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# Quantum Algorithm for Mining Frequent Patterns for Association Rule Mining

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## Abstract

Maximum frequent pattern generation from a large database of transactions and items for association rule mining is an important research topic in data mining. Association rule mining aims to discover interesting correlations, frequent patterns, associations, or causal structures between items hidden in a large database. By exploiting quantum computing, we propose an efficient quantum search algorithm design to discover the maximum frequent patterns. We modified Grover's search algorithm so that a subspace of arbitrary symmetric states is used instead of the whole search space. We presented a novel quantum oracle design that employs a quantum counter to count the maximum frequent items and a quantum comparator to check with a minimum support threshold. The proposed derived algorithm increases the rate of the correct solutions since the search is only in a subspace. Furthermore, our algorithm significantly scales and optimizes the required number of qubits in design, which directly reflected positively on the performance. Our proposed design can accommodate more transactions and items and still have a good performance with a small number of qubits.

## Keywords

Data Mining, Association Rule Mining, Frequent Pattern, Apriori Algorithm, Quantum Counter, Quantum Comparator, Grover's Search Algorithm

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## 1. Introduction

We live in a digitalized era where vast amounts of data are collected daily. Data mining is a process of extracting interesting information, which is called knowledge discovery (KDD) in a database. According to [1], data mining is a field related to machine learning, but data mining is more applied than machine learn-

ing. Data mining has a broader spectrum of applications in engineering, science, business, medical applications, and many other areas. Data mining is used to process the raw data on a larger scale of data. There are various types of data mining techniques, such as association rules, classification, and clustering [2]. Association rule mining (ARM) is one of the most important research topics in data mining. ARM aims to discover interesting correlations, frequent patterns, associations, or causal structures between items hidden in a large database. Association rule mining is a branch of unsupervised learning processes that discover hidden patterns in data in the form of easily recognizable rules. Association rule mining is often termed as market basket analysis which studies the buying behaviors of customers by searching for sets of items that are frequently purchased together. Association rule mining is widely used in the retail analysis of transactions [3] [4], recommendation engines [5] [6] [7], web mining [8] [9], medical diagnosis, bioinformatics [10], and other applications [11] in various areas.

- Retail analysis of transactions: The data from past transactions can be used to generate items that the customers most like to be purchased together. The retailer can then adjust the store layout, sales strategy, bundling prices, and inventory control to take advantage of the extracted rules that are generated from association rule mining.
- Recommendation engines: Recommendation systems such as entertainment, news, and social media can be designed using association rule mining to recommend the most interesting content based on the user's past behavior.
- Web mining: Web usage mining is used in e-commerce applications to get useful information about the behavior of customers. Association rule mining is applied to the data from past behavior of the customers, and then rules based on customer preferences are generated. The developers can optimize and improve websites to personalize the web portals based on the association rules.
- Medical diagnosis: Association rule mining can be used to help diagnose patients. The symptoms of diseases and illnesses can be identified to find the conditional probability of the occurrence of illness using associate rule mining.
- Bioinformatics: There are many applications in bioinformatics problems, such as protein interaction networks, gene expression data, and others [10], that can be applied to association rule mining to identify biologically relevant patterns. These patterns can be translated into a biological context.

Association rule mining increases revenue by ensuring customer satisfaction based on customized web portals, as well as enhances medical treatment by relating the severity of the sickness and its symptoms.

Given a set of transactions in a database, the goal is to find the association rules that connect between itemsets. For example,  $X \Rightarrow Y$  ( $X$  implies  $Y$ ), which means the customer who buys the items in  $X$  also tends to buy the items in  $Y$ .

The implication means the co-occurrence of  $X$  and  $Y$  items. If patterns within transaction data tell us that baby formula and diapers are usually purchased together in the same transaction, a retailer can take advantage of this association for bundle pricing, product placement, and even shelf space optimization within the store layout. Association rules are considered interesting and called strong if they satisfy the user-predefined thresholds, which are minimum support (*min-sup*) and minimum confidence (*minconf*) thresholds. These threshold values are pre-defined by users or domain experts.

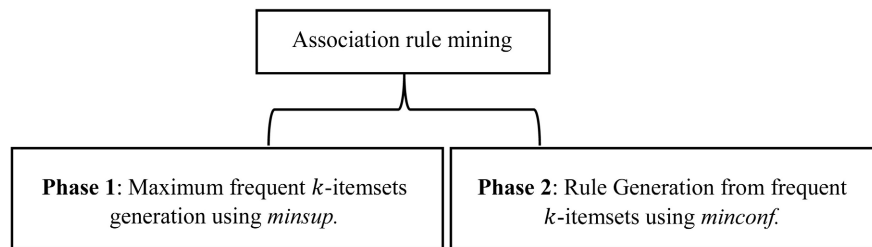
The original association rule mining problem was first introduced in [12]. Let  $I = \{I_1, I_2, \dots, I_M\}$  be the set of all items. Let  $T$  be a set of database transactions where  $T = \{T_1, T_2, \dots, T_N\}$  and  $T \subseteq I$ . Each transaction is associated with an identifier, called a *TID*. A set of items is referred to as an itemset. An itemset that contains  $k$  items is called a  $k$ -itemset.  $k$ -itemsets that occur frequently are called a frequent  $k$ -itemsets. Association rules of the form  $X \Rightarrow Y$  ( $X$  implies  $Y$ ) is measured by support, the percentage of transactions that contain both  $X$  and  $Y$ , the union of itemsets  $X$  and  $Y$ . The support is taken to be the probability,  $P(X \cup Y)$ .

$$\begin{aligned} \text{support}(X \Rightarrow Y) &= P(X \cup Y) \\ &= \frac{\text{number of transactions containing both } X \text{ and } Y}{\text{Total number of transactions}} \\ \text{support}(X) &= \frac{\text{number of transactions containing } X}{\text{Total number of transactions}} \end{aligned}$$

The support in the above equation is called *relative support*, where the frequency or occurrence of an item is called an *absolute support* or a *support count*. Another objective measure for association rules is *confidence*, which assesses the degree of certainty of the detected association [13]. The rule  $X \Rightarrow Y$  has confidence, the percentage of transactions that containing  $X$  also contains  $Y$ . The confidence is taken to be the conditional probability,  $P(Y | X)$ .

$$\begin{aligned} \text{confidence}(X \Rightarrow Y) &= P(Y | X) \\ &= \frac{\text{number of transactions containing } X \text{ and } Y}{\text{number of transaction containing } X} = \frac{\text{support}(X \cup Y)}{\text{support}(X)} \end{aligned}$$

The main objective of ARM is to discover the itemsets that frequently appear in the transactions. The support (occurrence frequency) for each of these itemsets is generated from a number of candidate itemsets and not less than a pre-defined threshold [13] [14]. In **Figure 1**, association rule mining is decomposed into two phases: First, find out all the frequent itemsets such that each of these itemsets will occur at least as frequently as the pre-defined minimum support threshold. Those itemsets are called frequent or large itemsets. Second, generate association rules from those frequent itemsets with the constraints of minimum confidence threshold. There are many algorithms for mining frequent itemsets; the first phase of the association rule mining task. This first phase dominates the complexity of the whole process.



**Figure 1.** Association rule mining phases.

## 2. Related Works

### 2.1. Classical Algorithms for Association Rule Mining

The AIS (Agrawal, Imielinski, Swami) algorithm was the first algorithm proposed for mining association rules in [12]. In the AIS algorithm, the database was scanned many times to get maximum frequent or large itemsets. During the first pass,  $C_1$ , the candidate 1-itemsets are generated, and the support count of each individual item was accumulated. From candidate 1-itemsets,  $F_1$  frequent 1-itemsets are generated by eliminating itemsets whose support count less than the value of *minsup*. Candidate 2-itemsets are generated by extending frequent 1-itemsets with other items in the same transaction. During the second pass over the database, the support counts of those candidate 2-itemsets are accumulated and checked against the *minsup*. Similarly, those candidate  $(k + 1)$ -itemsets are generated by extending frequent  $k$ -itemsets with items in the same transaction. However, extending the itemsets that are not present in the previous pass results in unnecessarily generating and counting too many candidate itemsets that turn out to be small.

A number of ARM algorithms were proposed. Among these, the most well-known algorithm is the Apriori algorithm [14] that makes additional use of prune property to those candidates which have an infrequent subset before counting their supports. This optimization is possible because the support values of all subsets of a candidate are known in advance. The Apriori algorithm employs an iterative approach known as level-wise search, where  $k$ -itemsets are used to explore  $(k + 1)$ -itemsets. First, the set of candidate 1-itemsets is found by scanning the database to accumulate the count for each item and collecting those items that satisfy the minimum support threshold. The resulting set is denoted by  $F_1$ , the set of frequent 1-itemsets. Next,  $F_1$  is used to find  $C_2$ , the set of candidate 2-itemsets, which is used to find  $F_2$ , and so on, until no more frequent  $k$ -itemsets can be found. The finding of each  $C_k$  requires one full scan of the database, which becomes the dilemma of performance in ARM when the transaction database is very large.

In the Apriori algorithm, finding of each  $C_k$  requires one full scan of the database. To improve the efficiency of the level-wise generation of frequent itemsets, an important property called the Apriori property is used to reduce the search space. Apriori property is:

- If an itemset is frequent, then all its subsets must also be frequent.



- If an itemset is not frequent, then all its supersets cannot be frequent.

To construct candidate  $C_k$  combine frequent itemsets of size  $k$ . If  $k = 1$ , take all 1-itemset. If  $k > 1$ , join pairs of itemset that differ by just one item. For each generated candidate itemset ensure that all subsets of size  $k$  are frequent. The first pass of the Apriori algorithm simply counts item occurrences to determine the frequent 1-itemsets. A subsequent pass, say pass  $k$ , consists of two phases. First, the frequent itemsets  $F_{k-1}$  found in the  $k-1$  pass are used to generate the candidate itemsets  $C_k$  using two step processes: self-join and prune.

- Self-join  $F_{k-1}$ : Generate set  $C_k$  by joining  $F_{k-1}$  itemsets that share the first  $k-1$  items.
- Prune: Remove from  $C_k$  the itemsets that contain a subset  $k$ -itemset that is not frequent.

