_v in the j^{th} layer of the BSQDD B on any path $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ is equal to the initial state of the node $\tilde{a}_v$ on the path v where a_v is the node in the BSQDD B that the path v terminates at and $\tilde{a}_v$ is the node in the BSQDD $\tilde{B}$ that the path v terminates at. The inductive proof will also show that the operation G of the node a_v is equal to the operation $\tilde{G}$ of the node $\tilde{a}_v$. Let the starting state be $|\psi_0\rangle = |b_1, \ldots, b_n\rangle$. Note that because the starting state $|\psi_0\rangle$ is required to be a basis state, $|b_k\rangle = |0\rangle$ or $|b_k\rangle = |1\rangle$ for all $k = 1, \ldots, n$. Let $|\psi\rangle$ be the quantum superposition represented by the BSQDD B. Since $B \approx \tilde{B}$, $|\psi\rangle$ is also represented by the BSQDD $\tilde{B}$. Consider the basis case where $j = 1$. Then $v = ()$. Let the operation of the node $a_{()}$ be G and let the operation of the node $\tilde{a}_{()}$ be $\tilde{G}$ where $G\,|b_{i_1}\rangle = \delta_0\,|0\rangle + \delta_1\,|1\rangle$ and $\tilde{G}\,|b_{i_1}\rangle = \tilde{\delta}_0\,|0\rangle + \tilde{\delta}_1\,|1\rangle$. Consider the quantum arrays generated by the BSQDDs B and $\tilde{B}$ according to definition 7.1. By theorem 7.3, applying either of these quantum arrays to the starting state $|\psi_0\rangle$ results in the desired quantum superposition $|\psi\rangle$. Because the control function of the root node $a_{()}$ of the BSQDD B is $f_{()}() = 1$ and no other layers in the BSQDD B operate on the variable x_{i_1}, the probability of observing $|0\rangle$ when the qubit $|x_{i_1}\rangle$ is measured in the quantum superposition $|\psi\rangle$ is $|\delta_0|^2$. Now the control function of the root node $\tilde{a}_{()}$ of the BSQDD $\tilde{B}$ is $\tilde{f}_{()}() = 1$ and no other layers in the BSQDD $\tilde{B}$ operate on the variable x_{i_1} so the probability of observing $|0\rangle$ when the qubit $|x_{i_1}\rangle$ is measured in the quantum superposition $|\psi\rangle$ is $\left|\tilde{\delta}_0\right|^2$. Therefore, $|\delta_0|^2 = \left|\tilde{\delta}_0\right|^2$ so since amplitudes are non-negative, $|\delta_0| = \left|\tilde{\delta}_0\right|$. Now $G, \tilde{G} \in F$ and the corresponding elements of gates in F have unique amplitudes. Therefore, $G = \tilde{G}$ which implies that the initial state of the root node $a_{()}$ of the BSQDD B on the path $()$ is equal to the initial state of the root node $\tilde{a}_{()}$ of the BSQDD $\tilde{B}$ on the path $()$. This proves the basis case. Consider the inductive case where the initial state of the node a_v in the j^{th} layer of the BSQDD Bon any path $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ is equal to the initial state of the node $\tilde{a}_v$ on the path v where a_v is the node in the BSQDD B that the path v terminates at and $\tilde{a}_v$ is the node in the BSQDD $\tilde{B}$ that the path v terminates at. Also, $G = \tilde{G}$ where G is the operation of the node a_v and $\tilde{G}$ is the operation of the node $\tilde{a}_v$. Let $\hat{v} = (\hat{v}_{i_1}, \ldots, \hat{v}_{i_j})$ be a path to a node $a_{\hat{v}}$ in the $j+1^{\text{th}}$ layer of the BSQDD B. Let $\tilde{a}_{\hat{v}}$ be the node in the BSQDD $\tilde{B}$ that the path $\hat{v}$ terminates at. Let the operation of the node $a_{\hat{v}}$ be G and let the operation of the node $\tilde{a}_{\hat{v}}$ be $\tilde{G}$ where $G\left|b_{i_{j+1}}\right\rangle = \delta_0 |0\rangle + \delta_1 |1\rangle$ and $\tilde{G}\left|b_{i_{j+1}}\right\rangle = \tilde{\delta}_0 |0\rangle + \tilde{\delta}_1 |1\rangle$. Let $v = (\hat{v}_{i_1}, \ldots, \hat{v}_{i_{j-1}})$. Because $\hat{v} \neq ()$ and the control function of the node $a_{\hat{v}}$ is $f_{\hat{v}}(x_{i_1}, \ldots, x_{i_j}) = 1$ the initial state of the node $a_{\hat{v}}$ on the path $\hat{v}$ in the BSQDD B is $\left|\hat{\psi}_{\hat{v},B}\right\rangle = \left(I_{2^{i_{j+1}-1}} \otimes G \otimes I_{2^{n-i_{j+1}}}\right)\left|\hat{\psi}^{\hat{v}_{i_j}}_{v,B}\right\rangle$ by definition 5.5 where B has been added to the subscripts of $\hat{\psi}$ to indicate that this initial state is from the BSQDD B. Since the qubit $\left|x_{i_{j+1}}\right\rangle$ is still equal to $\left|b_{i_{j+1}}\right\rangle$ in $\left|\hat{\psi}_{v,B}\right\rangle$ the probability of observing $|0\rangle$ when the qubit $\left|x_{i_{j+1}}\right\rangle$ is measured in the quantum superposition $\left|\hat{\psi}_{\hat{v},B}\right\rangle$ is $|\delta_0|^2$. Since $\hat{v} \neq ()$ and the control function of the node $\tilde{a}_{\hat{v}}$ is $\tilde{f}_{\hat{v}}(x_{i_1}, \ldots, x_{i_j}) = 1$ the initial state of the node $\tilde{a}_{\hat{v}}$ on the path $\hat{v}$ in the BSQDD $\tilde{B}$ is $\left|\hat{\psi}_{\hat{v},\tilde{B}}\right\rangle = \left(I_{2^{i_{j+1}-1}} \otimes \tilde{G} \otimes I_{2^{n-i_{j+1}}}\right)\left|\hat{\psi}^{\hat{v}_{i_j}}_{v,\tilde{B}}\right\rangle$ by definition 5.5 where $\tilde{B}$ has been added to the subscripts of $\hat{\psi}$ to indicate that this initial state is from the BSQDD $\tilde{B}$. Since the qubit $\left|x_{i_{j+1}}\right\rangle$ is still equal to $\left|b_{i_{j+1}}\right\rangle$ in $\left|\hat{\psi}_{v,\tilde{B}}\right\rangle$ the probability of observing $|0\rangle$ when the qubit $\left|x_{i_{j+1}}\right\rangle$ is measured in the quantum superposition $\left|\hat{\psi}_{\hat{v},\tilde{B}}\right\rangle$ is $\left|\tilde{\delta}_0\right|^2$. Let $\left|\overline{\ell}\right\rangle$ denote $\left|\hat{\ell}\right\rangle$ where $\hat{\ell}$ is equal to the binary string that corresponds to the number ℓ. Let $|\psi\rangle = \sum_{\ell=0}^{2^n-1} \alpha_\ell \left|\overline{\ell}\right\rangle$ be the quantum superposition represented by the BSQDD B. Let $|\gamma\rangle = \sum_{\ell=0}^{2^n-1} \beta_\ell \left|\overline{\ell}\right\rangle$ where $\beta_\ell = \alpha_\ell$ if $\hat{v}_{i_k} = 1$ in $\left|\overline{\ell}\right\rangle$ for all $k = 1, \ldots, j$ and $\beta_\ell = 0$ otherwise. Since the layers after the $j+1^{\text{th}}$ layer do not change the qubits $|x_{i_k}\rangle$ for $k = 1, \ldots, j+1$ and the BSQDD B represents $|\psi\rangle$, the probability of observing $|0\rangle$ when the qubit $\left|x_{i_{j+1}}\right\rangle$ is measured in the quantum superposition $|\gamma\rangle$ is equal to the probability $|\delta_0|^2$ of observing $|0\rangle$ when the qubit $\left|x_{i_{j+1}}\right\rangle$ is measured in the quantum superposition $\left|\hat{\psi}_{\hat{v},B}\right\rangle$. Because the BSQDD $\tilde{B}$ also represents the quantum superposition $|\psi\rangle$, the probability of observing $|0\rangle$ when the qubit $\left|x_{i_{j+1}}\right\rangle$ is measured in the quantum superposition $|\gamma\rangle$ is equal to the probability $\left|\tilde{\delta}_0\right|^2$ of observing $|0\rangle$ when the qubit $\left|x_{i_{j+1}}\right\rangle$ is measured in the quantum superposition $\left|\hat{\psi}_{\hat{v},\tilde{B}}\right\rangle$. Thus, $|\delta_0|^2 = \left|\tilde{\delta}_0\right|^2$ so since amplitudes are non-negative, $|\delta_0| = \left|\tilde{\delta}_0\right|$. Now $G, \tilde{G} \in F$ and the corresponding elements of gates in F have unique amplitudes. Therefore, $G = \tilde{G}$. By the inductive hypothesis, $\left|\hat{\psi}_{v,B}\right\rangle = \left|\hat{\psi}_{v,\tilde{B}}\right\rangle$ so $\left|\hat{\psi}^{\hat{v}_{i_j}}_{v,B}\right\rangle = \left|\hat{\psi}^{\hat{v}_{i_j}}_{v,\tilde{B}}\right\rangle$ by definition 5.5 which implies that $\left|\hat{\psi}_{\hat{v},B}\right\rangle = \left|\hat{\psi}_{\hat{v},\tilde{B}}\right\rangle$. This proves the inductive case. Therefore, by the principle of mathematical induction, the initial state of the node a_v in the j^{th} layer of the BSQDD B on any path $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ is equal to the initial state of the node $\tilde{a}_v$ on the path v where a_v is the node in the BSQDD B that the path v terminates at and $\tilde{a}_v$ is the node in the BSQDD $\tilde{B}$ that the path v terminates at. It will now be proven by induction that the node a_v in the j^{th} layer of the BSQDD B on any path $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ is equal to the node $\tilde{a}_v$ on the path v where a_v is the node in the BSQDD B that the path v terminates at and $\tilde{a}_v$ is the node in the BSQDD $\tilde{B}$ that the path v terminates at. Consider the basis case where $j = n$. Then a_v and $\tilde{a}_v$ are leaf nodes and have no children. Therefore, since the control function of a_v is $f_v(x_{i_1}, \ldots, x_{i_{n-1}}) = 1$ and the control function of $\tilde{a}_v$ is $\tilde{f}_v(x_{i_1}, \ldots, x_{i_{n-1}}) = 1$, $a_v = \tilde{a}_v$ if and only if $G = \tilde{G}$ where G is the operation of the node a_v and $\tilde{G}$ is the operation of $\tilde{a}_v$ by definition 5.1. Since it was just proven that $G = \tilde{G}$, $a_v = \tilde{a}_v$ so the basis case holds. Assume that the node a_v in the j^{th} layer of the BSQDD B on any path $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ is equal to the node $\tilde{a}_v$ on the path v where a_v is the node in the BSQDD B that the path v terminates at and $\tilde{a}_v$ is the node in the BSQDD $\tilde{B}$ that the path v terminates at. Let $\hat{v} = (v_{i_1}, \ldots, v_{i_{j-2}})$. Let $a_{\hat{v}}$ be the node in the BSQDD B that the path $\hat{v}$ terminates at and $\tilde{a}_{\hat{v}}$ be the node in the BSQDD $\tilde{B}$ that the path $\hat{v}$ terminates at. Let t be the tuple denoting the children of the node $a_{\hat{v}}$ and let $\tilde{t}$ be the tuple denoting the children of the node $\tilde{a}_{\hat{v}}$. By the inductive hypothesis the corresponding children of the nodes $a_{\hat{v}}$ and $\tilde{a}_{\hat{v}}$ are equal so $t = \tilde{t}$. Therefore, since the control function of $a_{\hat{v}}$ is $f_{\hat{v}}(x_{i_1}, \ldots, x_{i_{n-1}}) = 1$ and the control function of $\tilde{a}_{\hat{v}}$ is $\tilde{f}_{\hat{v}}(x_{i_1}, \ldots, x_{i_{n-1}}) = 1$, $a_{\hat{v}} = \tilde{a}_{\hat{v}}$ if and only if $G = \tilde{G}$ where G is the operation of a_v and $\tilde{G}$ is the operation of $\tilde{a}_v$ by definition 5.1. Since it was previously shown that $G = \tilde{G}$, $a_{\hat{v}} = \tilde{a}_{\hat{v}}$. Thus, the node a_v in the j^{th} layer of the BSQDD B on any path $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ is equal to the node $\tilde{a}_v$ on the path v where a_v is the node in the BSQDD B that the path v terminates at and $\tilde{a}_v$ is the node in the BSQDD $\tilde{B}$ that the path v terminates at. Therefore, $B = \tilde{B}$ by definition 6.3. □

