

## Article

# Development of Evolutionary Systems based on Quantum Petri Nets

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**Abstract:** The evolutionary systems (ES) include software applications that solve problems using heuristic methods instead of the deterministic ones. The classical computing used for ES development involves random methods to improve different kinds of genomes. The mappings of these genomes lead to individuals that correspond to the searched solutions. The individual evaluations by simulations serve for the improvement of their genotypes. Quantum computations, unlike the classical computations, can describe and simulate a large set of individuals simultaneously. This feature is used to diminish the time for finding the solutions. Quantum Petri Nets (QPNs) can model dynamical systems with probabilistic features that make them appropriate for the development of ES. Some examples of ES applications using the QPNs are given to show the benefits of the current approach.

**Keywords:** quantum computing; genetic algorithms; Petri nets; Quantum Petri nets; software development, analysis and verification

## 1. Introduction

The current research concerns applications, such as urban vehicle traffic, airplane traffic, weather, markets, electric power networks, fluids networks, telecommunications and data transmission, etc. that have stochastic behaviors. There are some entities that have to be controlled or managed to behave according to required specifications.

Quantum computers have different capabilities compared to classical computers and their use should cover the domains where these differences would lead to significant benefits. The authors of [1] review the quantum algorithms that have been discovered and reveal their features that outperform classical algorithms.

According to [2], tools are needed to create and debug quantum computers and their programs. These tools can help to elucidate hidden issues and drive towards design with the best chance for overall success.

The current approach developed methods that can sustain the heuristic search of evaluated solutions that exceed specified thresholds. The previously conceived ES methods are modified according to the features provided by the quantum algorithms.

The general objective in simulating a quantum system is to determine its structure or behavior, given knowledge of its components and the environment in which it exists.

In [2] the quantum computers are partitioned in three categories:

- Analogue quantum computers that directly manipulate the interactions between qubits without breaking the operations in logic gates.
- Digital noisy intermediate-scale quantum computers that use primitive gate operations on physical qubits.
- Fully error-corrected quantum computers that enable noisy physical qubits to emulate stable logical qubits.

The QPNs (Quantum Petri Nets) can be used to model the quantum software applications, to analyze their structure and to verify their behaviors [3]. After the simulations of the QPN models, the implementation of the quantum applications is expected to be achieved (compiled) without difficulties.

This article shows the links between quantum algorithms and their corresponding QPN models. These can sustain the quantum processor configuration and quantum program conception, verification and debugging.

The two directions for solving the problems concern the contraption of methods that use quantum computation methods implemented on classical computers and to create new concepts that allow the finding of the ES solutions using the quantum computers.

### 1.1. Current Research State of the Field

#### 1.1.1. Quantum Algorithms

Quantum computing is recommended to be used in applications where it outperforms the classical computation. Some reviews ([26], [7]) present as main QC directions: breaking cryptosystems [10], unstructured search problems, finding accurate approximate solutions to optimization problems, finding the minimum of an unsorted list of integers, determining a graph connectivity, solving linear equations, quantum annealing, etc.

The search in an unstructured database is obtained in [8] using a function  $F(x)$ ,  $x \in X = \{0, 1, \dots, (n-1)\}$ , with  $F(x) = 0$ , for  $\forall x \in X$ ,  $x \neq j$  where  $F(j) = 1$ . The problem consists of finding  $j$ . The exponential speedup of the search compared to the classical computation is an undoubted benefit.

Shor's algorithm solves the factorization problem [9]. It is given  $F(x) = a^x \bmod N$  with  $a \in \mathbb{R}$ ,  $1 < a < N$ . The request is the finding of the smallest integer  $r$  such that  $a^r \bmod N = 1$ . Again, the algorithm's exponential search determines its use in many applications, such as the use of QC in cryptography [10], [11].

The inverse transform of a matrix introduced in [12] is used for solving linear equations of the form  $A \cdot x = b$ , where  $A$  is a Hermitean  $N \times N$  matrix and  $b$  a given unit vector. QC solves such problems that appear in many practical applications with exponential speedup.