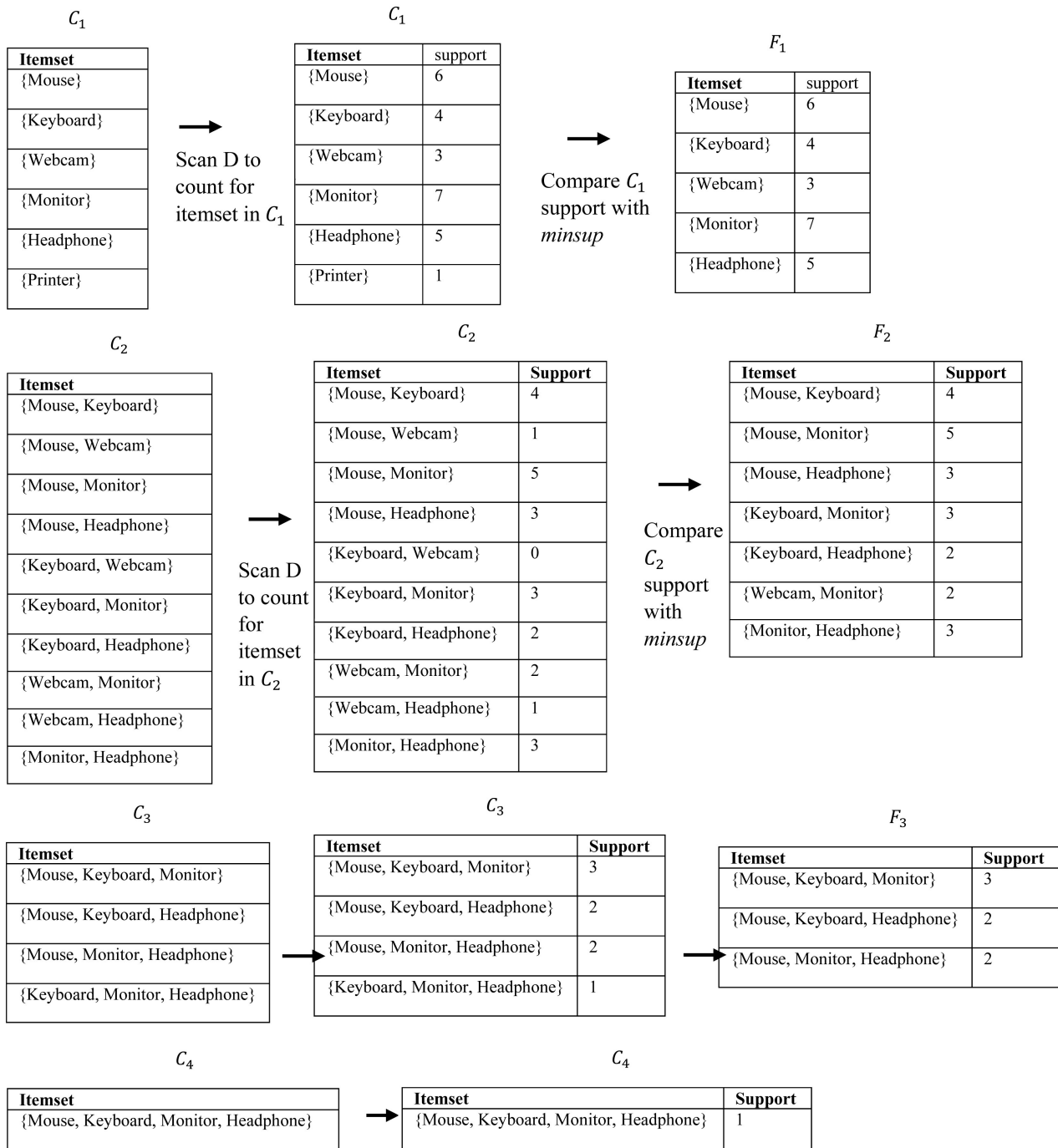
Second, the database is scanned and the support of candidates in  $C_k$  is counted.

**Example:** Let a store promote certain computer accessories, and the store manager bundles some accessories with other discounted accessories. The manager wants to know which accessories the customers pay mostly when purchased together. **Table 1** contains transactions with items.

Let  $minsup = 2$  and  $minconf = 70\%$ . We need first to generate a maximum frequent itemset. The transaction database in **Table 1** is applied in the Apriori algorithm, as can be seen in **Figure 2**. The set of candidate 1-itemsets,  $C_1$ , obtained and then scanned the database to count the support of each itemset. The set of frequent 1-itemsets,  $F_1$ , whose support is equal to or greater than 2, the  $minsup$  value, are generated from  $C_1$ . Items in  $F_1$  are joined to get candidate 2-itemsets,  $C_2$ . The database is scanned, and the support of each candidate itemset in  $C_2$  is counted. The set of frequent 2-itemsets,  $F_2$ , is determined based on the support count of each candidate 2-itemset in  $C_2$ . From  $F_2$  pairs of itemset are joined that differ by just one item to get candidate 3-itemsets,  $C_3$ . The support of each itemset

**Table 1.** Transaction with items.

Transaction ID	Computer accessories items
$T_1$	Mouse, Keyboard, Monitor, Headphone
$T_2$	Webcam, Monitor
$T_3$	Mouse, Keyboard, Monitor
$T_4$	Printer
$T_5$	Mouse, Keyboard, Headphone
$T_6$	Webcam, Headphone
$T_7$	Mouse, Monitor, Headphone
$T_8$	Monitor, Headphone
$T_9$	Mouse, Keyboard, Monitor
$T_{10}$	Mouse, Webcam, Monitor



**Figure 2.** Generating maximum frequent itemsets using the apriori algorithm.

in  $C_3$  is counted by scanning the database and  $F_3$  is generated based on the min-sup value. The candidate of 4-itemset,  $C_4$ , is created by joining itemsets that differ by just two items in  $F_3$ . The support count of  $C_4$  itemset is less than the min-sup value, so there is no frequent 4-itemsets,  $F_4$ . Thus, in this case the maximum frequent itemset is  $F_3$ . So, the maximum frequent itemset are: {Mouse, Keyboard, Monitor}, {Mouse, Keyboard, Headphone} and {Mouse, Monitor, Headphone} as can see in **Figure 2**.

Let generate association rules based on  $minconf = 70\%$  for {Mouse, Keyboard, Monitor}:

Rule 1: {Mouse, Keyboard}  $\rightarrow$  {Monitor}

$$\begin{aligned} & confidence(\{Mouse, Keyboard\} \rightarrow \{Monitor\}) \\ &= \frac{support\{Mouse, Keyboard, Monitor\}}{support\{Mouse, Keyboard\}} = \frac{3}{4} = 75\% \end{aligned}$$

Rule 2: {Mouse, Monitor}  $\rightarrow$  {Keyboard}

$$\begin{aligned} & confidence(\{Mouse, Monitor\} \rightarrow \{Keyboard\}) \\ &= \frac{support\{Mouse, Keyboard, Monitor\}}{support\{Mouse, Monitor\}} = \frac{3}{5} = 60\% \end{aligned}$$

Rule 3: {Keyboard, Monitor}  $\rightarrow$  {Mouse}

$$\begin{aligned} & confidence(\{Keyboard, Monitor\} \rightarrow \{Mouse\}) \\ &= \frac{support\{Mouse, Keyboard, Monitor\}}{support\{Keyboard, Monitor\}} = \frac{3}{3} = 100\% \end{aligned}$$

Rule 4: {Mouse}  $\rightarrow$  {Keyboard, Monitor}

$$\begin{aligned} & confidence(\{Mouse\} \rightarrow \{Keyboard, Monitor\}) \\ &= \frac{support\{Mouse, Keyboard, Monitor\}}{support\{Mouse\}} = \frac{3}{6} = 50\% \end{aligned}$$

Rule 5: {Keyboard}  $\rightarrow$  {Mouse, Monitor}

$$\begin{aligned} & confidence(\{Keyboard\} \rightarrow \{Mouse, Monitor\}) \\ &= \frac{support\{Mouse, Keyboard, Monitor\}}{support\{Keyboard\}} = \frac{3}{4} = 75\% \end{aligned}$$

Rule 6: {Monitor}  $\rightarrow$  {Mouse, Keyboard}

$$\begin{aligned} & confidence(\{Monitor\} \rightarrow \{Mouse, Keyboard\}) \\ &= \frac{support\{Mouse, Keyboard, Monitor\}}{support\{Monitor\}} = \frac{3}{7} = 42.9\% \end{aligned}$$

If the desired  $minconf$  is 70%, then all interested rules that satisfy the  $minconf$  are rules 1, 3, and 5. Based on rule 1, 75% of the customers who purchase {Mouse, Keyboard} also purchase a Monitor. Also, based on rule 3, 100% of the customers who purchase {Keyboard, Monitor} always purchase {Mouse}.

Although the research in the Apriori algorithm has grown the recent years [15], the drawback of the Apriori algorithm is the necessity of scanning the whole database many times. Based on the Apriori algorithm, many new algorithms were designed with some modifications or improvements. Generally, there were two approaches: one is to reduce the number of passes over the whole database or replace the whole database with only part of it based on the current frequent itemsets, and another approach is to explore different kinds of pruning techniques to make the number of candidate itemsets much smaller [16]. Direct

hash and pruning (DHP) [17] and partitioning [18] are modifications of the Apriori algorithm. Another mining technique is to simultaneously mine both frequent and infrequent itemsets [19].

Associate rule mining aims to extract interesting correlations from a raw dataset that contains a huge number of database transactions and items in each transaction. Computing such a large scale of raw data in classical computing is very expensive. Leveraging the quantum search algorithm can solve such a problem significantly faster than the classical algorithm. Grover's search algorithm gives a quadratic speedup compared to an exhaustive classical algorithm for the same problem.

## 2.2. Quantum Algorithms for Association Rule Mining

Quantum algorithms for association rule mining [20] [21] was proposed using a quantum counting algorithm [22]. The quantum circuit design that was proposed in [20] [21] presented experimental implementation for  $2 \times 2$  (two transactions and two items). The experiment for  $2 \times 2$  required 9 qubits. Let  $T$ , the number of the transaction and  $I$ , the number of the items, the required number of qubits is equal to  $2TI + 1$  for each iteration to find the maximum frequent  $k$ -itemset. Also, for each iteration, the whole database is a search space.

To find the maximum frequent  $k$ -itemsets from  $n$  items, we are interested only in the subspace of states of Hamming weight  $k$ . We propose an efficient method that the search space is reduced from  $2^n$ -dimensional Hilbert space to an  $\binom{n}{k}$ -dimensional subspace. Also, we presented an efficient quantum circuit design that the required number of qubits reduced significantly compared with [20] [21]. We present a new quantum design method for association rule mining to generate the maximum frequent  $k$ -itemsets, which required fewer qubits, and the search space based only on the candidate  $k$ -itemset to discover the maximum frequent  $k$ -itemsets. We modified Grover's search algorithm [12] by employing the Dicke state [23] to create the superposition for  $k$ -itemset, quantum counter [24] [25] to count the frequent of  $k$ -itemset and quantum comparator to check the frequent  $k$ -itemset equal or greater than to *minsup* threshold. We start to transform the transaction database into a binary matrix such that the item value is "1" if the item is present in a transaction and "0" otherwise. The database is converted to binary matrix  $A_{N \times M}$ , where each row corresponds to transaction in  $T$ , each column corresponds to an item in the set of all items  $I$ , and  $N$  is the number of transactions, and  $M$  is the number of items. A Boolean function in the sum-of-product (SOP) form is generated from the binary matrix such that each row of the matrix corresponds to one product term of the SOP function expression. In the presented case, the term is a product of variables for all items that have a value of one.

Apriori algorithm for associate rule mining, the maximum frequent  $k$ -itemset is required to scan the database for every 1-itemset, 2-itemset, etc. until to find the maximum  $k$ -itemset. The candidate itemset generated during an early itera-

tion are generally of larger magnitude than the maximum frequent  $k$ -itemset, which likelihood can be found in later iterations. Therefore, the initial candidate itemset generation is the key issue in improving the performance of association rule mining [17]. In this case, we started the search from the maximum  $k$ -itemsets as the candidate to search the maximum frequent  $k$ -itemsets, which may be a better chance to be the actual or close to the maximum frequent  $k$ -itemsets rather than starting the search from candidate 1-itemsets. Thus, the database size and the computation cost are reduced substantially. We choose only all the terms that have the maximum  $k$ -itemset from the SOP function. We built the quantum oracle design from the optimized SOP function that contained only the maximum  $k$ -itemset combined with the quantum counter and quantum comparator. We run an experiment and perform analysis using QISKIT, an IBM quantum simulator [26].

### 3. Quantum Oracle Design

First, let us create a binary matrix in **Table 2** such that the item value is “1” if the item is present in a transaction and “0” otherwise. The binary matrix is based on items from **Table 1**.