This canonical form is quite general and works for many sets of gates. Examples include any set of gates $\{U, I, X\}$ where $|u_{ij}| \neq 0$ and $|u_{ij}| \neq 1$. This includes sets of gates such as $\{H, I, X\}$ and $\{V, I, X\}$ where $V = \frac{1}{2}\left[\begin{smallmatrix} 1+i & 1-i \\ 1-i & 1+i \end{smallmatrix}\right]$ is the square root of NOT. Another interesting set of gates for which the canonical form holds is $\left\{G_\theta = \left[\begin{smallmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{smallmatrix}\right] \;\middle|\; 0 \leq \theta \leq \frac{\pi}{2}\right\}$ which is used in the Long-Sun algorithm [6].

Theorem 10.2. *Let $F \neq \emptyset$ be a set of gates such that the corresponding elements of the* *gates in the set F have unique amplitudes as defined in theorem 10.1. Let B and $\hat{B}$ be equivalent BSQDDs where $B = (A, (L_1, \ldots, L_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_n}), F)$ and $\hat{B} = (\hat{A}, (\tilde{L}_1, \ldots, \tilde{L}_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_n}), F)$ have no repeated variables. Then B can be transformed into $\hat{B}$ using transformation rules 8.1 and 8.2.*

Proof. The theorem will be proven by showing that the BSQDDs B and $\hat{B}$ can be transformed into canonical form. First transformation rule 8.1 is used to split the nodes in B and $\hat{B}$ until each node has exactly one parent. Let these two new sets of nodes be denoted by $\dot{A}$ and $\ddot{A}$ respectively. Now consider a node $a = (G, f(x_{i_1}, \ldots, x_{i_{j-1}}), t)$ where $a \in \dot{A}$ or $a \in \ddot{A}$. If $f(x_{i_1}, \ldots, x_{i_{j-1}})$ is not equal to the constant function $\tilde{f}(x_{i_1}, \ldots, x_{i_{j-1}}) = 1$, then a can be replaced by a new node $\tilde{a} = (\tilde{G}, \tilde{f}(x_{i_1}, \ldots, x_{i_{j-1}}) = 1, t)$ where $\tilde{G} = G$ if $f(x_{i_1}, \ldots, x_{i_{j-1}}) = 1$ on the path to a from the root and $\tilde{G} = I$ if $f(x_{i_1}, \ldots, x_{i_{j-1}}) = 0$ on the path to a from the root using transformation rule 8.2. Merging equal nodes in each layer then results in two new BSQDDs B_c and $\hat{B}_c$ that are obtained from B and $\hat{B}$ respectively as described above. Because B_c and $\hat{B}_c$ are in canonical form by theorem 10.1, $B_c = \hat{B}_c$. Because transformation rules 8.1 and 8.2 can each be applied in both directions, the BSQDD $\hat{B}_c = B_c$ can be transformed into $\hat{B}$ using transformation rules 8.1 and 8.2. Therefore the BSQDD B can be transformed into the BSQDD $\hat{B}$ using transformation rules 8.1 and 8.2. □

Theorem 10.2 shows that a BSQDD B of the form shown in theorem 10.1 that has no repeated variables can be transformed into any equivalent BSQDD using transformation rules 8.1 and 8.2. Algorithm 2 can be used to construct a BSQDD in the canonical form given in theorem 10.1 that represents a desired quantum superposition for a given order of variables and starting state provided that the set of gates used for synthesis satisfy the constraints in theorem 10.1. Since a quantum superposition can be represented as a list of all terms with non-zero coefficients, this algorithm is in the complexity class $\Theta(mn)$ where m is the number of terms non-zero coefficients in the desired quantum superposition. Algorithm 3 can be used to convert any BSQDD that satisfies the conditions in theorem 10.1 and has all of its control functions equal to the constant 1 into canonical form using transformation rule 8.1. The restriction on the control functions is used because it makes the algorithm much more efficient. If the number of nodes in the j^{th} layer of the BSQDD B is given by ℓ_j, then algorithm 3 is in the complexity class $\Theta(\ell_1 + \ldots + \ell_n) = \Theta(|A|)$ since each iteration over all pairs of equal nodes can be implemented in linear time by constructing a hash table that contains all nodes in the current layer.