Hybrid methods involving quantum and classical computers can be used as Variational Quantum Eigensolver [13], [14]. The eigenvalues and eigenvectors of a Hamiltonian are used to transform a system iteratively to a desired specified one.

Quantum annealing is an optimization method for combinatorial problems where the superposition is used for avoiding the focalization in local minimums [15].

Quantum walk opens ways for algorithm construction that solves search problems on a graph [16].

According to [18] the classical random walk concept has been used as a computational framework for designing classical algorithms for complex problems, while quantum variants provide speed-up in computational power for various algorithms with distinct elements in spatial search or graph connectivity.

As example is the optimization of search based on random walk that requires the reduction of the number of necessary repetitions [20], [23].

Some quantum walker approaches tackle the Quantum Discrete Random Walkers in an infinite space or finite space [25]. Other researchers studied the quantum continuous random walkers (in an infinite space) [24], [29]. They are widely used in practical applications [26]. An application of quantum discrete walker ranking in a grid nodes is given in [27].

The reference [58] contains some variants of QRW approaches and different variants of generalized coin tossing. In [28] two entangled coins were used to control the walker's move in a one-dimension space.

One goal in walker problems is the reducing of the hitting time and diminishing mixing time [30].

Quantum walk can be used for search of element distinctness (e. g. find two equal elements) [21].

The comprehensive review [63] divides the quantum walker approaches as: Schrodinger and combinatorial. To be noted the decoherence definition as a physical phenomenon that typically arises from the interaction of quantum systems and their environment. This interaction can be used for quantum process control as it will be seen further for controlling the walker moves.

Quantum Approximate Optimization Algorithm (QAOA) uses the mapping of the objective function to Hamiltonian that brings the problem into Hilbert space [31], [32], [33]. The expectation value of Hamiltonian is improved by using quantum mechanical techniques in the Hilbert space. QAOA can be extended by adding constraints. A relevant problem is the so called MaxCut where a graph  $G = (V, E)$  with  $V$  vertices and  $E$  edges has to be cut in such a manner, that it maximizes the number of edges crossing the cut.

As conclusion, the main quantum walk research directions and their practical applications focus on *the hitting times*, *the quantum amplification control* and *the marked element detection*.

### 1.1.2. Evolutionary Systems

Evolutionary Algorithms (EAs) are applied to problems where pure stochastic algorithms fail or find it difficult to solve due to the high number of dimensions or function complexities [36]. Their main utilizations cover the domains of variable optimization, new structural design and improvement. EAs include: evolutionary strategies, genetic algorithms, genetic programming, genetic improvement, grammatical evolution, linear genetic programming, Chartistian genetic programming, differential evolution and gene expression evolution.

The evolutionary systems implemented on classical computers are often used for solving problems concerning:

- combinatorial requirements,
- optimization of system parameters,
- dynamic behavior optimizations and
- algorithm synthesis such as for controlling plants or for reacting to events produced by their environments.

Related to the use of QC in EA some questions arise: What are the benefits of using QC in EA? What are the modifications required for application of QC in EA? Where and how can Quantum Evolutionary Algorithms (QEAs) be applied in practical applications? References [37] and [34] offers some answers to this.

The use of QC in EAs led to three main development directions: quantum inspired evolutionary algorithms ([38], [39], [40], [41], [42], [43], [44], [45], [46], [47], [48], [49], [50], [51]), quantum evolutionary algorithms ([52], [53], [54], [55], [56], [57], [17]) and hybrid quantum-classic evolutionary algorithms ([60], [61], [62]).

Successfully detailed implementations at the QLC level are developed and deeply analyzed in [64] and [65].

Some QEA used animal behaviors for searching the solutions [67], [68], [44]. Remarkable are the characteristics of the systems that can be approached: they could have various complexities, including non-linear, non-convex, multi-modality, non-differentiable functions and large-scale dimensionality.

Quantum control based on machine learning in an open quantum system is another direction of QC application development [59].

Closest to the view point of quantum state superposition, created by QC, is the Particle Swarm Optimization (PSO) method [22].