To simplify, we change each item name to a letter so that we can build the SOP function. Let us observe that the SOP expressions used here are different from those applied in binary circuit synthesis. This is because here we can use repeated products or products included in other products, which can’t happen in SOP expressions used for binary circuit synthesis. Therefore, our expression compiled from **Table 2** is as follows:

$$abde + cd + abd + f + abe + ce + ade + de + abd + acd$$

Let  $minsup = 2$  and we need to find the maximum frequent 3-itemset. First, extract all itemsets equal to or greater than the 3-itemset.

**Table 2.** Binary matrix corresponds from **Table 1**.

Transaction ID	a	b	c	d	e	f
	Mouse	Keyboard	Webcam	Monitor	Headphone	Printer
$T_1$	1	1		1	1	
$T_2$			1	1		
$T_3$	1	1		1		
$T_4$						1
$T_5$	1	1			1	
$T_6$			1		1	
$T_7$	1			1	1	
$T_8$				1	1	
$T_9$	1	1		1		
$T_{10}$	1		1	1		

$$abde + abd + abe + ade + abd + acd$$

Second, we decompose any itemset that is greater than 3-itemset. In this case, we have  $abde$  which is decomposed into  $abd + abe + ade + bde$  such that:

$$abd + abe + ade + bde + abd + abe + ade + abd + acd$$

Third, we build the quantum oracle for SOP function expression:

$$abd + abe + ade + bde + abd + abe + ade + abd + acd \geq 2 \quad (1)$$

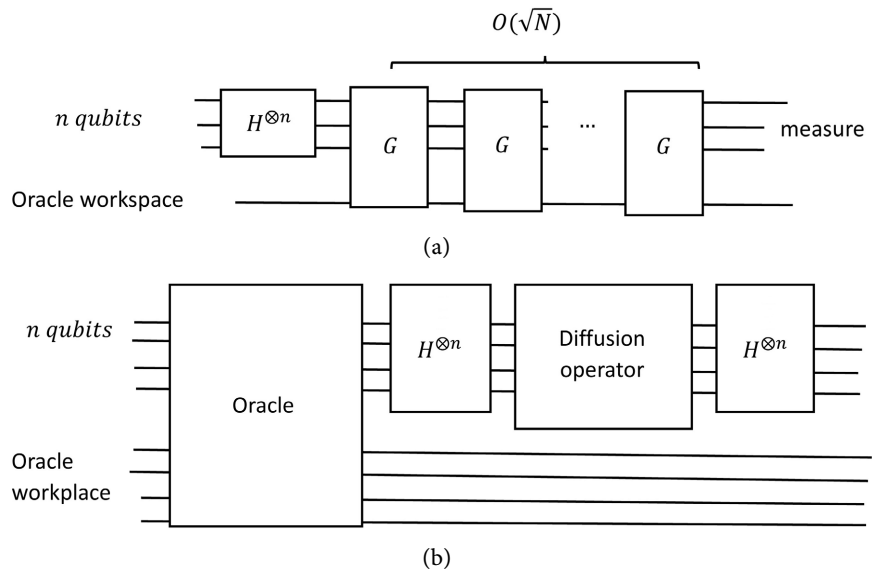
Each term in the traditional quantum oracle design for the SOP function is a Toffoli gate, and the outcome is stored in an additional ancilla qubit. One large Toffoli gate that is controlled for all results is used to compute the output of the SOP function. The problem with the traditional quantum oracle architecture is that one additional ancilla qubit is needed for each term. We proposed that each term of the SOP function be connected to a quantum counter and then mirror the term back before computing the next term. In [13] [14], more information on this design is provided.

### 3.1. Grover's Search Algorithms

Grover's Algorithm [22] searches an unordered array of  $N$  elements to find a particular element with a given property. In classical computations, in the worst case, this search takes  $N$  queries (tests, evaluations of the classical oracle). In the average case, the particular element will be found in  $N/2$  queries. Grover's algorithm can find the element in  $\sqrt{N}$  queries. Thus, Grover's algorithm can be used to search the maximum frequent  $k$ -itemset for associate rule mining. Grover's algorithm is a quantum search algorithm, which speeds up a classical search algorithm of complexity  $O(N)$  to  $O(\sqrt{N})$  in the space of  $N$  objects, hence Grover gives a quadratic speed up.

The SOP Boolean function in Equation (1) contains  $n$  variables from the given binary matrix in **Table 2**, which is used to represent the search space of  $N = 2^n$  elements. To apply the SOP Boolean function in Grover's algorithm, these  $N$  elements are applied in a superposition state which is the input to the oracle. If the oracle recognizes an element as the solution, then the phase of the desired state is inverted. This is called the Phase inversion of the marked element. Grover's search algorithm uses another trick called inversion about the mean (average), which is also known as diffusion operation or amplitude amplification. Inversion about the mean amplifies the amplitude of the marked states and shrinks the amplitudes of other items. The amplitude amplification increases the probability of marked states, so that measuring the final states will return the target solution with a high probability near 1.

As shown in **Figure 3(a)**, the  $n$  qubits in the superposition state result from applying a vector of Hadamard gates to initial state  $|0\rangle^n$ . Next applied is repeated operator  $G$  which is called the Grover Loop. After the iteration of the Grover Loop operator  $O(\sqrt{N})$  times the output is measured for all input qubits. Oracle can use an arbitrary number of ancilla qubits, but all these qubits must be returned to value  $|0\rangle$  inside the oracle. The number of required iterations



**Figure 3.** (a) Schematic circuit for Grover’s algorithm [22]. (b) Grover operator  $G$ .

for the Grover operator is:  $R \leq \left\lceil \frac{\pi}{4} \sqrt{\frac{N}{M}} \right\rceil$  where  $N$  is number of all search space

elements and  $M$  is number of solutions. The Grover Loop  $G$  is a quantum sub-routine which can be broken into four steps as shown in **Figure 3(b)**.

1) Phase inversion: apply the oracle. If the oracle recognizes the solution, then the phase of the desired state is inverted.

2) Apply the Hadamard transform  $H^{\otimes n}$  ( $H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ ).

3) Zero state phase shift: Perform the condition phase shift, in which all states receive a phase shift of -1 except for the zero state  $|0\rangle$ .

4) Apply the Hadamard transform  $H^{\otimes n}$ .

Grover’s search algorithm is started to create the superposition by using Hadamard operator  $H$ . Hadamard operator of  $n$  qubits creates  $N = 2^n$  quantum states. Hadamard operator of  $H^{\otimes n}$  applied  $|0\rangle^{\otimes n}$ :

$$H^{\otimes n} |0\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle$$

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \quad H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

$$H^{\otimes 4} |0\rangle^{\otimes 4} = \frac{1}{\sqrt{16}} (|0000\rangle + |0001\rangle + \dots + |1111\rangle)$$

For maximum frequent  $k$ -itemsets, all  $N$  states are not solutions, but the solution would be only in Hamming weight  $k$ -itemsets. Hamming weight in binary is the number of ones in the binary number.  $k$ -itemsets is Hamming weight of  $k$ -itemset. For instance, finding the maximum frequent 2-itemset from 4 items, the solution will be only in 6 states with Hamming weight 2 which are equal to 0011, 0101, 0110, 1001, 1010, 1100. So, using the Hadamard operator for four

items creates 16 quantum states (0000, 0001, ..., 1111) which are not required to search from the possible solutions, but the possible solutions are only in 6 quantum states of Hamming weight 2.

### 3.2. Dicke State

The search space of search algorithms has a critical role in terms of performance in both classical and quantum computing. In Grover's search algorithm starts preparing superposition states for the search problems. The Hadamard operator is the traditional way to create  $2^n$  superposition states for  $n$  qubits. There are many real problems such as symmetric Boolean function [27], Johnson graph [28], and frequent patterns for associate rule mining that the possible solutions are in the form of Hamming weight, a pure symmetric state in  $\binom{n}{k}$  states. For problems such as these, a proper quantum superposition state can be achieved using the Dicke state [23]. Finding the maximum frequent  $k$ -itemsets from  $n$  items, we are interested only in the subspace of states of Hamming weight  $k$ . The Dicke state  $|D_k^n\rangle$  is an equal-weight superposition of all  $n$ -qubit states with Hamming Weight  $k$  (i.e., all strings of length  $n$  with exactly  $k$  ones over a binary).  $|D_k^n\rangle$  creates  $\binom{n}{k}$  symmetric states. Below we illustrate practical examples of the Dicke state.

$$|D_k^n\rangle = \frac{1}{\sqrt{\binom{n}{k}}} \sum_{x \in \{0,1\}^n, wt(x)=k} |X\rangle$$

where  $\binom{n}{k} = \frac{n!}{(n-k)!k!}$  and  $0 < k < n$ . There are  $n$  qubits and  $n-k$  of them are 0 and  $k$  are 1. For instance,

$$\begin{aligned} |D_2^4\rangle &= \frac{1}{\sqrt{6}} \sum_{x \in \{0,1\}^4, wt(x)=2} |X\rangle \\ &= \frac{1}{\sqrt{6}} (|0011\rangle + |0101\rangle + |0110\rangle + |1001\rangle + |1010\rangle + |1100\rangle) \end{aligned}$$

$|D_2^4\rangle$  is Dicke state of 4 qubits that has 6 symmetric states and each state have 2 ones.

$$\begin{aligned} |D_3^5\rangle &= \frac{1}{\sqrt{10}} \{ |00111\rangle + |01011\rangle + |10011\rangle + |01101\rangle + |10101\rangle \\ &\quad + |11001\rangle + |01110\rangle + |10110\rangle + |11010\rangle + |11100\rangle \} \end{aligned}$$

$|D_3^5\rangle$  is Dicke state of 5 qubits that has 10 symmetric states and each state have 3 ones.

Dicke state creates arbitrary symmetric pure states  $|0\rangle^{\otimes n-k} |1\rangle^{\otimes k}$ . Using the Dicke state increases the rate of the correct solution since the search is only in subspace. The classical bitstring can be converted to the Dicke state by a recursive unitary operation called Split & Cyclic Shift (SCS) unitary  $SCS_{n,k}$  [23]. To



build  $|D_k^n\rangle$  state, we start from  $SCS_{n,k}$  where the original sequence is multiplied by a factor of  $\sqrt{\frac{k}{n}}$  and then shift the first zero to the end and shift the whole sequence forward by multiplying by a factor of  $\sqrt{\frac{n-k}{n}}$ .

$$SCS_{n,k} : |0\rangle^{\otimes n-k} |1\rangle^{\otimes k} \rightarrow \sqrt{\frac{k}{n}} |0\rangle^{\otimes n-k} |1\rangle^{\otimes k} + \sqrt{\frac{n-k}{n}} |0\rangle^{\otimes n-k-1} |1\rangle^{\otimes k} |0\rangle$$

Dicke state given as input string  $|0\rangle^{\otimes n-k} |1\rangle^{\otimes k}$  generates the entire Dicke states  $|D_k^n\rangle$  by recursive unitary operation  $SCS_{n,k}$ .