11 Complexity of BSQDDs

This section will present two theorems that provide upper bounds on the number of nodes required in BSQDDs with and without repeated variables. A class of quantum superpositions will then be shown that require an exponential number of one and two qubit operations to be initialized using the Ventura-Martinez [11], SQUID [8] and Long-Sun [6] algorithms but only a linear number of one and two qubit operations when BSQDDs are used to find the initialization quantum array.

Algorithm 2 The algorithm for constructing a BSQDD in canonical form

Let the desired quantum superposition be $|\psi\rangle$, let $(x_{i_1}, \ldots, x_{i_n})$ be the desired order of variables, let the starting state be $|\psi_0\rangle = |b_1, \ldots, b_n\rangle$ and let F be a set of gates that satisfies the constraints in theorem 10.1
Let $a = \mathbf{construct}(|\psi\rangle, 1)$
if $|\phi\rangle = |\psi\rangle$ where $|\phi\rangle$ is the quantum superposition represented by the BSQDD with the root node a **then**
    return $\mathbf{bsqdd}(a, (x_{i_1}, \ldots, x_{i_n}), F)$ ▷ **bsqdd** is a function that takes a root node, the order of variables and the set of gates and stores them in a BSQDD which it then returns
else
    return Failure, this quantum superposition cannot be represented using this set of gates
end if
function $\mathbf{construct}(|\delta\rangle, j)$:
Let $|\delta\rangle = \sum_{i=0}^{2^n-1} \alpha_i \left|\bar{i}\right\rangle$
Let $\beta = \sqrt{\sum_{i=0}^{2^n-1} \beta_i^2}$ where $\beta_i = \alpha_i$ if $x_{i_j} = 0$ in $\left|\bar{i}\right\rangle$ and $\beta_i = 0$ otherwise
Let $\gamma = \sqrt{\sum_{i=0}^{2^n-1} \gamma_i^2}$ where $\gamma_i = \alpha_i$ if $x_{i_j} = 1$ in $\left|\bar{i}\right\rangle$ and $\gamma_i = 0$ otherwise
Let $|\zeta\rangle = \sum_{i=0}^{2^n-1} \beta_i \left|\bar{i}\right\rangle$ and $|\xi\rangle = \sum_{i=0}^{2^n-1} \gamma_i \left|\bar{i}\right\rangle$
Let $G \in F$ be the operator that satisfies $|g_0|^2 = \frac{\beta^2}{\beta^2+\gamma^2}$ and $|g_1|^2 = \frac{\gamma^2}{\beta^2+\gamma^2}$ where $G\left|b_{i_j}\right\rangle = g_0|0\rangle + g_1|1\rangle$ ▷ Note that because the gates in the set F have unique amplitudes, the operator G is unique if it exists
if no such operator G exists **then**
    return Failure, this quantum superposition cannot be represented using this set of gates
else if $j = n$ **then**
    return $(G, f(x_{i_1}, \ldots, x_{i_{j-1}}) = 1, ())$
else if $\beta \neq 0$ and $\gamma \neq 0$ **then**
    return $(G, f(x_{i_1}, \ldots, x_{i_{j-1}}) = 1, (\mathbf{construct}(|\zeta\rangle, j+1), \mathbf{construct}(|\xi\rangle, j+1)))$
else if $\beta \neq 0$ and $\gamma = 0$ **then**
    return $(G, f(x_{i_1}, \ldots, x_{i_{j-1}}) = 1, (\mathbf{construct}(|\zeta\rangle, j+1)))$
else if $\beta = 0$ and $\gamma \neq 0$ **then**
    return $(G, f(x_{i_1}, \ldots, x_{i_{j-1}}) = 1, (\mathbf{construct}(|\xi\rangle, j+1)))$
end if

Algorithm 3 The algorithm for converting a BSQDD into canonical form

1: Let $B = (A, (L_1, \ldots, L_n), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_n}), F)$ be a BSQDD that satisfies the constraints in theorem 10.2 and the control function for each node a in the j^{th} layer is $f(x_{i_1}, \ldots, x_{i_{j-1}}) = 1$
2: **for all** $j = n, \ldots, 1$ **do**
3:     **for all** pairs of nodes a and $\hat{a}$ in the j^{th} layer where $a = \hat{a}$ **do**
4:         Apply transformation rule 8.1 to merge the nodes a and $\hat{a}$
5:     **end for**
6: **end for**

Theorem 11.1. *Let $B = (A, (L_1, \ldots, L_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_m}), F)$ be a BSQDD. Then the maximum number of nodes in the BSQDD B is $(m-n)2^{n-1}+2^n-1$.*

Proof. Let $B = (A, (L_1, \ldots, L_m), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_m}), F)$ be a BSQDD. By definition 5.3, each node a in the j^{th} layer of the BSQDD B has at least one path $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ that terminates at a. Therefore, the number of nodes in the j^{th} layer is bounded above by the number of paths to nodes in the j^{th} layer. From definition 5.3, each $v_{i_k} \equiv \overline{x}_{i_k}$ or $v_{i_k} \equiv x_{i_k}$ so the number of paths to nodes in the j^{th} layer is at most 2^{j-1}. Therefore, there are at most $\sum_{j=1}^{n} 2^{j-1} = 2^n - 1$ nodes in the first n layers. By definition 5.3, if $x_{i_j} \equiv x_{i_k}$ for some $k < j$ and $v = (v_{i_1}, \ldots, v_{i_{j-1}})$ and $\hat{v} = (\hat{v}_{i_1}, \ldots, \hat{v}_{i_{j-1}})$ are paths to the j^{th} layer with $v_{i_\ell} \equiv \hat{v}_{i_\ell}$ for $\ell < j$ and $\ell \neq k$ then $v_{i_k} \equiv \hat{v}_{i_k}$. This implies that only $n-1$ of the variables v_{i_k} where $k < j$ and $j > n$ can be chosen because the rest are determined by definition 5.3. Therefore, the j^{th} layer has at most 2^{n-1} nodes. Since there are $m - n$ layers where $j > n$, the number of nodes in layers where $j > n$ is at most $(m-n)2^{n-1}$. Therefore, the total of nodes in the BSQDD B is at most $(m-n)2^{n-1} + 2^n - 1$. □

Theorem 11.2. *Let $B = (A, (L_1, \ldots, L_n), \{x_1, \ldots, x_n\}, (x_{i_1}, \ldots, x_{i_n}), F)$ be a BSQDD with no repeated variables. Then the maximum number of nodes in the BSQDD B is $2^n - 1$.*

Proof. Because the number of layers in the BSQDD B is $m = n$, the maximum number of nodes in the BSQDD B is $2^n - 1$ by theorem 11.1. □

It will now be shown that quantum superpositions that correspond to an an exclusive or (EXOR) of the variables that correspond to qubits in the quantum superposition can be represented using a BSQDD that requires only a linear number of nodes.