Final principal conclusions:

Analyzing the QEAs, it can be concluded that the genotypes are coded based on the quantum superposition fulfilling the Hilbert condition. The genotypes are initialized

to meet some diversity requirements and covering the search domain. The individual (i. e. genotypes) are improved using unitary transformation matrix. The individual improvements can be based on a single (usually the best) individual or combining features from two individuals (i. e. crossover). Some evolution methods need genotype (or individual) repair mechanisms. There are improvements consisting of the search step adaptations, usually related to the generation iterations. It is difficult to prove the benefits of using the quantum vector representation instead of classical ones. There would be clear benefits if it can be proved that the number of searches and evaluations is smaller in the case of quantum description. The comparisons based on experiments of different QEA methods for solving particular problems can be supposed to be biased to particular characteristics.

The approaches of discrete oriented and un-oriented random walker problems were used to show the benefits of the QPN models.

## 2. Materials and Methods

### 2.1. Quantum State versus Classical State

The classical bits take values in the domain  $\{0, 1\}$ . They are used to compose the digital information. A number of  $r$  bits can cover a domain of  $2^r$  values.

The quantum replacement of the classical bit is the qubit denoted here  $|b_k\rangle$ :  $|b_k\rangle = \alpha_k|0\rangle + \beta_k|1\rangle$  where the complex numbers  $\alpha_k$  and  $\beta_k$  satisfy the relation  $|\alpha_k|^2 + |\beta_k|^2 = 1$  and  $|0\rangle, |1\rangle$  represent their quantum state.

The quantum system  $Q$  with finite dimension  $r$  state set  $Q = \{q_0, q_1, \dots, q_{r-1}\}$  is represented by the  $r$ -dimensional row vector:

$$\langle\psi| = \sum_{i=0}^{r-1} c_i \langle q_i| \quad (1)$$

with  $c_i$  complex number from the set  $\mathbb{C}$  fulfilling the relation:  $\sum_{i=0}^{r-1} |c_i|^2 = 1$ .

Denoting by  $|\psi\rangle$  the conjugate-transpose of  $\langle\psi|$ , the Hilbert space  $\mathcal{H}_q$  has the base  $|q_i\rangle : i = 0, 1, \dots, (r-1)$  spanning in  $\mathcal{H}_q = \text{span}\{|q_i\rangle : i = 0, 1, \dots, (r-1)\}$ .

Let  $|\psi_1\rangle = \sum_{i=0}^{r-1} c_i^1 |q_i\rangle$  and  $|\psi_2\rangle$  be two vectors in Hilbert space. Then:

$$|\psi_2\rangle = A|\psi_1\rangle = A \sum_{i=0}^{r-1} c_i^1 |q_i\rangle = \sum_{i=0}^{r-1} c_i^1 A|q_i\rangle \quad (2)$$

$A$  is a matrix that generates transformation of superposed quantum state.  $AA^\dagger = A^\dagger A = I$ , where  $A^\dagger$  is the conjugate transpose of  $A$ .  $A$  is a so-called unitary matrix. This property of  $A$  grants that the transformation  $C_2^T = A \cdot C_1^T$  with  $C_i = [c_0^i, c_1^i, \dots, c_{r-1}^i]$ , ( $i = 1, 2$ ) is a valid one.

The qubits (similar to the bits) can be organized in registers. The content of a register composed of  $g$  (length) qubits can store information using  $2^g$  states from the set  $Q = \{|q_0\rangle, |q_1\rangle, \dots, |q_r\rangle\}$  with  $r = 2^g - 1$ .

A register content can be described by the superposed state vector in a Hilbert space ( $\mathcal{H}$ ) at the computational base:

$$|\psi\rangle = \sum_{k=0}^{r-1} c_k |q_k\rangle \quad (3)$$

with  $c_k, i = 0, \dots, r$  complex numbers from the set  $\mathbb{C}$  fulfilling the relation:  $\sum_{k=0}^r |c_k|^2 = 1$ . These coefficients are denoted amplitudes and they represent the probability distribution of the quantum state. The value  $|c_k|^2$  provides the probability of the quantum process to be in the quantum state  $|q_k\rangle$ . This conception of storing the quantum information based on the quantum state amplitudes (i. e. the coefficients  $c_i$ ) can sustain the opposite behavior manners named *quantum interference*.