$$\begin{aligned} SCS_{5,3} : |00111\rangle &\rightarrow \sqrt{\frac{3}{5}} |00111\rangle + \sqrt{\frac{2}{5}} |01110\rangle \\ &\sqrt{\frac{3}{5}} |00111\rangle \rightarrow \sqrt{\frac{3}{5}} \{|0011\rangle\} \otimes |1\rangle \\ &\rightarrow \sqrt{\frac{3}{5}} \left\{ \sqrt{\frac{2}{4}} |0011\rangle + \sqrt{\frac{2}{4}} |0110\rangle \right\} \otimes |1\rangle \\ &\rightarrow \sqrt{\frac{3}{5}} \left\{ \sqrt{\frac{2}{4}} \left[ \sqrt{\frac{1}{3}} |001\rangle + \sqrt{\frac{2}{3}} |010\rangle \right] \otimes |1\rangle \right. \\ &\quad \left. + \sqrt{\frac{2}{4}} \left[ \sqrt{\frac{2}{3}} |011\rangle + \sqrt{\frac{1}{3}} |110\rangle \right] \otimes |0\rangle \right\} \otimes |1\rangle \\ &\rightarrow \sqrt{\frac{3}{5}} \left\{ \sqrt{\frac{2}{4}} \left[ \sqrt{\frac{1}{3}} |001\rangle + \sqrt{\frac{2}{3}} \left( \sqrt{\frac{1}{2}} |01\rangle + \sqrt{\frac{1}{2}} |10\rangle \right) \otimes |0\rangle \right] \otimes |1\rangle \right. \\ &\quad \left. + \sqrt{\frac{2}{4}} \left[ \sqrt{\frac{2}{3}} \left( \sqrt{\frac{1}{2}} |01\rangle + \sqrt{\frac{1}{2}} |10\rangle \right) \otimes |1\rangle + \sqrt{\frac{1}{3}} |110\rangle \right] \otimes |0\rangle \right\} \otimes |1\rangle \\ &\rightarrow \sqrt{\frac{3}{5}} \left\{ \sqrt{\frac{2}{4}} \left[ \sqrt{\frac{1}{3}} |001\rangle + \sqrt{\frac{1}{3}} (|010\rangle + |100\rangle) \right] \otimes |1\rangle \right. \\ &\quad \left. + \sqrt{\frac{2}{4}} \left[ \sqrt{\frac{1}{3}} (|011\rangle + |101\rangle) + \sqrt{\frac{1}{3}} |110\rangle \right] \otimes |0\rangle \right\} \otimes |1\rangle \\ &\rightarrow \sqrt{\frac{3}{5}} \left\{ \sqrt{\frac{2}{4}} \left[ \sqrt{\frac{1}{3}} |001\rangle + \sqrt{\frac{1}{3}} |010\rangle + \sqrt{\frac{1}{3}} |100\rangle \right] \otimes |1\rangle \right. \\ &\quad \left. + \sqrt{\frac{2}{4}} \left[ \sqrt{\frac{1}{3}} (|011\rangle + |101\rangle) + \sqrt{\frac{1}{3}} |110\rangle \right] \otimes |0\rangle \right\} \otimes |1\rangle \\ &\rightarrow \sqrt{\frac{3}{5}} \left\{ \sqrt{\frac{2}{4}} \left[ \sqrt{\frac{1}{3}} |0011\rangle + \sqrt{\frac{1}{3}} |0101\rangle + \sqrt{\frac{1}{3}} |1001\rangle \right] \right. \\ &\quad \left. + \sqrt{\frac{2}{4}} \left[ \sqrt{\frac{1}{3}} |0110\rangle + \sqrt{\frac{1}{3}} |1010\rangle + \sqrt{\frac{1}{3}} |1100\rangle \right] \right\} \otimes |1\rangle \\ &\rightarrow \sqrt{\frac{1}{10}} \{|00111\rangle + |01011\rangle + |10011\rangle + |01101\rangle + |10101\rangle + |11001\rangle\} \end{aligned}$$

$$\begin{aligned}
 & \sqrt{\frac{2}{5}}|01110\rangle \rightarrow \sqrt{\frac{2}{5}}\{|0111\rangle\} \otimes |0\rangle \\
 & \rightarrow \sqrt{\frac{2}{5}}\left\{\sqrt{\frac{3}{4}}|0111\rangle + \sqrt{\frac{1}{4}}|1110\rangle\right\} \otimes |0\rangle \\
 & \rightarrow \sqrt{\frac{2}{5}}\left\{\sqrt{\frac{3}{4}}\left[\sqrt{\frac{2}{3}}|011\rangle + \sqrt{\frac{1}{3}}|110\rangle\right] \otimes |1\rangle + \sqrt{\frac{1}{4}}|1110\rangle\right\} \otimes |0\rangle \\
 & \rightarrow \sqrt{\frac{2}{5}}\left\{\sqrt{\frac{3}{4}}\left[\sqrt{\frac{2}{3}}\left(\sqrt{\frac{1}{2}}|01\rangle + \sqrt{\frac{1}{2}}|10\rangle\right) \otimes |1\rangle + \sqrt{\frac{1}{3}}|110\rangle\right] \otimes |1\rangle + \sqrt{\frac{1}{4}}|1110\rangle\right\} \otimes |0\rangle \\
 & \rightarrow \sqrt{\frac{2}{5}}\left\{\sqrt{\frac{3}{4}}\left[\sqrt{\frac{1}{3}}|011\rangle + \sqrt{\frac{1}{3}}|101\rangle + \sqrt{\frac{1}{3}}|110\rangle\right] \otimes |1\rangle + \sqrt{\frac{1}{4}}|1110\rangle\right\} \otimes |0\rangle \\
 & \rightarrow \sqrt{\frac{2}{5}}\left\{\sqrt{\frac{1}{4}}|0111\rangle + \sqrt{\frac{1}{4}}|1011\rangle + \sqrt{\frac{1}{4}}|1101\rangle + \sqrt{\frac{1}{4}}|1110\rangle\right\} \otimes |0\rangle \\
 & \rightarrow \sqrt{\frac{1}{10}}\{|01110\rangle + |10110\rangle + |11010\rangle + |11100\rangle\} \\
 & |00111\rangle \rightarrow \sqrt{\frac{1}{10}}\{|00111\rangle + |01011\rangle + |10011\rangle + |01101\rangle + |10101\rangle \\
 & \quad + |11001\rangle + |01110\rangle + |10110\rangle + |11010\rangle + |11100\rangle\}
 \end{aligned}$$

The transformation or mapping of  $SCS_{n,k}$  is constructed by 1-controlled and 2-controlled  $Y$ -rotation  $R_y(2\theta)$  gate between two  $CNOT$ , where  $R_y(2\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$ . Dicke state is constructed recursively by smaller  $|D_l^n\rangle$ , where  $l \leq k$ .

$$\begin{aligned}
 & |0\rangle^{\otimes n-k-1} |0\rangle^{\otimes k+1-l} |1\rangle^{\otimes l} \\
 & \rightarrow \sqrt{\frac{l}{n}}|0\rangle^{\otimes n-k-1} |0\rangle^{\otimes k+1-l} |1\rangle^{\otimes l} + \sqrt{\frac{n-l}{n}}|0\rangle^{\otimes n-k-1} |0\rangle^{\otimes k-l} |1\rangle^{\otimes l} |0\rangle
 \end{aligned}$$

In **Figure 4** and **Figure 5** presented are the explicit constructions of  $SCS_{n,k}$ . To get more in-depth view of this construction can refer to [23]. The  $R_y$  gate is a single qubit rotation gate through angle  $\theta$  radian. The  $R_y$  gate rotation is around  $Y$ -axis by angle  $\theta$ . If the controlled qubits for  $R_y$  gate are all active, then the original sequence is multiplied by a factor of  $\sqrt{\frac{l}{n}}$  and then shift the first zero to end and shift the whole sequence forward by multiplying by a factor of  $\sqrt{\frac{n-l}{n}}$ . If the controlled qubits for  $R_y$  gate are not all active, then the two  $CNOT$  gates cancel each other.

The full circuit of Dicke state  $|D_3^5\rangle$  is constructed recursively by  $SCS_{n,k}$  as can be seen in **Figure 6** which contains  $R_y$  gate in between two  $CNOT$  gates. The  $R_y$  gates are controlled either one-qubit or two-qubits.

$$\begin{aligned}
 |00\rangle_{n-1} &\rightarrow |00\rangle_{n-1} \\
 |11\rangle_{n-1} &\rightarrow |11\rangle_{n-1} \\
 |01\rangle_{n-1} &\rightarrow \frac{1}{\sqrt{n}}|01\rangle_{n-1} + \sqrt{\frac{n-1}{n}}|10\rangle_{n-1}
 \end{aligned}$$

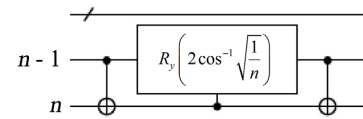


Figure 4. Construction of  $SCS_{n,l}$  of a two-qubit gate [23].

$$\begin{aligned}
 |00\rangle_{n-l}|0\rangle_n &\rightarrow |00\rangle_{n-l}|0\rangle_n \\
 |01\rangle_{n-l}|0\rangle_n &\rightarrow |01\rangle_{n-l}|0\rangle_n \\
 |00\rangle_{n-l}|1\rangle_n &\rightarrow |00\rangle_{n-l}|1\rangle_n \\
 |11\rangle_{n-l}|1\rangle_n &\rightarrow |11\rangle_{n-l}|1\rangle_n \\
 |01\rangle_{n-l}|1\rangle_n &\rightarrow \frac{l}{\sqrt{n}}|01\rangle_{n-l}|1\rangle_n + \sqrt{\frac{n-l}{n}}|11\rangle_{n-l}|0\rangle_n
 \end{aligned}$$

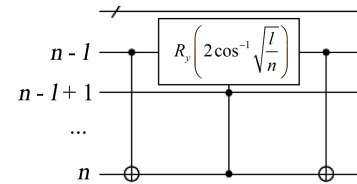


Figure 5. Construction of  $SCS_{n,l}$  of a three-qubit gate [23].

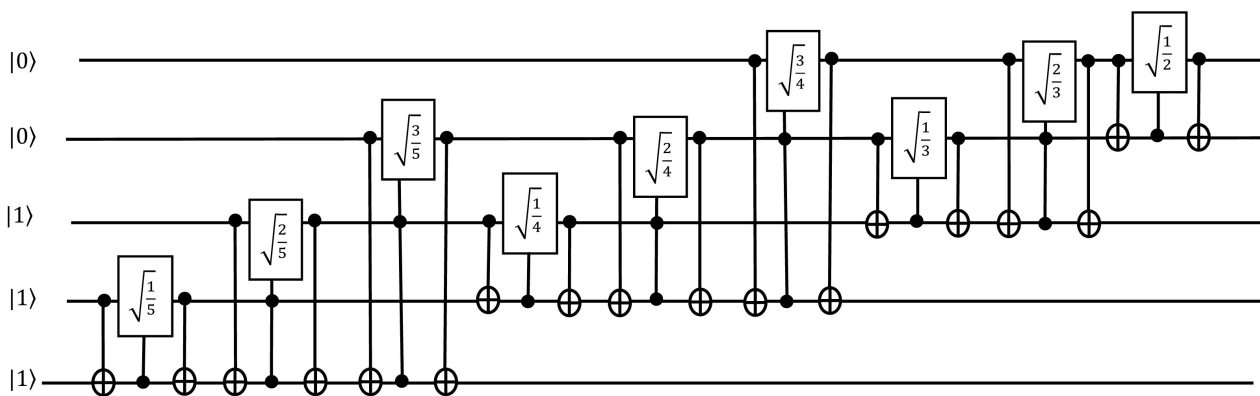


Figure 6. Dicke state  $|D_3^5\rangle$  circuit, where  $\sqrt{\frac{l}{n}}$  gates are shorthand for  $Y$ -rotation  $R_y\left(2\cos^{-1}\sqrt{\frac{l}{n}}\right)$  [23].