Theorem 11.3. *Let $\{|x_1\rangle, \ldots, |x_n\rangle\}$ be a set of qubits and let $g(x_1, \ldots, x_n) = \bigoplus_{k=1}^{n} x_k$ where $\bigoplus$ denotes summation using the EXOR operation. Let $u_{i,1}, \ldots, u_{i,n}$ denote the binary representation of the number $0 \leq i \leq 2^n - 1$. Let $|\psi\rangle = \sum_{i=0}^{2^n-1} \alpha_i \left|\bar{i}\right\rangle$ where $\left|\bar{i}\right\rangle$ denotes $\left|\hat{i}\right\rangle$, $\hat{i}$ is equal to the binary string that corresponds to the number i and $\alpha_i = \frac{1}{\sqrt{2^{n-1}}}$ if $g(u_{i,1}, \ldots, u_{i,n}) = 1$ and $\alpha_i = 0$ otherwise. Then the quantum state $|\psi\rangle$ can be represented by $B = (A, (L_1, \ldots, L_n), \{x_1, \ldots, x_n\}, (x_1, \ldots, x_n), \{H, I, X\})$*

where B is a BSQDD in the canonical form of theorem 10.1 that has $2n-1$ nodes and the starting state $|\psi_0\rangle = |0^n\rangle$.

Proof. First a BSQDD $B = (A, (L_1, \ldots, L_n), \{x_1, \ldots, x_n\}, (x_1, \ldots, x_n), \{H, I, X\})$ will be constructed. In this BSQDD, the j^{th} layer L_j will contain two nodes if $j > 1$ and one node if $j = 1$. These nodes will be denoted by $a_{j,\ell}$ where j is the index of the layer that contains the node and ℓ is an index that distinguishes nodes within the same layer so that $\ell = 0$ or $\ell = 1$ for $j > 1$ and $\ell = 0$ for $j = 1$. The control function is $f(x_1, \ldots, x_{j-1}) = 1$ for each node $a_{j,\ell}$ in the j^{th} layer. The operation of each node $a_{j,\ell}$ in the j^{th} layer is H for $j < n$. The operation of the node $a_{n,0}$ is X and the operation of the node $a_{n,1}$ is I. The children of the nodes will now be defined. Let $t_{j,\ell}$ be the tuple from definition 5.1 denoting the children of the node $a_{j,\ell}$. The tuple $t_{j,\ell}$ will now be defined. If $n = 1$ then the root node $a_{1,0}$ is the only node in the BSQDD B and $t_{1,0} = ()$. For $j < n$, $t_{j,0} = (a_{j+1,0}, a_{j+1,1})$ and $t_{j,1} = (a_{j+1,1}, a_{j+1,0})$. For $j = n$, $t_{n,0} = ()$ and $t_{n,1} = ()$ if $n \neq 1$. Let the starting state be $|\psi_0\rangle = |0^n\rangle$. Let $v = (v_1, \ldots, v_{j-1})$ be a path to a node $a_{j,\ell}$ in the j^{th} layer of the BSQDD B. The BSQDD B is shown in figure 6(a) for the case where $n = 3$. Let $u_k = 0$ if $v_k \equiv \overline{x}_k$ and $u_k = 1$ if $v_k \equiv x_k$ for each $k = 1, \ldots, j-1$. Also, let $s_{j,\ell} = \bigoplus_{k=1}^{j-1} u_k$. It will be proven by induction that for $j < n$ the initial state of the node $a_{j,\ell}$ on the path v is

$$\left|\hat{\psi}_v\right\rangle = \frac{1}{\sqrt{2^j}} \left|u_1 \ldots u_{j-1} 0^{n-j+1}\right\rangle + \frac{1}{\sqrt{2^j}} \left|u_1 \ldots u_{j-1} 1 0^{n-j}\right\rangle \tag{16}$$

Furthermore, it will also be shown that $\ell = s_{j,\ell}$ for all $j = 1, \ldots, n$. Consider the basis case where $j = 1$. Then $v = ()$ since this is the only possible path to the root node and the root node is the only node in the first layer. Since the starting state is $|\psi_0\rangle = |0^n\rangle$, the initial state of the root node on the path $()$ is $\left|\hat{\psi}_{()}\right\rangle = \frac{1}{\sqrt{2}} |0^n\rangle + \frac{1}{\sqrt{2}} \left|10^{n-1}\right\rangle$ by definition 5.5 so equation (16) is satisfied. Since $v = ()$ and the root node is $a_{1,0}$, $\ell = 0$ and $s_{1,0} = 0$ so $\ell = s_{1,0}$ as well and the basis case is proven. For the inductive case, assume that equation (16) holds for every path $v = (v_1, \ldots, v_{j-1})$ to a node $a_{j,\ell}$ in the j^{th} layer of the BSQDD B and $\ell = s_{j,\ell}$ for each such node. Let $\hat{v} = (\hat{v}_1, \ldots, \hat{v}_j)$ be a path to a node $a_{j+1,\hat{\ell}}$ in the $j+1^{\text{th}}$ layer. Let $a_{j,\ell}$ be the parent node of $a_{j+1,\hat{\ell}}$ on the path $\hat{v}$. Let $\hat{u}_k = 0$ if $\hat{v}_k \equiv \overline{x}_k$ and $\hat{u}_k = 1$ if $\hat{v}_k \equiv x_k$ for each $k = 1, \ldots, j$. By the inductive hypothesis, the initial state of the node $a_{j,\ell}$ on the path v is $\left|\hat{\psi}_v\right\rangle = \frac{1}{\sqrt{2^j}} \left|\hat{u}_1 \ldots \hat{u}_{j-1} 0^{n-j+1}\right\rangle + \frac{1}{\sqrt{2^j}} \left|\hat{u}_1 \ldots \hat{u}_{j-1} 1 0^{n-j}\right\rangle$ where $v = (\hat{v}_1, \ldots, \hat{v}_{j-1})$. Therefore, $\left|\hat{\psi}_v^{\hat{v}_j}\right\rangle = \frac{1}{\sqrt{2^j}} \left|\hat{u}_1 \ldots \hat{u}_j 0^{n-j}\right\rangle$ by definition 5.5. It follows by definition 5.5 that the initial state of the node $a_{j+1,\hat{\ell}}$ is $\left|\hat{\psi}_{\hat{v}}\right\rangle = \frac{1}{\sqrt{2^{j+1}}} \left|\hat{u}_1 \ldots \hat{u}_j 0^{n-j}\right\rangle + \frac{1}{\sqrt{2^{j+1}}} \left|\hat{u}_1 \ldots \hat{u}_j 1 0^{n-j-1}\right\rangle$ which satisfies equation (16). Observe that by definition, if $\ell = \hat{\ell}$ then $\hat{u}_j = 0$ so $s_{j+1,\hat{\ell}} = s_{j,\ell} \oplus 0$ which is equal to $\ell = \hat{\ell}$. Also, by definition if $\ell \neq \hat{\ell}$ then $\ell = \hat{\ell} \oplus 1$ and $\hat{u}_j = 1$ so $s_{j+1,\hat{\ell}} = s_{j,\ell} \oplus 1$ which is equal to $\ell \oplus 1 = \hat{\ell}$. This proves the inductive case so by the principle of mathematical induction, the initial state of the node $a_{j,\ell}$ on the path v is given by equation (16) for $j < n$ and $\ell = s_{j,\ell}$ for all $j = 1, \ldots, n$. Let $\hat{v} = (\hat{v}_1, \ldots, \hat{v}_{n-1})$ be a path to a node $a_{n,\hat{\ell}}$ in the n^{th} layer. Let $a_{n-1,\ell}$ be the parent node of the node $a_{n,\hat{\ell}}$ on the path