Another manner of describing the register content is based on the qubit vectors of the form:

$$V = [|b_0\rangle|b_1\rangle \dots |b_{g-1}\rangle] = [(\alpha_0, \beta_0)(\alpha_1, \beta_1) \dots (\alpha_{g-1}, \beta_{g-1})] \quad (4)$$

While  $|\psi\rangle$  requires  $2^8$  complex coefficients,  $V$  involves only  $2g$  complex coefficients. These coefficients are linked by the relations:

[illegible]

181 The conversion of  $V$  to  $\Psi$  can always be performed, while the reversal (i. e. from  $\Psi$  to  $V$ )  
182 can be done only for some particular (pure) states.

183 *2.2. Quantum Systems versus Classic Dynamic Systems*

Let  $|\psi_x\rangle = \sum_{k=0}^{r-1} c_k^x |q_k\rangle$  be a quantum vector and  $\mathbf{x} = [x_0, x_1, \dots, x_{r-1}]^T$  a vector with real number elements in the classic system theory. The relations between the quantum vector and the classic vector is set in the current approach by  $|c_k^x|^2 = x_k$  for all  $k = 0, 1, \dots, r-1$ . As it can be seen, the values  $x_k$  ( $k = 0, 1, \dots, r-1$ ) correspond to the system probabilities to be in the quantum states  $|q_k\rangle$  ( $k = 0, 1, \dots, r-1$ ). The *conventional position*  $X \in [0, r-1]$  on the circle can be calculated by the formula:  $X = \sum_{k=0}^{r-1} x_k \cdot k$ .

A classic dynamic system can be described by  $\mathbf{x}(\tau+1) = U \cdot \mathbf{x}(\tau)$  with  $\tau = 0, 1, \dots$  the discrete time. If  $U$  is a unitary matrix, the position  $X$  remains on the circle domain. Operations such as permutation, circular positive shift (denoted by  $SH^+$ ) and negative circular shift (denoted by  $SH^-$ ) maintain the relation  $\sum_{k=0}^{r-1} x_k = 1$  and thus  $X$  remains on the circle.

Let  $a_0$  and  $a_1$  be two real numbers that fulfill the relation  $a_0 + a_1 = 1$ . Then  $\mathbf{x}' = a_0 \cdot SH^+(\mathbf{x}) + a_1 \cdot SH^-(\mathbf{x})$  will lead to an  $X'$  positioned on the circle.

197 If  $|\psi_o\rangle = \sum_{k=0}^1 c_k^o |q_k\rangle$  is a Hilbert vector, then  $|\psi_x^o\rangle = |\psi_o\rangle \otimes |\psi_x\rangle$  is a Hilbert vector  
198 too. The classic system obtained by setting  $a_0 = |c_0^o|^2$  and  $a_1 = |c_1^o|^2$  corresponds to a  
199 system that moves on the circle. It can be noticed that  $c_0^o$  and  $c_1^o$  are complex numbers,  
200 while  $a_0$  and  $a_1$  are real numbers.

A quantum system  $|\psi_x(\tau+1)\rangle = A \cdot |\psi_x(\tau)\rangle$  can model an un-oriented walker, while  $\psi_x^o(\tau+1) = A^o \cdot \psi_x^o(\tau)$  can model an oriented one. The un-oriented walker has the state  $|\psi_x\rangle$  equivalent to  $\mathbf{x}$ , while the oriented walker has the state  $|\psi_x^o\rangle$  equivalent to  $(a_0, a_1, \mathbf{x})$ . The matrices  $A$  and  $A^o$  have to be unitary for the walker system to remain in the Hilbert space.

206 Instead of the synthesis of the matrices  $A$  and  $A^0$  for implementing the walker  
207 evolution, it is simpler to use some control coefficients  $(k_0, k_1)$  and the shift operators,  
208 or to use them for changing the walker's orientation, and to continue with the shift  
209 operators.