### 3.3. Quantum Counter

Quantum counter [24] [25] is used to count the number of terms in the SOP Boolean function. Quantum counter block is a sequence of  $n$ -Toffoli followed by Feynman ( $CNOT$ ) gates which is called Peres gate [29], as shown in Figure 7. The first qubit is applied a constant 1 with other variables combined, and the Peres gate is then turned into a quantum counter. (This qubit will be next taken from the term of the SOP formula to activate the counter block realized from Peres gates). For simplicity of explanation, we assume that the counter block is built from Toffoli and CNOT gates, as shown in Figure 7.

Here  $z$  is the least significant qubit and  $x$  the most significant. The outputs of CNOT and two of the Toffoli gates are  $1 \oplus z$ ,  $1 \cdot z \oplus y$ , and  $1 \cdot z \cdot y \oplus x$ , respectively. When  $xyz = 000$ , the first Toffoli gate outputs

$$1 \cdot z \cdot y \oplus x = 1 \cdot 0 \cdot 0 \oplus 0 = 0 \oplus 0 = 0 \quad \text{and the second } 1 \cdot z \oplus y = 1 \cdot 0 \oplus 0 = 0 \oplus 0 = 0.$$

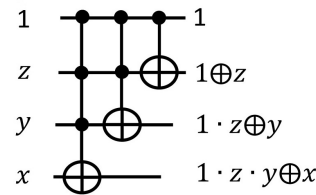


Figure 7. Three-qubit quantum counter.

The outputs of the qubits  $y$  and  $x$  are both zeros. The output of the qubit  $z$  is  $1 \oplus z = 1 \oplus 0 = 1$ . Hence the circuit incremented  $000$  by  $1$  to  $001$ . Quantum counter circuit indeed outputs the value input  $+1$ .

If we connect the first control input of the quantum counter block to a circuit, then the output of the connected circuit (a term of the SOP) will either activate or deactivate the counter. When the output of the connected circuit is equal to  $1$ , the output of the counter block is incremented by  $1$ . When the output of the circuit is equal to  $0$ , the output of the counter block is unchanged.

### 3.4. Quantum Comparator

In **Table 3**, the truth table of one-bit comparator which contains equal, greater than and less than.

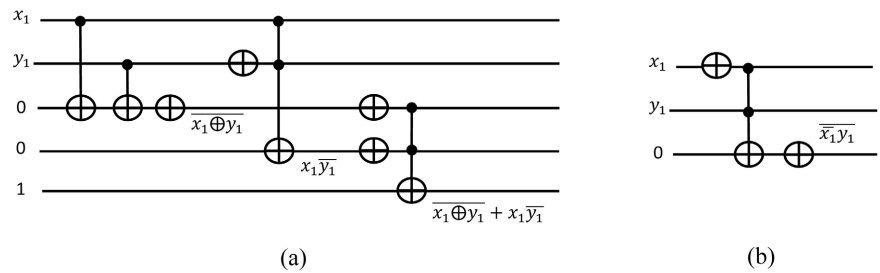
For 1-qubit comparator, to check equal  $(x_1 \oplus y_1)$  or greater than  $(x_1 \overline{y_1})$ , we add both values  $\overline{x_1 \oplus y_1} + x_1 \overline{y_1}$ . To build this circuit requires 5 qubits, 2 Toffoli, 4NOT, and 2CNOT gates, as can be seen in **Figure 8(a)**. For more than 1-qubit comparator, the circuit would be huge in terms of the number of qubits and gates. To minimize the required qubits and gates, we use “not less than” such  $\overline{x_1 y_1}$  which required only 3 qubits, 1 Toffoli, and 2 NOT gates as can be seen in **Figure 8(b)**. The output from the quantum counter would be compared with the *minsup* value. In this case we have 4-bit quantum counter compared with  $\text{minsup} = 2$  (0010). Every qubit from the quantum counter output is compared with every bit of the *minsup* value. For instance, let  $x_4 x_3 x_2 x_1$  quantum counter output and  $y_4 y_3 y_2 y_1$  *minsup* values, we build the quantum circuit for 4-bit comparator  $(\overline{x_4 y_4})(\overline{x_3 y_3})(\overline{x_2 y_2})(\overline{x_1 y_1})$ . In **Figure 9** for 4-bit quantum comparator, we rename  $x_4 x_3 x_2 x_1$  to  $\text{counter}_3 \text{counter}_2 \text{counter}_1 \text{counter}_0$  and  $y_4 y_3 y_2 y_1$  to  $\text{comparator}_3 \text{comparator}_2 \text{comparator}_1 \text{comparator}_0$ . The quantum comparator output is  $\text{out}_0$ .

In **Figure 9**, the four-bit comparator is compared the *minsup* value 0010 with the out of quantum counter. Every  $n$ -qubit comparator requires  $3n + 1$  qubits. The  $n$ -ancilla <sub>$i$</sub>  qubits are used to store the obtained value from the comparison.

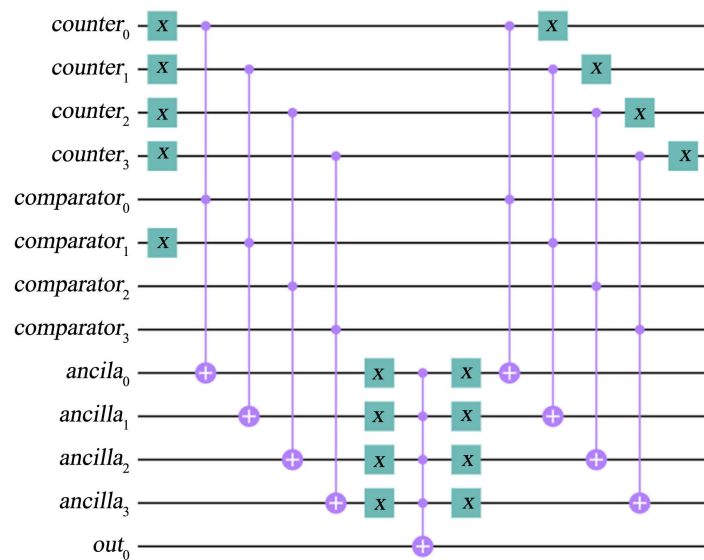
**Figure 10** is the complete quantum oracle circuit design for associate rule mining. The oracle circuit contains the circuit for each term in the SOP function expression connected with the quantum counter for each term and the quantum comparator connected with the quantum counter output. The  $q_4 q_3 q_2 q_1 q_0$  represent the items and  $\text{control\_counter}_0$  is the control bit for the quantum

**Table 3.** Truth Table of one-bit comparator.

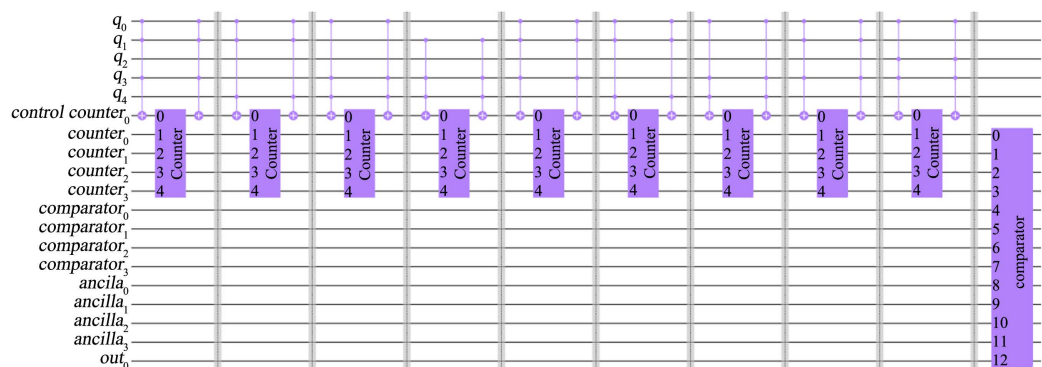
$x_1y_1$	$x_1 = y_1 \Rightarrow \overline{x_1 \oplus y_1}$	$x_1 > y_1 \Rightarrow \overline{x_1 y_1}$	$x_1 < y_1 \Rightarrow \overline{\bar{x}_1 \bar{y}_1}$
00	1	0	0
01	0	0	1
10	0	1	0
11	1	0	0



**Figure 8.** One-qubit comparator (a) equal or greater than. (b) Not less than.



**Figure 9.** Four-bit quantum comparator build using IBM Qiskit simulator.



**Figure 10.** Full quantum oracle circuit for  $abd + abe + ade + bde + abd + abe + ade + abd + acd \geq 2$ .

counter. If the control bit is active (1), then the counter value is incremented by 1. If the control bit is 0, then the counter keeps its value. The number of required qubits for the quantum counter is equal to  $\lceil \log_2 T \rceil + 1$ , where the number of required qubits for the quantum comparator required is  $3\lceil \log_2 T \rceil + 1$ . Note that if  $\log_2 T$  is integer value, then add 1 to the  $\log_2 T$  value. The SOP function  $abd + abe + ade + bde + abd + abe + ade + abd + acd \geq 2$  contains 9 terms that requires  $\lceil \log_2 9 \rceil = 4$  qubits for the quantum counter. The quantum comparator compares the output of the quantum counter 4-qubit with *minsup* value 4-qubit. The quantum comparator required four additional ancilla qubits for computation and one qubit for the output. In associate rule mining, we need the maximum frequent of *k*-itemset that is equal to or greater than to *minsup* = 2. In this case, 4-qubit from the quantum counter compared with 0010. The output is *out<sub>0</sub>* is equal to 1 when frequent of *k*-itemset equal to or greater than 2.

Let us observe that the SOP function above is not used as a logical function, but it used as a pattern matching for our problem. This general idea can be used for other problems that require counting matching patterns or counting satisfied constraints. Some constraint satisfaction problems that can be formulated as such the SOP function above can refer to [30].

Figure 11 is the complete quantum algorithm circuit design for the associate rule mining, which is a modification of Grover’s search algorithm. The Dicke state is used for superposition preparation, oracle, and diffuser to recognize the solution states. We applied this oracle in Grover’s search algorithms for  $R = 2$

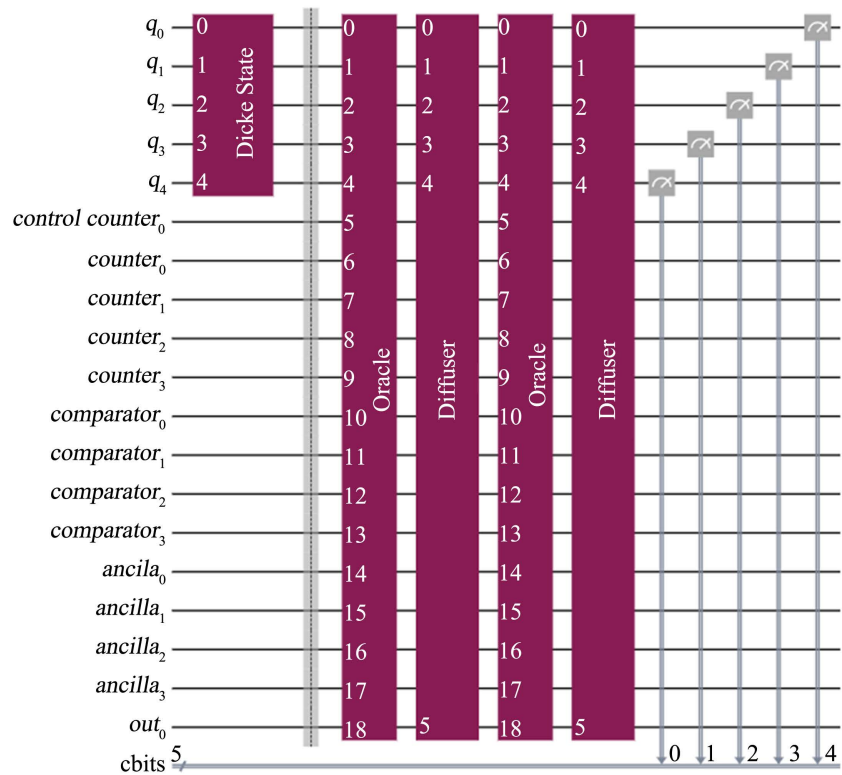


Figure 11. Full quantum algorithm circuit design for the associate rule mining.