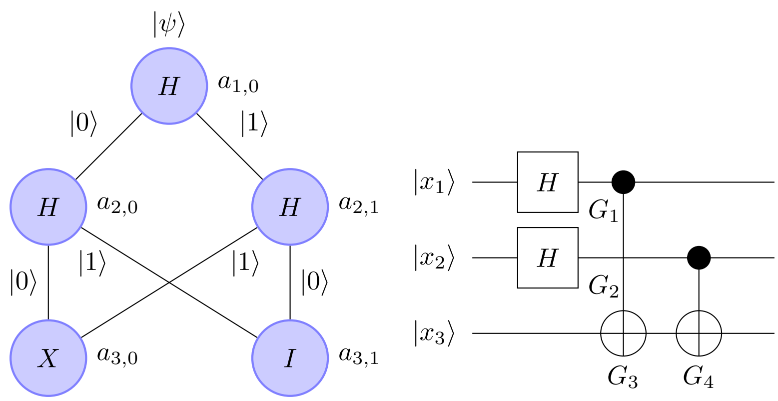
$\hat{v}$. It was shown that the initial state of $a_{n-1,\ell}$ on the path $v = (\hat{v}_1, \ldots, \hat{v}_{n-2})$ is given by equation (16). Suppose that $\hat{\ell} = 0$. Since the operation of the node $a_{n,0}$ is X, the initial state of the node $a_{n,\hat{\ell}}$ on the path $\hat{v}$ is $\left|\hat{\psi}_{\hat{v}}\right\rangle = \frac{1}{\sqrt{2^{n-1}}} \left|\hat{u}_1 \ldots \hat{u}_{n-1} 1\right\rangle$. Because $s_{n,0} = 0$, it follows that $g(\hat{u}_1, \ldots, \hat{u}_{n-1}, 1) = 1$. Now suppose that $\hat{\ell} = 1$. Since the operation of the node $a_{n,1}$ is I, the initial state of the node $a_{n,\hat{\ell}}$ on the path $\hat{v}$ is $\left|\hat{\psi}_{\hat{v}}\right\rangle = \frac{1}{\sqrt{2^{n-1}}} \left|\hat{u}_1 \ldots \hat{u}_{n-1} 0\right\rangle$. Because $s_{n,1} = 1$, it follows that $g(\hat{u}_1, \ldots, \hat{u}_{n-1}, 0) = 1$. Therefore since the amplitude of each basis state in the quantum superposition represented by the BSQDD B is $\frac{1}{\sqrt{2^{n-1}}}$ and the function $g(x_1, \ldots, x_n)$ has an output of 1 for exactly 2^{n-1} assignments to its inputs, it follows that the BSQDD B represents the quantum superposition $|\psi\rangle$. Since the BSQDD B has $2n-1$ nodes and satisfies the conditions in 10.1 the proof is complete. $\square$

Applying algorithm 1 to the BSQDD B from the proof of theorem 11.3, a quantum array that uses $n-1$ single qubit H operations and $n-1$ two qubit Feynman operations is obtained. This quantum array is shown in figure 6(b) for the case where $n = 3$. Thus, the quantum superposition $|\psi\rangle$ from theorem 11.3 can be represented using a BSQDD with a linear number of nodes that generates a quantum array with a linear number of one and two qubit operations. Because other approaches to initializing this quantum superposition rely on representing the quantum superposition using minterms in the case of the Ventura-Martinez [11] and phase groups in the case of the SQUID [8], both of these algorithms require an exponential number of one and two qubit operations to initialize the quantum superposition $|\psi\rangle$ from theorem 11.3 while BSQDDs can be used to accomplish this task using only a linear number of one and two qubit operations. Therefore, in this case BSQDDs are an exponential improvement over the Ventura-Martinez [11], SQUID [8] and Long-Sun [6] algorithms. The ESQUID algorithm [9] can initialize the quantum state $|\psi\rangle$ from theorem 11.3 using only a linear number of one and two qubit operations assuming the correct sequence of generalized phase groups is used. However, it still uses extra qubits and requires more operations than if BSQDDs are used. Furthermore, finding an efficient sequence of generalized phase groups is a difficult problem that the ESQUID algorithm [9] does not address and the ESQUID algorithm [9] can only be used for quantum superpositions of the form $|\psi\rangle = \sum_{i=0}^{2^n-1} \frac{t_i}{\sqrt{m}} |i\rangle$ where $t_i \in \{-1, 0, 1\}$ while BSQDDs can be used for arbitrary quantum superpositions as is proven in theorem 12.1.

12 BSQDDs are Universal

In this section, it will be shown that BSQDDs are universal in the sense that a BSQDD can represent an arbitrary quantum superposition given an appropriate set of gates.

Theorem 12.1. *A BSQDD operating on the set of qubits* $\{|x_1\rangle, \ldots, |x_n\rangle\}$ *using the set of gates* $\left\{G_{\theta,\varphi} = \begin{bmatrix} \cos\theta & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta \end{bmatrix} \,\middle|\, \theta, \varphi \in \mathbb{R}\right\}$, *the order of variables* $(x_1, \ldots, x_n)$ *and the starting state* $|\psi_0\rangle = |0^n\rangle$ *can represent an arbitrary quantum superposition.*



(a) A BSQDD that represents $|\psi\rangle$

(b) The quantum array generated by the BSQDD

Figure 6: The BSQDD and quantum array for $|\psi\rangle$

This set of gates is adapted from the Long-Sun algorithm [6]. This theorem will now be proven by constructing a BSQDD that initializes an arbitrary quantum superposition.

Proof. Note that $G_{\theta,\varphi} = G^{\dagger}_{\theta,\varphi}$ so $G_{\theta,\varphi}$ is Hermitian and as well as unitary. Let $|\psi\rangle = \sum_{k=0}^{2^n-1} \alpha_k \left|\overline{k}\right\rangle$ be an arbitrary quantum superposition where $\alpha_k \in \mathbb{C}$, $\sum_{k=0}^{2^n-1} |\alpha_k|^2 = 1$ and $\left|\overline{k}\right\rangle$ denotes $\left|\hat{k}\right\rangle$ with $\hat{k}$ equal to the binary string that corresponds to the number k. Then $|\psi\rangle = \sum_{k=0}^{2^n-1} r_k e^{i\phi_k} \left|\overline{k}\right\rangle$ where each $\alpha_k = r_k e^{i\phi_k}$ and $\sum_{k=0}^{2^n-1} r_k^2 = 1$. Because global phase is irrelevant, the quantum superposition

$$\left|\tilde{\psi}\right\rangle = e^{-i\phi_0} |\psi\rangle \tag{17}$$

$$= \sum_{k=0}^{2^n-1} r_k e^{i\varphi_k} \left|\overline{k}\right\rangle \tag{18}$$

is equivalent to $|\psi\rangle$ where each $\varphi_k = \phi_k - \phi_0$. Consider the BSQDD B that has the order of variables $(x_1, \ldots, x_n)$ where each node that is not a leaf node has two children and the control function of each node is always equal to 1. This implies that the path from the root to any node in this BSQDD is unique. Let a_v be a node in the j^{th} layer that the path $v = (v_1, \ldots, v_{j-1})$ terminates at. Let $u_k = 0$ if $v_k \equiv \overline{x}_k$ and $u_k = 1$ if $v_k \equiv x_k$ for each $k = 1, \ldots, j-1$. Let $x = u_1 \ldots u_{j-1}0^{n-j+1}$, $y = u_1 \ldots u_{j-1}1^{n-j+1}$ and $z = u_1 \ldots u_{j-1}10^{n-j}$ where the expressions $u_1 \ldots u_{j-1}0^{n-j+1}$, $u_1 \ldots u_{j-1}10^{n-j}$ and $u_1 \ldots u_{j-1}1^{n-j+1}$ are interpreted as binary numbers. For the rest of this proof, the node a_v at which a path v terminates will be denoted by $a_{x,y}$ where x and y are as defined above. Assume that $a_{x,y}$ is not a leaf node. Then $z - 1 = u_1 \ldots u_{j-1}01^{n-j}$ which implies that the tuple from definition 5.1 that denotes that children of the node $a_{x,y}$ is $(a_{x,z-1}, a_{z,y})$ since the paths to the children of the node $a_{x,y}$ are $(v_1, \ldots, v_{j-1}, \overline{x}_j)$ and $(v_1, \ldots, v_{j-1}, x_j)$. Also note that by definition of x and z, $z = x + 2^{n-j}$. This property will be used later in this proof. The operation of the node $a_{x,y}$ is denoted by $U_{x,y} = G_{\theta_{x,y}, \varphi_{x,y}}$ where $\theta_{x,y} = \cos^{-1}\alpha_{x,y}$, $\varphi_{x,y} = \varphi_z - \varphi_x$, $\alpha_{x,y} = \sqrt{\frac{\sum_{k=x}^{z-1} r_k^2}{\sum_{k=x}^{y} r_k^2}}$, $\beta_{x,y} = \sqrt{\frac{\sum_{k=z}^{y} r_k^2}{\sum_{k=x}^{y} r_k^2}}$ and x, y and z are as previously defined. If the denominator in the formulas for $\alpha_{x,y}$ and $\beta_{x,y}$ is 0, then $\alpha_{x,y}$ is taken to be 1 and $\beta_{x,y}$ is taken to be 0. The BSQDD B is shown in figure 7 for the case where $n = 3$. It will now be proven that the BSQDD B represents $\left|\tilde{\psi}\right\rangle$. Because each path from the root to a node in the BSQDD B is unique, it is not necessary to specify the path to when referring to the initial state of a node. Several identities are used in this proof which will now be shown. From trigonometry, $\sin\cos^{-1}x = \sqrt{1 - x^2}$. Also, from the definitions of $\alpha_{x,y}$ and $\beta_{x,y}$, $\alpha_{x,y} = \sqrt{1 - \beta_{x,y}^2}$ and $\beta_{x,y} = \sqrt{1 - \alpha_{x,y}^2}$. It will now be proven by induction on the layers of the BSQDD B that the initial state of a node $a_{x,y}$ on the path v in the j^{th} layer of the BSQDD B is