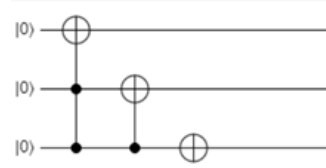
## 210 2.3. Quantum Computation

Unlike the classical computation that uses logical gates, the processing of quantum information is performed by quantum processors composed of quantum logical gates. A quantum logic gate acting on a qubit is a  $2 \times 2$  matrix. For example, the Hadamard (or diffusion) matrix:

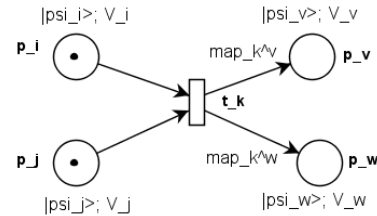
$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad (6)$$

211 acting on the qubit  $|b\rangle = \alpha|0\rangle + \beta|1\rangle$  provides  $|b'\rangle = \frac{1}{\sqrt{2}}(\alpha + \beta)|0\rangle + \frac{1}{\sqrt{2}}(\alpha - \beta)|1\rangle$  that  
 212 verifies the quantum coefficients (i.e. Hilbert) condition.

A single quantum logic gate acts on a qubit while multiple quantum gates composing a *quantum logic circuit* act on a register (vector) of qubits performing an operation of



**Figure 1.** Quantum logic circuit representation.



**Figure 2.** Quantum Petri Net model.

the form  $|\psi'\rangle = A|\psi\rangle$ . Any such transformation of information has to fulfill the quantum coefficient condition that is met if the corresponding matrix  $A$  is unitary.

According to [6], a single qubit quantum gate can be applied to a register of  $r$  qubits on a single qubit of a quantum vector. If the qubit is in the  $k$  position, the full quantum gate matrix  $H$  is described by:

$$A_k = \bigotimes_{j=0}^{r-1} \begin{cases} H, & \text{if } j = k \\ I, & \text{otherwise} \end{cases} \quad (7)$$

where  $I$  is the identity matrix.

For  $g = 3$  qubits ( $|b_0\rangle|b_1\rangle|b_2\rangle$ ) the application of  $H$  on the middle qubit leads to the matrix  $A_1 = I \otimes H \otimes I$  which is a matrix of  $8 \times 8$  size.

Figure 1 represents a quantum logic circuit that acts on a vector composed of 3 qubits performing an increment operation detailed by the AND and exclusive OR operations.

#### 2.4. Quantum Petri Nets

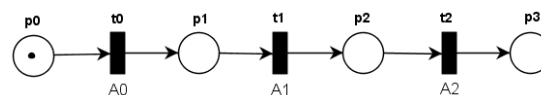
A quantum program involves modifications of the information stored in a set of quantum registers by the quantum gate circuits that link them. This can be modeled by *Quantum Petri Nets* (QPNs) [3]. Figure 2 shows an example of a QPN model that is used for their definition.

Another QPN formal definition and modeling method can be found in [4].

Figure 3 shows an example of a quantum gate circuit that sequentially applies the mappings (i. e. gate operations)  $A_0, A_1, A_2$  to the qubits  $|b_0\rangle, |b_1\rangle$  and  $|b_2\rangle$  respectively performing the operations  $|\psi_3\rangle = A_2 \cdot |\psi_2\rangle = A_2 \cdot A_1 \cdot |\psi_1\rangle = A_2 \cdot A_1 \cdot A_0 \cdot |\psi_0\rangle$ .

For the QPNs (see Figure 3.) the following notations and concepts are used:

- $N = (P, T, F)$  is a net with two kinds of disjoint node sets,
- a finite place set  $P = \{p_1, p_2, \dots, p_m\}, (m \geq 1)$ ,
- a finite transition set  $T = \{t_1, t_2, \dots, t_n\}, (n \geq 1)$ ,
- $F \subseteq P \times T \cup T \times P$  is the flow relation,



**Figure 3.** Quantum Petri Net model of a QLC.



- 237 •  ${}^{\circ}t = \{p \in P | (p, t) \in F\}$  describes the transition  $t$  input place set,
- 238 •  $t^{\circ} = \{p \in P | (t, p) \in F\}$  describes the transition  $t$  output place set.