iterations from this formula:  $R \leq \left\lceil \frac{\pi}{4} \sqrt{\frac{N}{M}} \right\rceil$  where  $M = 3$  is the number of

solutions in **Figure 2** in the Apriori algorithm, and  $N = 10$  is the number of all search space elements from the Dicke state of  $|D_3^5\rangle$ . We measured only  $q_4q_3q_2q_1q_0$  for the items but for verification the measurement can be added to  $out_0$  which is equal to 1 only if the  $k$ -itemset is greater than or equal to the *min-sup*. As can be seen in **Figure 12** the values with high probability are 10,011, 11,001 and 11,010 for *abcde* respectively based on this SOP function:

$$abd + abe + ade + bde + abd + abe + ade + abd + acd \geq 2$$

In **Figure 13**, we generalized our design to handle for associate rule mining to generate the maximum frequent  $k$ -itemset. As can be seen from **Figure 13**, the input of Dicke state is  $|0\rangle^{\otimes n-k} |1\rangle^{\otimes k}$ , where  $n$  is the number of items and  $k$  is the

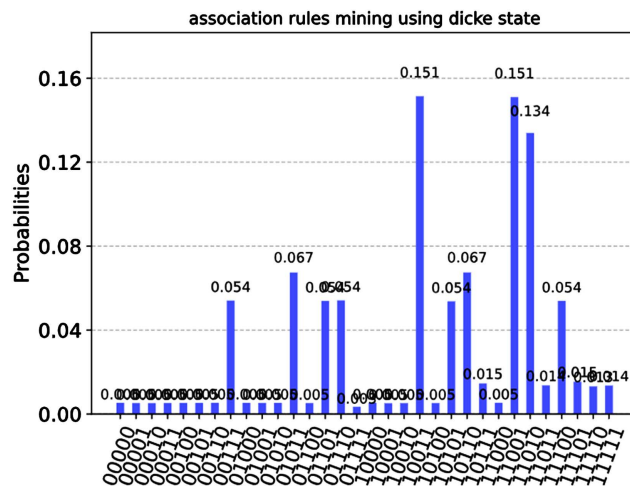


Figure 12. Histogram of measured value from Figure 11.

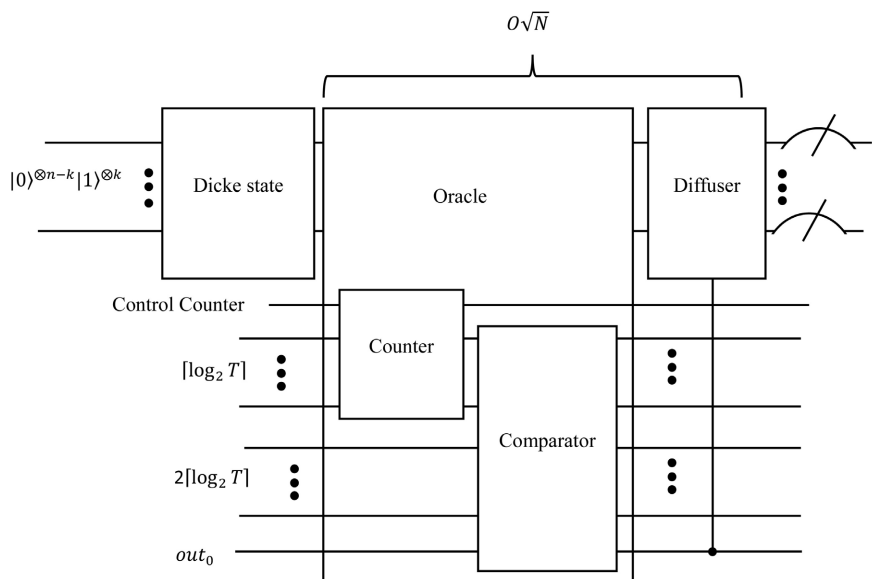


Figure 13. Proposed algorithm design for associate rule mining.

large itemset to check whether is the maximum frequent  $k$ -itemset or not. Each term from the SOP function is connected to the first qubit (Control Counter) of the quantum counter. The remaining number of qubits for the quantum counter is equal to  $\lceil \log_2 T \rceil$ , and the number of qubits of the quantum comparator is equal to  $3\lceil \log_2 T \rceil + 1$ , where  $T$  is the number of terms in the SOP function. Note that if the  $\log_2 T$  is integer value, then add 1 to the  $\log_2 T$  value. The  $out_0$  is connected to the diffuser to amplify the solution. If  $out_0$  is equal to one, then the oracle has recognized the solution. Finally, the Dicke state qubits for the items are measured. For checking purposes, the  $out_0$  can be added to the measurement in order to check the solutions with a high probability that  $out_0$  is equal to 1.

Scaling the required number of qubits in design is critical in the current generation of quantum computers because the number of qubits determines the degree of computational complexity. The more qubits a quantum processor possesses, the more complex and valuable the quantum circuits can run [31]. Thus, to scale and optimize the number of qubits that can accommodate in quantum algorithm design is directly reflected on the performance.

We compare the number of qubits that need in our design and the proposed design in [20] [21]. The number of required qubits in [20] [21] is equal to:

$$2TI + 1 \tag{2}$$

Our proposed design, the number of required qubits is:

$$\begin{cases} I + 3(\lceil \log_2 T \rceil + 1) + 2, & \text{If } \log_2 T \text{ is integer value} \\ I + 3\lceil \log_2 T \rceil + 2, & \text{If } \log_2 T \text{ not integer} \end{cases} \tag{3}$$

where  $T$  is the number of transactions and  $I$  is the number of items. For instance,  $8 \times 5$  (8 transactions and 5 items), the number of required qubits in [20] [21] is equal to 81 qubits, while our design requires only 19 qubits.

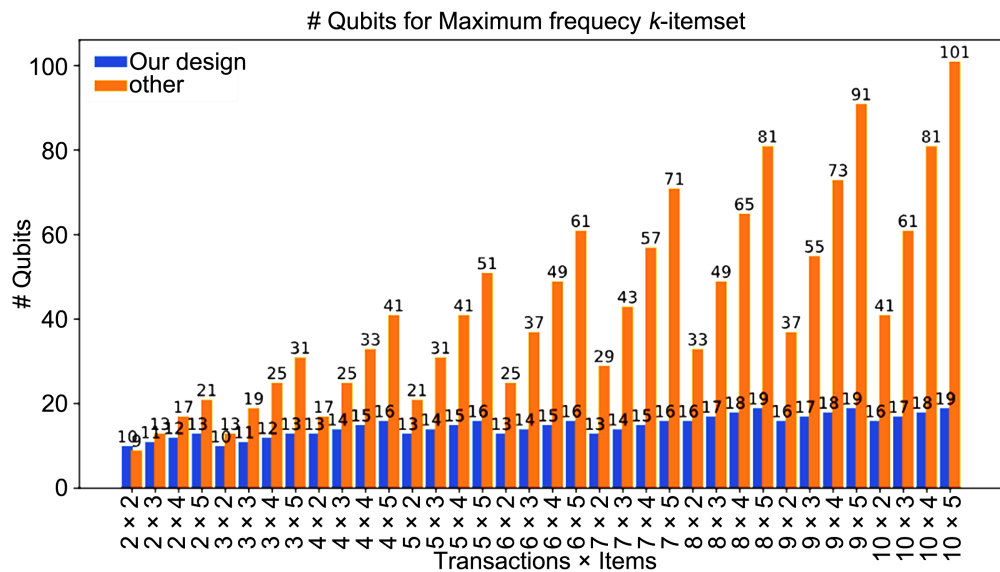


Figure 14. Histogram between our purposed design and other design in [20] [21].



As can be seen in the histogram in **Figure 14**, based on the equations in (2) and (3), for 10 transactions and 5 items,  $10 \times 5$  requires 101 qubits for the design in [20] [21], while our proposed design just requires 19 qubits. According to the design in [20] [21], one qubit is needed for every item, as well as one qubit for every transaction and one qubit for the output qubit. A large transaction database typically contains massive transactions and large item sets. As a result, the number of qubits will be unreasonably high, even for large quantum computers. Our proposed quantum architecture employs the Dicke state, which reduces the search space into a sub-search space. In addition, we employ a quantum counter and a quantum comparator that can handle more transactions and items while still performing well with a small number of qubits.

#### 4. Conclusion

We presented a novel quantum design for association rule mining to discover the maximum frequent  $k$ -itemset. We converted the transaction database into a new type of SOP Boolean function and then reduced the SOP function into large  $k$ -items with only Hamming weight that satisfies the minimum support threshold. In addition, we proposed using the Dicke state to prepare the superposition  $\binom{n}{k}$  states for Grover's search algorithm instead of the conventional Hadamard operator, which would require  $2^n$  states. We reduced the SOP function to large  $k$ -items where the likelihood of the maximum frequent  $k$ -itemset can be found. Then we design an advanced quantum oracle with a quantum counter and quantum comparator. Using these three different quantum blocks, Dicke state, quantum counter, and quantum comparator, we achieved to reduce search space and the required number of qubits in the design. We have then shown a full implementation of our design on the IBM Qiskit simulator and observed the correct results. We compared our proposal design with [20] [21] design that our design requires fewer qubits. We can solve many transactions and items by scaling and optimizing the search space and required qubits. For future improvement, a fully quantum design for association rule mining can be developed using our proposed design to generate association rules from a maximum frequent  $k$ -itemset.

#### Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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# What in Fact Proves the Violation of the Bell-Type Inequalities?

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## Abstract

A. Peres constructed an example of particles entangled in the state of spin singlet. He claimed to have obtained the CHSH inequality and concluded that the violation of this inequality shows that in a measurement in which some variables are tested, other variables, not tested, have no defined value. In the present paper is proved that the correct conclusion of the violation of the CHSH inequality is different. It is proved that the classical calculus of probabilities of test results, obeying the Kolmogorov axioms, is unfit for the quantum formalism, dominated by probability amplitudes.

## Keywords

CHSH Inequalities, Kolmogorov Axioms, Photon Singlet of Polarization, Malus Law

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## 1. Introduction

J. S. Bell developed in his famous work [1] an inequality for three observables, and it was extended to more observables [2]. These inequalities were found to disagree with the quantum mechanics (QM). The violation of these inequalities was proved by the experiment, [3]-[11], and is typically interpreted as indicating that the quantum world allows nonlocal influences between measurement results of entangled quantum objects [1] [3] [4] [5] [6] [12]-[18] (see also the references in [18] and also a generalization of the Bell-type inequalities in [19]).

In his famous article “Unperformed experiments have no results” [20] (see also [21]) A. Peres claimed to have deduced from the violation of Bell-type inequalities, a new conclusion, namely, that incompatible observables cannot take definite values in the same test. By incompatible is understood that the operators corresponding to the observables don’t commute. So, Peres concluded that if the observables  $A$  and  $B$  are measured and produce definite values,

the wave-function (w-f) cannot predict definite values for non-measured observables,  $A'$  and  $B'$ , not commuting with  $A$  respectively  $B$ .