$$\left|\hat{\psi}_v\right\rangle = \gamma_{x,y}\alpha_{x,y}e^{i\varphi_x}\left|\overline{x}\right\rangle + \gamma_{x,y}\beta_{x,y}e^{i\varphi_z}\left|\overline{z}\right\rangle \tag{19}$$

where $\gamma_{x,y} = \sqrt{\sum_{k=x}^{y} r_k^2}$. For the basis case $j = 1$, $x = 0$, $y = 2^n - 1$ and $z = 2^{n-1}$ so by definition 5.5 the initial state of the root node is

$$\left|\hat{\psi}_{()}\right\rangle = (U_{0,2^n-1} \otimes I_{2^{n-1}})\left|0^n\right\rangle \tag{20}$$

$$= (G_{\theta_{0,2^n-1}, \varphi_{0,2^n-1}} \otimes I_{2^{n-1}})\left|0^n\right\rangle \tag{21}$$

$$= \left(\begin{bmatrix} \cos\theta_{0,2^n-1} & \sin\theta_{0,2^n-1}e^{-i\varphi_{0,2^n-1}} \\ \sin\theta_{0,2^n-1}e^{i\varphi_{0,2^n-1}} & -\cos\theta_{0,2^n-1} \end{bmatrix} \otimes I_{2^{n-1}}\right)\left|0^n\right\rangle \tag{22}$$

$$= \left(\begin{bmatrix} \alpha_{0,2^n-1} & \sqrt{1 - \alpha_{0,2^n-1}^2}e^{-i\varphi_{2^{n-1}}} \\ \sqrt{1 - \alpha_{0,2^n-1}^2}e^{i\varphi_{2^{n-1}}} & -\alpha_{0,2^n-1} \end{bmatrix} \otimes I_{2^{n-1}}\right)\left|0^n\right\rangle \tag{23}$$

$$= \left(\begin{bmatrix} \alpha_{0,2^n-1} & \beta_{0,2^n-1}e^{-i\varphi_{2^{n-1}}} \\ \beta_{0,2^n-1}e^{i\varphi_{2^{n-1}}} & -\alpha_{0,2^n-1} \end{bmatrix} \otimes I_{2^{n-1}}\right)\left|0^n\right\rangle \tag{24}$$

$$= \alpha_{0,2^n-1}e^0\left|0^n\right\rangle + \beta_{0,2^n-1}e^{i\varphi_{2^{n-1}}}\left|10^{n-1}\right\rangle \tag{25}$$

$$= \gamma_{0,2^n-1}\alpha_{0,2^n-1}e^{\varphi_0}\left|\overline{0}\right\rangle + \gamma_{0,2^n-1}\beta_{0,2^n-1}e^{i\varphi_{2^{n-1}}}\left|\overline{2^{n-1}}\right\rangle \tag{26}$$

Thus, equation (19) holds so the basis case is proven. The inductive case will now be proved. Assume that the initial state of any node $a_{x,y}$ in the j^{th} layer of the BSQDD B is given by equation (19). Let $\hat{a}_{\hat{x},\hat{y}}$ be a node in the $j + 1^{\text{th}}$ layer of the BSQDD B, let $a_{x,y}$ be the parent node of $\hat{a}_{\hat{x},\hat{y}}$ and let $\hat{v} = (\hat{v}_1, \ldots, \hat{v}_j)$ be the path to the node $\hat{a}_{\hat{x},\hat{y}}$ from the root node. Let $v = (\hat{v}_1, \ldots, \hat{v}_{j-1})$. Suppose that $\hat{v}_j \equiv \overline{x}_j$. Then $\hat{x} = x$, $\hat{y} = z - 1$ and $\hat{z} = \hat{x} + 2^{n-j-1}$ by definition of x, y and z. Therefore, by definition

5.5 the initial state of the node $\hat{a}_{\hat{x},\hat{y}}$ is

$$\begin{aligned}
\left|\hat{\psi}_{\hat{v}}\right\rangle =&(I_{2^j} \otimes U_{\hat{x},\hat{y}} \otimes I_{2^{n-j-1}}) \left|\hat{\psi}_{v}^{\overline{x}_j}\right\rangle && (27)\\
=&(I_{2^j} \otimes G_{\theta_{\hat{x},\hat{y}},\varphi_{\hat{x},\hat{y}}} \otimes I_{2^{n-j-1}})\gamma_{x,y}\alpha_{x,y}e^{i\varphi_x} \left|\overline{x}\right\rangle && (28)\\
=&\left(I_{2^j} \otimes \begin{bmatrix} \cos\theta_{\hat{x},\hat{y}} & \sin\theta_{\hat{x},\hat{y}}e^{-i\varphi_{\hat{x},\hat{y}}} \\ \sin\theta_{\hat{x},\hat{y}}e^{i\varphi_{\hat{x},\hat{y}}} & -\cos\theta_{\hat{x},\hat{y}} \end{bmatrix} \otimes I_{2^{n-j-1}}\right) && (29)\\
&\cdot \gamma_{x,z-1}e^{i\varphi_x} \left|\overline{x}\right\rangle \\
=&\left(I_{2^j} \otimes \begin{bmatrix} \alpha_{\hat{x},\hat{y}} & \sqrt{1-\alpha_{\hat{x},\hat{y}}^2}e^{-i\varphi_{\hat{x},\hat{y}}} \\ \sqrt{1-\alpha_{\hat{x},\hat{y}}^2}e^{i\varphi_{\hat{x},\hat{y}}} & -\alpha_{\hat{x},\hat{y}} \end{bmatrix} \otimes I_{2^{n-j-1}}\right) && (30)\\
&\cdot \gamma_{\hat{x},\hat{y}}e^{i\varphi_{\hat{x}}} \left|\overline{x}\right\rangle \\
=&\left(I_{2^j} \otimes \begin{bmatrix} \alpha_{\hat{x},\hat{y}} & \beta_{\hat{x},\hat{y}}e^{-i(\varphi_{\hat{z}}-\varphi_{\hat{x}})} \\ \beta_{\hat{x},\hat{y}}e^{i(\varphi_{\hat{z}}-\varphi_{\hat{x}})} & -\alpha_{\hat{x},\hat{y}} \end{bmatrix} \otimes I_{2^{n-j-1}}\right) && (31)\\
&\cdot \gamma_{\hat{x},\hat{y}}e^{i\varphi_{\hat{x}}} \left|\overline{x}\right\rangle \\
=&\gamma_{\hat{x},\hat{y}}\alpha_{\hat{x},\hat{y}}e^{i\varphi_{\hat{x}}} \left|\overline{x}\right\rangle + \gamma_{\hat{x},\hat{y}}\beta_{\hat{x},\hat{y}}e^{i\varphi_{\hat{z}}} \left|\overline{x+2^{n-j-1}}\right\rangle && (32)\\
=&\gamma_{\hat{x},\hat{y}}\alpha_{\hat{x},\hat{y}}e^{i\varphi_{\hat{x}}} \left|\overline{\hat{x}}\right\rangle + \gamma_{\hat{x},\hat{y}}\beta_{\hat{x},\hat{y}}e^{i\varphi_{\hat{z}}} \left|\overline{\hat{z}}\right\rangle && (33)
\end{aligned}$$