It may though be that there are effects beyond the predictions of the w-f, e.g. that the QM admits a substructure. For example, if the quantum object behaves according to Bohm's mechanics [22], some observables may take values although the w-f does not acknowledge them.

It is argued in the present article that what in fact is proved by the violation of the Bell-type inequalities is another feature, namely, that the classical calculus of distribution of probabilities, satisfying the Kolmogorov axioms, is incompatible with the predictions of the w-f. The assumption of locality of measurement results yields just a particular case of such a distribution.

The next sections are organized as follows: Section 2 defines the most general distribution of probabilities of variables' values, for which the Bell-type inequalities can be derived; no locality assumption is made. Section 3 derives the CHSH inequality using this general distribution. Section 4 compares the consequences of this distribution with the quantum predictions, and a contradiction is found. Section 5 contains conclusions.

## 2. A Probability Distribution under the Komogorov Axioms

Consider a set of events  $\{E_1, E_2, \dots, E_n\}$  with probabilities  $P$  from a common space satisfying the Kolmogorov axioms

- 1)  $0 \leq P(E_i) \leq 1$ ,
- 2)  $P(E_i \text{ OR } E_j \text{ OR } \dots \text{ OR } E_k) = P(E_i) + P(E_j) + \dots + P(E_k)$ .

In this text we will have to do with four binary variables:  $A$  and  $A'$  belong to a photon 1,  $B$  and  $B'$  belong to a photon 2. All the four variables are polarizations,  $A$  and  $A'$  along the directions  $\mathbf{a}$  respectively  $\mathbf{a}'$ ,  $B$  and  $B'$  along the directions  $\mathbf{b}$  respectively  $\mathbf{b}'$ . We will denote the polarization along a direction  $\mathbf{u}$  by “+ $\mathbf{u}$ ” and perpendicular to  $\mathbf{u}$  by “- $\mathbf{u}$ ”. So, in a measurement of the variable  $A$  for photon 1 and  $B$  for photon 2 we will get the result “+ $\mathbf{a}$ ” for  $A$  and “- $\mathbf{b}$ ” for  $B$  with the probability  $P(+_{\mathbf{a}} -_{\mathbf{b}})$ .

*Assumption A:* in a test of the two particles, each one along some direction, all the four variables take definite values, *i.e.* the non-measured variables take values as well as the measured ones.

Therefore we will have to do with probabilities of the form  $P_{AB'}(+_{\mathbf{a}} +_{\mathbf{a}'} +_{\mathbf{b}} -_{\mathbf{b}'})$  where the indexes  $A$  and  $B'$  after  $P$  indicate which observables were in fact measured.

Applying then the Komogorov axioms one has

$$P_{AB'}(+_{\mathbf{a}} -_{\mathbf{b}'}) = P_{AB'}(+++-) + P_{AB'}(++--)+ P_{AB'}(+--+)+ P_{AB'}(+---). \quad (1)$$

We omitted here and so we will do in the rest of the article, the indexes inside the round parentheses in the four-variable probabilities, but we will keep the convention that the order of the results is  $\pm_{\mathbf{a}} \pm_{\mathbf{a}'} \pm_{\mathbf{b}} \pm_{\mathbf{b}'}$ .

*Assumption B:* the distribution of four-variable probabilities is independent of which variables are actually measured.

That means

$$\begin{aligned}
 P_{AB}(q_a, q_{a'}, q_b, q_{b'}) &= P_{A'B}(q_a, q_{a'}, q_b, q_{b'}) = P_{AB'}(q_a, q_{a'}, q_b, q_{b'}) \\
 &= P_{A'B'}(q_a, q_{a'}, q_b, q_{b'}),
 \end{aligned}
 \tag{2}$$

with  $q_a, q_{a'}, q_b, q_{b'} \in [+, -]$ . That gives us the possibility to omit the specification of the actual measurement in the four-variable probability, e.g. we will write simply  $P(q_a, q_{a'}, q_b, q_{b'})$ . We will also omit the specification of the actual measurement in the two-variable measurement, because it appears inside the parentheses, *i.e.*  $P_{AB}(q_a, q_b) = P(q_a, q_b)$ .

### 3. A General Derivation of the CHSH Inequality

With the distribution of probability developed in the previous section we can obtain the following results

$$\begin{aligned}
 P(+_a +_b) &= P(++++) + P(+++-) + P(+--+ +) + P(+--+ -), \\
 P(+_a -_b) &= P(++-+) + P(++-- +) + P(+--- +) + P(+--- -), \\
 P(-_a +_b) &= P(-+++) + P(-++- +) + P(---+ +) + P(---+ -), \\
 P(-_a -_b) &= P(-+-+) + P(-+-- +) + P(---- +) + P(---- -),
 \end{aligned}$$

The average  $\overline{AB}$  of the results of the joint measurement of  $A$  and  $B$  can be expressed according to the above equalities as

$$\begin{aligned}
 \overline{AB} &= \{P(++++) + P(+++-) + P(+--+ +) + P(+--+ -)\} \\
 &\quad - \{P(++-+) + P(++-- +) + P(+--- +) + P(+--- -)\} \\
 &\quad - \{P(-+++) + P(-++- +) + P(---+ +) + P(---+ -)\} \\
 &\quad + \{P(-+-+) + P(-+-- +) + P(---- +) + P(---- -)\}
 \end{aligned}
 \tag{3}$$

One can similarly express in terms of four-variable probabilities, the averages  $\overline{A'B}$ ,  $\overline{AB'}$ ,  $\overline{A'B'}$

$$\begin{aligned}
 \overline{A'B} &= P(+_{a'} +_b) - P(+_{a'} -_b) - P(-_{a'} +_b) + P(-_{a'} -_b), \\
 \overline{AB'} &= P(+_a +_{b'}) - P(+_a -_{b'}) - P(-_a +_{b'}) + P(-_a -_{b'}), \\
 \overline{A'B'} &= P(+_{a'} +_{b'}) - P(+_{a'} -_{b'}) - P(-_{a'} +_{b'}) + P(-_{a'} -_{b'}).
 \end{aligned}
 \tag{4}$$

e.g.

$$\begin{aligned}
 \overline{A'B} &= \{P(++++) + P(+++-) + P(-+++) + P(-++-)\} \\
 &\quad - \{P(++-+) + P(++-- +) + P(---+ +) + P(---+ -)\} \\
 &\quad - \{P(+--+ +) + P(+--+ -) + P(---- +) + P(---- -)\} \\
 &\quad + \{P(+--- +) + P(+--- -) + P(---- +) + P(---- -)\}.
 \end{aligned}
 \tag{5}$$

Since  $\sum_{A, A', B, B'} P(A, A', B, B') = 1$ , one has

$$\begin{aligned}
 &P(++++) + P(+++-) + P(+--+ +) + P(+--+ -) \\
 &+ P(+--+ +) + P(+--+ -) + P(+--- +) + P(+--- -) \\
 &+ P(-+++) + P(-++- +) + P(---+ +) + P(---+ -) \\
 &+ P(-+-+) + P(-+-- +) + P(---- +) + P(---- -) = 1
 \end{aligned}
 \tag{6}$$

From the Equalities (3) and (4) one can find by direct substitution and reduc-

ing identical terms that

$$\begin{aligned} & \overline{AB + A'B - AB' + A'B'} \\ &= 2\{P(++++) + P(+++-) - P(++-+) - P(++--)) \\ & \quad - P(+--+)) + P(+---) - P(+---) + P(+---) \\ & \quad + P(-+++)) - P(-++-) + P(-++-) - P(-++-) \\ & \quad - P(-++-) - P(-++-) + P(-++-) + P(-++-)\}. \end{aligned} \tag{7}$$

Comparing with (6) one can see that

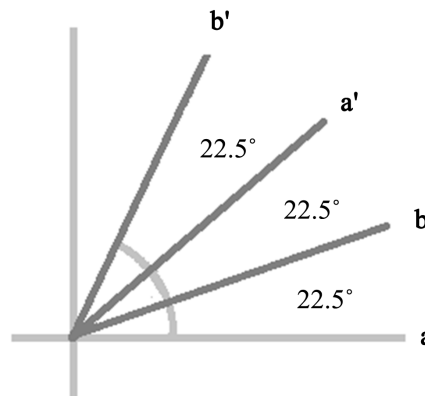
$$\overline{AB + A'B - AB' + A'B'} \leq 2. \tag{8}$$

Indeed, if the sum of all the four-variable probabilities is equal to 1, the sum in which some of the probabilities appear with minus should be in general less than 1.

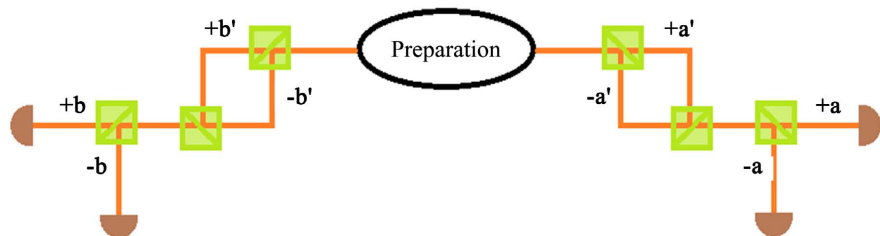
The inequality (8) is the CHSH inequality.

#### 4. Then What in Fact Prove the Bell-Type Inequalities?

It is known that the CHSH inequality is violated if one considers the photon singlet. For a measurement of the polarization of the photon 1 along a direction  $\mathbf{u}$ , and a measurement of the polarization of photon 2 along a direction  $\mathbf{v}$ , the averaged product of the two results is equal to  $\cos(2\theta_{uv})$ , where  $\theta_{uv}$  is the angle between the two directions. Choosing for the observables  $A$  and  $A'$  the polarization of the photon 1 along the directions  $\mathbf{a}$  and  $\mathbf{a}'$ , and for the observables  $B$  and  $B'$  the polarization of the photon 2 along the directions  $\mathbf{b}$  and  $\mathbf{b}'$ , as in the **Figure 1** and **Figure 2**, the quantum formalism predicts



**Figure 1.** Four coplanar directions. See explanations in the text.



**Figure 2.** Arrangement of a CHSH experiment involving different polarization directions.

The wave-packet of the photon 1 (2) is split according to the polarization directions  $\mathbf{a}'$  and perpendicular to  $\mathbf{a}'$  ( $\mathbf{b}'$  and perpendicular to  $\mathbf{b}'$ ). Then, the two wave-packets are merged back into one and split according to the polarization axes  $\mathbf{a}$  and perpendicular to  $\mathbf{a}$  ( $\mathbf{b}$  and perpendicular to  $\mathbf{b}$ ).

$$\langle AB \rangle + \langle A'B \rangle - \langle AB' \rangle + \langle A'B' \rangle = 2\sqrt{2}, \quad (9)$$

This result disagrees with the inequality (8).

This violation proves that some of the assumptions made in the derivation of the distribution  $P(q_a, q_a', q_b, q_b')$  in Section 2 must be wrong. These assumptions are the Kolmogorov axioms 1 and 2 and the assumptions A and B. Some of them must disagree with the QM, and it is known that QM was never disproved by the experiment.