Now Suppose that $\hat{v}_j \equiv x_j$ on the path $\hat{v}$ from the root to $\hat{a}_{\hat{x},\hat{y}}$. Then $\hat{x} = z$, $\hat{y} = y$ and $\hat{z} = \hat{x} + 2^{n-j-1}$. Therefore, by definition 5.5 the initial state of $\hat{a}_{\hat{x},\hat{y}}$ is

$$\begin{aligned}
\left|\hat{\psi}_{\hat{v}}\right\rangle =&(I_{2^j} \otimes U_{\hat{x},\hat{y}} \otimes I_{2^{n-j-1}}) \left|\hat{\psi}_{v}^{x_j}\right\rangle && (34)\\
=&(I_{2^j} \otimes G_{\theta_{\hat{x},\hat{y}},\varphi_{\hat{x},\hat{y}}} \otimes I_{2^{n-j-1}})\gamma_{x,y}\beta_{x,y}e^{i\varphi_z} \left|\overline{z}\right\rangle && (35)\\
=&\left(I_{2^j} \otimes \begin{bmatrix} \cos\theta_{\hat{x},\hat{y}} & \sin\theta_{\hat{x},\hat{y}}e^{-i\varphi_{\hat{x},\hat{y}}} \\ \sin\theta_{\hat{x},\hat{y}}e^{i\varphi_{\hat{x},\hat{y}}} & -\cos\theta_{\hat{x},\hat{y}} \end{bmatrix} \otimes I_{2^{n-j-1}}\right) \gamma_{z,y}e^{i\varphi_z} \left|\overline{z}\right\rangle && (36)\\
=&\left(I_{2^j} \otimes \begin{bmatrix} \alpha_{\hat{x},\hat{y}} & \sqrt{1-\alpha_{\hat{x},\hat{y}}^2}e^{-i\varphi_{\hat{x},\hat{y}}} \\ \sqrt{1-\alpha_{\hat{x},\hat{y}}^2}e^{i\varphi_{\hat{x},\hat{y}}} & -\alpha_{\hat{x},\hat{y}} \end{bmatrix} \otimes I_{2^{n-j-1}}\right) && (37)\\
&\cdot \gamma_{\hat{x},\hat{y}}e^{i\varphi_{\hat{x}}} \left|\overline{z}\right\rangle \\
=&\left(I_{2^j} \otimes \begin{bmatrix} \alpha_{\hat{x},\hat{y}} & \beta_{\hat{x},\hat{y}}e^{-i(\varphi_{\hat{z}}-\varphi_{\hat{x}})} \\ \beta_{\hat{x},\hat{y}}e^{i(\varphi_{\hat{z}}-\varphi_{\hat{x}})} & -\alpha_{\hat{x},\hat{y}} \end{bmatrix} \otimes I_{2^{n-j-1}}\right) \gamma_{\hat{x},\hat{y}}e^{i\varphi_{\hat{x}}} \left|\overline{z}\right\rangle && (38)\\
=&\gamma_{\hat{x},\hat{y}}\alpha_{\hat{x},\hat{y}}e^{i\varphi_{\hat{x}}} \left|\overline{\hat{x}}\right\rangle + \gamma_{\hat{x},\hat{y}}\beta_{\hat{x},\hat{y}}e^{i\varphi_{\hat{z}}} \left|\overline{\hat{x}+2^{n-j-1}}\right\rangle && (39)\\
=&\gamma_{\hat{x},\hat{y}}\alpha_{\hat{x},\hat{y}}e^{i\varphi_{\hat{x}}} \left|\overline{\hat{x}}\right\rangle + \gamma_{\hat{x},\hat{y}}\beta_{\hat{x},\hat{y}}e^{i\varphi_{\hat{z}}} \left|\overline{\hat{z}}\right\rangle && (40)
\end{aligned}$$

This proves that inductive case. Thus, for a node $a_{x,y}$ in the n^{th} layer of the BSQDD B, $y = x + 1$ and $z = x + 1$ so by equation (19) the initial state of the node $a_{x,y}$ on the path v from the root is

$$\left|\hat{\psi}_v\right\rangle = \gamma_{x,x+1}\alpha_{x,x+1}e^{i\varphi_x}\left|\overline{x}\right\rangle + \gamma_{x,x+1}\beta_{x,x+1}e^{i\varphi_{x+1}}\left|\overline{x+1}\right\rangle \tag{41}$$

$$= \gamma_{x,x}e^{i\varphi_x}\left|\overline{x}\right\rangle + \gamma_{x+1,x+1}e^{i\varphi_{x+1}}\left|\overline{x+1}\right\rangle \tag{42}$$

$$= r_x e^{i\varphi_x}\left|\overline{x}\right\rangle + r_{x+1}e^{i\varphi_{x+1}}\left|\overline{x+1}\right\rangle \tag{43}$$

Thus, the quantum superposition represented by the BSQDD B is

$$\sum_{k=0}^{2^{n-1}-1} r_{2k}e^{i\varphi_{2k}}\left|\overline{2k}\right\rangle + r_{2k+1}e^{i\varphi_{2k+1}}\left|\overline{2k+1}\right\rangle = \sum_{k=0}^{2^n-1} r_k e^{i\varphi_k}\left|\overline{k}\right\rangle \tag{44}$$

$$= \left|\tilde{\psi}\right\rangle \tag{45}$$

Since $\left|\tilde{\psi}\right\rangle$ is equivalent to $|\psi\rangle$, the BSQDD B represents the quantum superposition $|\psi\rangle$. □

This theorem is important because it shows that BSQDDs can represent any quantum superposition up to global phase. In conjunction with theorem 7.3, this theorem shows that BSQDDs can be used to synthesize quantum arrays for initializing arbitrary quantum superpositions from the starting state $|0^n\rangle$ by constructing a BSQDD of form defined in the proof of theorem 12.1. Basis states other than $|0^n\rangle$ can also be used. To find a BSQDD that represents an arbitrary quantum superposition with respect to the starting state $|\psi_0\rangle$ where $|\psi_0\rangle$ is any basis state, use the method from theorem 12.1 to find a BSQDD that represents the desired quantum superposition with respect to the starting state $|0^n\rangle$. This BSQDD can then be modified by replacing the operation U of each node with the product $U \cdot X$ in layers where the corresponding qubit in the starting state $|\psi_0\rangle$ is equal to $|1\rangle$. This will result in a BSQDD that represents the desired quantum superposition with respect to the starting state $|\psi_0\rangle$.

13 Representing Quantum Superpositions Using a Class of BSQDDs with Canonical Forms

This section will present a theorem which shows that a BSQDD that uses the set of gates $\left\{D_\theta = \left[\begin{smallmatrix}\cos\theta & \sin\theta \\ \sin\theta & -\cos\theta\end{smallmatrix}\right] \,\middle|\, 0 \le \theta \le \frac{\pi}{2}\right\}$ with no repeated variables can initialize any quantum superposition with non-negative real coefficients. Although this is not as general as theorem 12.1, this set of gates is used in the Long-Sun algorithm [6] and satisfies the conditions in theorems 10.1 and 10.2. This implies that BSQDDs that use this set of gates and do not have repeated variables have canonical forms and can be transformed into any equivalent BSQDD.

Theorem 13.1. *A BSQDD operating on the set of qubits* $\{|x_1\rangle, \ldots, |x_n\rangle\}$ *using the set of gates* $\left\{D_\theta = \left[\begin{smallmatrix}\cos\theta & \sin\theta \\ \sin\theta & -\cos\theta\end{smallmatrix}\right] \,\middle|\, 0 \le \theta \le \frac{\pi}{2}\right\}$*, the order of variables* $(x_1, \ldots, x_n)$ *and the starting state* $|\psi_0\rangle = |0^n\rangle$ *can represent any quantum superposition with non-negative real coefficients.*

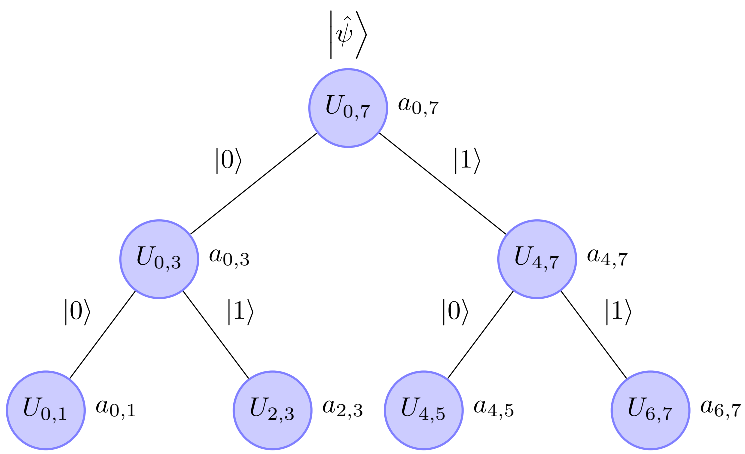


Figure 7: A BSQDD that represents $\left|\hat{\psi}\right\rangle$ for $n = 3$

Proof. Let the desired quantum superposition be denoted by $|\psi\rangle$. Recall that in the proof for theorem 12.1, the operation of each node $a_{x,y}$ was $U_{x,y} = G_{\theta_{x,y},\varphi_{x,y}}$ where $\theta_{x,y} = \cos^{-1}\alpha_{x,y}$, $\varphi_{x,y} = \varphi_z - \varphi_x$, $\alpha_{x,y} = \sqrt{\frac{\sum_{k=x}^{z-1} r_k^2}{\sum_{k=x}^{y} r_k^2}}$ and x, y and z are as defined in theorem 12.1 and $G_{\theta,\varphi} = \begin{bmatrix} \cos\theta & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta \end{bmatrix}$. Since $x \le z - 1 < y$, $0 \le \sum_{k=x}^{z-1} r_k^2 \le \sum_{k=x}^{y} r_k^2$. Therefore, $0 \le \frac{\sum_{k=x}^{z-1} r_k^2}{\sum_{k=x}^{y} r_k^2} \le 1$ so $0 \le \alpha_{x,y} \le 1$. Hence, $0 \le \theta_{x,y} \le \frac{\pi}{2}$. Recall that the quantum superposition represented in the proof of theorem 12.1 was $\left|\tilde{\psi}\right\rangle = \sum_{k=0}^{2^n-1} r_k e^{i\varphi_k} \left|\overline{k}\right\rangle$ as shown in equation (17) where each $\varphi_k = \phi_k - \phi_0$ and the original quantum superposition before the global phase was factored out was $|\psi\rangle = \sum_{k=0}^{2^{n-1}} r_k e^{i\phi_k} \left|\overline{k}\right\rangle$. Since the quantum superposition being represented now has only non-negative real coefficients, $\phi_k = 0$ for all $k = 0, \ldots, 2^n - 1$. Therefore, $\varphi_{x,y} = 0$ for each node $a_{x,y}$. Then $D_{\theta_{x,y}} = G_{\theta_{x,y},\varphi_{x,y}}$ so since $|\psi\rangle = \left|\tilde{\psi}\right\rangle$ the construction used in the proof of theorem 12.1 can be used to represent the quantum superposition $|\psi\rangle$ with a BSQDD that operates on the set of qubits $\{|x_1\rangle, \ldots, |x_n\rangle\}$, uses the set of gates $\left\{D_\theta = \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix} \,\middle|\, 0 \le \theta \le \frac{\pi}{2}\right\}$, has the order of variables $(x_1, \ldots, x_n)$ and uses the starting state $|\psi_0\rangle = |0^n\rangle$. □

This theorem is useful because it shows that a class of BSQDDs that satisfy the conditions in theorems 10.1 and 10.2 can initialize a broad class of quantum superpositions. The construction from theorem 13.1 can be used to construct a BSQDD that represents any quantum superposition with non-negative real coefficients.

14 Conclusion

BSQDDs are a powerful data structure that can be used for synthesizing efficient quantum arrays for initializing arbitrary quantum superpositions and also for representing arbitrary quantum superpositions. The gates used in BSQDDs can be restricted to only those available for synthesis so that the generated quantum arrays do not require gates that are not available. A canonical form exists for a broad class of BSQDDs. Transformation rules also exist for reducing BSQDDs in order to decrease the number of gates in the resulting quantum array. BSQDDs have advantages over existing methods for initializing quantum superpositions. One advantage is that quantum arrays generated from BSQDDs do not require ancilla qubits unlike the Ventura-Martinez [11], SQUID [8] and ESQUID [9] algorithms. Furthermore, for some classes of quantum superpositions, BSQDDs can be used to generate quantum arrays that require exponentially fewer gates than the Ventura-Martinez [11], Long-Sun [6] and SQUID [8] algorithms. This makes BSQDDs a powerful and useful data structure for representing and initializing quantum superpositions.

References

[1] A. Abdaollahi and M. Pedram. Analysis and synthesis of quantum circuits by using quantum decision diagrams. In *Design, Automation and Test in Europe*, 2006.

[2] D. Biron, O. Biham, E. Biham, M. Grassl, and D. A. Lidar. Generalized grover search algorithm for arbitrary initial amplitude distribution. *Quantum Computing and Quantum Communications*, 1509/1999:140–147, 1999.

[3] R. E. Bryant. Graph-based algorithms for boolean function manipulation. *IEEE Transactions on Computers*, C-35:677–691, 1986.

[4] A. A. Ezhov, A. V. Nifanova, and D. Ventura. Quantum associative memory with distributed queries. *Information Sciences*, 128:271–293, 1999.

[5] L. K. Grover. A fast quantum mechanical algorithm for database search. In *Proceedings of the Annual ACM Symposium on Theory of Computing*, pages 212–219, 1996.

[6] G.-L. Long and Y. Sun. Efficient scheme for initializing a quantum register with an arbitrary superposed state. *Physical Review A*, 64:014303, 2001.

[7] D. M. Miller and M. A. Thornton. Qmdd: A decision diagram structure for reversible and quantum circuits. In *Proceedings of the 36th International Symposium on Multiple Valued Logic*, 2006.

[8] D. Rosenbaum and M. Perkowski. Superposed quantum state initialization using disjoint prime implicants. In *Proceedings of the 38th International Symposium on Multiple Valued Logic*, pages 144–149, 2008.

[9] D. Rosenbaum and M. Perkowski. Extended superposed quantum state initialization using disjoint prime implicants. *Physical Review A*, 79:052310, 2009.

[10] L. J. Schulman and U. V. Vazirani. Molecular scale heat engines and scalable quantum computation. In *Conference Proceedings of the Annual ACM Symposium on Theory of Computing*, pages 322–329, 1999.

[11] D. Ventura and T. Martinez. Initializing the amplitude distribution of a quantum state. *Foundations of Physics Letters*, 12:547–559, 1999.

[12] D. Ventura and T. Martinez. Quantum associative memory. *Information Sciences*, 124:273–296, 1999.

[13] G. F. Viamontes, I. L. Markov, and J. P. Hayes. Graph-based simulation of quantum computation in the density matrix representation. *Quantum Information and Computation*, 5:113–130, 2004.

[14] G. F. Viamontes, M. Rajagopalan, I. L. Markov, and J. P. Hayes. Gate-level simulation of quantum circuits. In *Proceedings of the 2003 Conference on Asia South Pacific Design Automation*, 2003.