Whether the assumptions A and B disagree with the QM is not obvious. But it is obvious that the axiom 2 of Kolmogorov does disagree with the QM. Indeed, by this axiom the probability of occurrence of a result  $q_1$  or  $q_2$  satisfies

$$\text{Prob}(q_1 \text{ OR } q_2) = \text{Prob}(q_1) + \text{Prob}(q_2). \quad (10)$$

However, in the quantum formalism the basic element in the calculus of probability of a result  $q$  is not the probability  $\text{Prob}(q)$ , but the amplitude of probability  $\mathbf{a}(q)$ , with

$$\text{Prob}(q_1) = |\mathbf{a}(q_1)|^2, \quad \text{Prob}(q_2) = |\mathbf{a}(q_2)|^2, \quad (11)$$

and instead of (10) one has by the QM

$$\begin{aligned} \text{Prob}(q_1 \text{ OR } q_2) &= |\mathbf{a}(q_1) + \mathbf{a}(q_2)|^2 \\ &= \text{Prob}(q_1) + \text{Prob}(q_2) + \mathbf{a}(q_1)^* \mathbf{a}(q_2) + \mathbf{a}(q_2)^* \mathbf{a}(q_1). \end{aligned} \quad (12)$$

Let's exemplify the problem on the probability  $P(+_a +_b)$ , *i.e.* the actual measurement is done in the base  $\{+_a, -_a\}$  for photon 1 and  $\{+_b, -_b\}$  for photon 2, and we retain the pairs producing the response “++”. We will show that QM and the Kolmogorov-type calculus yield different expressions, as do (10) and (12). For this purpose we write the w-f of the photon singlet putting in evidence the polarizations along  $\mathbf{a}'$ ,  $\mathbf{a}$ , and  $\mathbf{b}'$ ,  $\mathbf{b}$ , and we denote by  $\theta_{uv}$  the angle between directions  $\mathbf{u}$  and  $\mathbf{v}$ .

So, we start from the expression of the w-f in the polarization base  $\{+_a, -_a\}$  for photon 1, and  $\{+_b, -_b\}$  for photon 2

$$\begin{aligned} |\psi\rangle &= \frac{1}{\sqrt{2}} \{ \cos(\theta_{a'b'}) |+_a\rangle |+_b\rangle + \sin(\theta_{a'b'}) |+_a\rangle |-_b\rangle \\ &\quad - \sin(\theta_{a'b'}) |-_a\rangle |+_b\rangle + \cos(\theta_{a'b'}) |-_a\rangle |-_b\rangle \} \\ &= \mathbf{a}(+_a +_b) |+_a\rangle |+_b\rangle + \mathbf{a}(+_a -_b) |+_a\rangle |-_b\rangle \\ &\quad + \mathbf{a}(-_a +_b) |-_a\rangle |+_b\rangle + \mathbf{a}(-_a -_b) |-_a\rangle |-_b\rangle. \end{aligned} \quad (13)$$

Following the evolution of the pair in the apparatus, see **Figure 2**, let's pass to the base  $\{+_a, -_a\}$  for photon 1



$$\begin{aligned} |+_a\rangle &= \cos(\theta_{a'a})|+_a\rangle + \sin(\theta_{a'a})|-_a\rangle \\ |-_a\rangle &= -\sin(\theta_{a'a})|+_a\rangle + \cos(\theta_{a'a})|-_a\rangle \end{aligned} \quad (14)$$

$$\begin{aligned} |\psi\rangle &= \frac{1}{\sqrt{2}} \left\{ \cos(\theta_{a'b'}) [\cos(\theta_{a'a})|+_a\rangle|+_b\rangle + \sin(\theta_{a'a})|-_a\rangle|+_b\rangle] \right. \\ &\quad + \sin(\theta_{a'b'}) [\cos(\theta_{a'a})|+_a\rangle|-_b\rangle + \sin(\theta_{a'a})|-_a\rangle|-_b\rangle] \\ &\quad - \sin(\theta_{a'b'}) [-\sin(\theta_{a'a})|+_a\rangle|+_b\rangle + \cos(\theta_{a'a})|-_a\rangle|+_b\rangle] \\ &\quad \left. + \cos(\theta_{a'b'}) [-\sin(\theta_{a'a})|+_a\rangle|-_b\rangle + \cos(\theta_{a'a})|-_a\rangle|-_b\rangle] \right\} \\ &= \mathbf{a}(+_a+_a+_b')|+_a\rangle|+_b\rangle + \mathbf{a}(+_a-_a+_b')|-_a\rangle|+_b\rangle \\ &\quad + \mathbf{a}(+_a+_a-_b')|+_a\rangle|-_b\rangle + \mathbf{a}(+_a-_a-_b')|-_a\rangle|-_b\rangle \\ &\quad + \mathbf{a}(-_a+_a+_b')|+_a\rangle|+_b\rangle + \mathbf{a}(-_a-_a+_b')|-_a\rangle|+_b\rangle \\ &\quad + \mathbf{a}(-_a+_a-_b')|+_a\rangle|-_b\rangle + \mathbf{a}(-_a-_a-_b')|-_a\rangle|-_b\rangle. \end{aligned} \quad (15)$$

Finally we pass from the base  $\{|+_b, -_b\rangle\}$  for the photon 2 to the base  $\{|+_b, -_b\rangle\}$

$$\begin{aligned} |+_b\rangle &= \cos(\theta_{b'b})|+_b\rangle + \sin(\theta_{b'b})|-_b\rangle \\ |-_b\rangle &= -\sin(\theta_{b'b})|+_b\rangle + \cos(\theta_{b'b})|-_b\rangle \end{aligned} \quad (16)$$

and get

$$|\psi\rangle = \{\mathbf{a}(++++) + \mathbf{a}(+++ -) + \mathbf{a}(+ - + +) + \mathbf{a}(+ - - -)\}|+_a\rangle|+_b\rangle + \dots \quad (17)$$

where the order inside the round parentheses is  $q_a, q_{a'}, q_b, q_{b'}$ , and

$$\begin{aligned} \mathbf{a}(++++) &= \cos(\theta_{a'b'})\cos(\theta_{a'a})\cos(\theta_{b'b})/\sqrt{2} \\ \mathbf{a}(+++ -) &= -\sin(\theta_{a'b'})\cos(\theta_{a'a})\sin(\theta_{b'b})/\sqrt{2} \\ \mathbf{a}(+ - + +) &= \sin(\theta_{a'b'})\sin(\theta_{a'a})\cos(\theta_{b'b})/\sqrt{2} \\ \mathbf{a}(+ - - -) &= \cos(\theta_{a'b'})\sin(\theta_{a'a})\sin(\theta_{b'b})/\sqrt{2} \end{aligned} \quad (18)$$

According to the QM from these amplitudes of probability one can calculate the probability of getting the result  $+_a+_b$

$$P(+_a+_b) = |\mathbf{a}(++++) + \mathbf{a}(+++ -) + \mathbf{a}(+ - + +) + \mathbf{a}(+ - - -)|^2. \quad (19)$$

Substituting in (19) the expressions in (18) one gets after a simple calculus of trigonometry

$$P(+_a+_b) = \cos^2(\theta_{ab})/2. \quad (20)$$

However, if we equate  $P(q_a q_{a'} q_b q_{b'}) = |\mathbf{a}(q_a q_{a'} q_b q_{b'})|^2$ , one can immediately see that the sum of the absolute squares of the amplitudes in (18) does not lead to the quantum result (20).

A similar problem of disagreement between the classical probability calculus and the quantum formalism was posed by Tarozzi [23] and later by Božić *et al.* [24]. Both referred to the two-slit experiment in which the intensity of the image on a screen  $\mathcal{S}$  beyond the slits  $B$  and  $C$ ,  $|\psi(\mathbf{r}, t)|^2$ , differs from the sum of the intensities of the images created with only one of the slits open,  $|\varphi_B(\mathbf{r}, t)|^2$  and  $|\varphi_C(\mathbf{r}, t)|^2$ . Indeed,

$$|\psi(\mathbf{r}, t)|^2 = |\varphi_B(\mathbf{r}, t) + \varphi_C(\mathbf{r}, t)|^2 = |\varphi_B(\mathbf{r}, t)|^2 + |\varphi_C(\mathbf{r}, t)|^2 + X(\mathbf{r}, t),$$

where  $X(\mathbf{r}, t)$  is the interference term  $X(\mathbf{r}, t) = 2 \operatorname{Re}[\varphi_B^*(\mathbf{r}, t)\varphi_C(\mathbf{r}, t)]$ .

For solving the dilemma why the whole differs from the sum of its parts, Božić *et al.* suggested to regard the experiment in which both slits are open as having a different configuration than the experiments in which only one slit is open and in consequence, what passes through the apparatus is different in the two types of experiment. They suggested to write for the interference experiment  $|\psi(\mathbf{r}, t)|^2 = |\tilde{\varphi}_B(\mathbf{r}, t)|^2 + |\tilde{\varphi}_C(\mathbf{r}, t)|^2$ , where each one of  $\tilde{\varphi}_B(\mathbf{r}, t)$  and  $\tilde{\varphi}_C(\mathbf{r}, t)$  contains also a part from  $X(\mathbf{r}, t)$ .

This idea seems appealing for the experiment in the **Figure 2** too. That means, to construct a distribution of probabilities in which  $P(q_a, q_{a'}, q_b, q_{b'})$  contains besides the absolute square of the respective four-variable amplitude, a part of the interference terms.

But that turns to be impossible. Let's take as an example the probability  $P(q_a, q_{a'}, q_b, q_{b'}) = |++\rangle$ , which according to (18) should be equal to  $\sin^2(\theta_{a'b'})\sin^2(\theta_{a'a})\cos^2(\theta_{b'b})$ . This expression cannot be modified since it is dictated by the Malus law. It says that if the particle 1 took the path  $-a'$ , the particle 2 takes the path  $+b'$  with probability  $\sin^2(\theta_{a'b'})$ . Next, the particle 1 takes the path  $+a$  with probability  $\sin^2(\theta_{a'a})$  and the particle 2 takes the path  $+b$  with probability  $\cos^2(\theta_{b'b})$ . There is no possibility for changing  $P(q_a, q_{a'}, q_b, q_{b'})$ .

## 5. Conclusions

In his article "Unperformed experiments have no results" [20], Peres concluded that the assumption A, see Section 2, is wrong. However, as shown here, the correct cause of the violation of the CHSH inequality is the incompatibility between the classical calculus of probabilities, governed by the Kolmogorov axioms, and the quantum probabilities governed by the calculus of amplitudes of probability.

It has to be mentioned that 16 years after the publication of Peres' article, Berndl et Goldstein also concluded [25], in an examination of the celebrated Hardy's article "Quantum Mechanics, Local Realistic Theories, and Lorenz-Invariant Realistic Theories" [26], that observables that were not measured may have no definite values in a test in which other observables were actually measured. But, again, this conclusion does not result from the violation of the Bell-type inequality.

No locality was assumed in the derivation of the distribution  $P(q_a, q_{a'}, q_b, q_{b'})$  obtained here. The hypothesis of locality of measurement results leads to a particular case of  $P(q_a, q_{a'}, q_b, q_{b'})$ . The distribution derived here covers not only distributions obtained in base of the locality assumption, but also distributions of results dependent both on a local setup as well as on a distant setup.

The fact that the quantum probabilistic formalism is based on superposition of amplitudes of probability stresses the wave nature of the quantum object.

## Conflicts of Interest

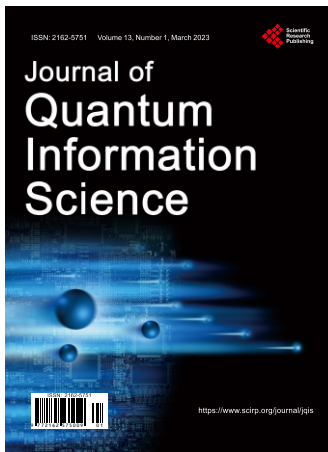
The author declares no conflicts of interest regarding the publication of this paper.

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