239 There are two referential systems denoted by  $V$  and  $\Psi$  that store in parallel the  
 240 information in the QPN places. The quantum logic circuits (i. e. the mappings  
 241  $mapV$ ) act on the  $V$  level (i. e. qubit registers) modifying the coefficient values  $V =$   
 242  $[(\alpha_0, \beta_0)(\alpha_1, \beta_1) \dots (\alpha_{g-1}, \beta_{g-1})]$ , while the mappings  $map\Psi$  act at the  $\Psi$  (computational)  
 243 level modifying the amplitudes  $[c_0 c_1 \dots c_{r-1}]$ . For each value  $V$  there is the trans-  
 244 formation (5) denoted by  $\mathcal{T}$  that converts the  $V$  vector in  $|\psi\rangle = \mathcal{T}(V)$  vector. For  
 245 some pure states of  $|\psi\rangle$  the transformation and the revers transformation (conversion)  
 246  $V = \mathcal{T}^{-1}(|\psi\rangle)$  can be defined.

247 Some quantum algorithms use and have defined mapping  $map\Psi$ , even if at the low  
 248 level they are implemented by mappings on quantum logic circuits (QLC). This requires  
 249 the synthesis of QLCs that perform the mappings  $map\Psi$ . Other quantum algorithms  
 250 have defined operations only at the qubit level. The conversion from  $V$  to  $\Psi$  is always  
 251 defined by the transformation of the type  $\mathcal{T}$ .

252 For quantum program verification (by simulation of QPN), the QLC synthesis is  
 253 not compulsory if there are interactions only from  $V$  level to  $\Psi$  level (and never needed  
 254 the reverse transformation  $\mathcal{T}^{-1}$ ).

255 As example, in Figure 8 the transition  $t1$  has defined the mapping  $mapV$ , while the  
 256 rest of the application (transitions) has the mappings of the type  $map\Psi$ . Performing the  
 257 transformation  $\mathcal{T}$  in  $p1$  the vector  $|\psi_1\rangle$  is obtained.

258 Related to QPN states, the following are specified:

- 259 • any place  $p_s \in P$  has assigned a pair of natural numbers  $(g_s, r_s)$ , with  $r_s = 2^{g_s} - 1$   
 260 specifying the dimensions of the tokens (i. e. vectors)  $|\psi_s\rangle$  and  $V_s$  respectively,
- 261 •  $Q = \{|q_0\rangle, |q_1\rangle, \dots, |q_{r-1}\rangle\}$  is the place quantum state set,
- 262 •  $|\psi_s\rangle = \sum_{l=0}^{r-1} c_l^s |q_l\rangle$  is the first part of the token that can be set in a place  $p_s$ ;
- 263 •  $V_s = [(\alpha_0^s, \beta_0^s)(\alpha_1^s, \beta_1^s) \dots (\alpha_{g-1}^s, \beta_{g-1}^s)]$  is the second part of the token set in the place  
 264  $p_s$ ,
- 265 • the marking of a place  $p_s$  is  $QM(p_s) = [|\psi_s\rangle, V_s]$ ,
- 266 • when the token is missing in a place  $p$ , the place marking is  $QM(p) = \Phi$  (i. e. the  
 267 empty set meaning nothing or the lack of information);
- the system quantum superposed state QS is

$$QS = [QM(p_1), QM(p_2), \dots, QM(p_m)] \quad (8)$$

and it is given by

$$QS = [|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_m\rangle] \quad (9)$$

or

$$QS = [V_1, V_2, \dots, V_m] \quad (10)$$

## 268 2.5. Transition admissibility and execution

269 The QPN places can store two kinds of tokens ( $V$  token and  $\Psi$  token) and its  
 270 transitions can execute two kinds of mappings ( $mapV$  and  $map\Psi$ ) depending on the  
 271 available tokens in their input places.

Any output arc  $(t_k, p_v) \in F$  of a transition  $t_k$  has assigned a mapping denoted  
 $map\Psi_k^v(\dots, |\psi_j\rangle, \dots)$ , and a mapping  $mapV_k^v(\dots, V_j, \dots)$  with  $|\psi_j\rangle$  and  $V_j$  tokens in  
 $QM(p_j)$ ,  $p_j \in {}^{\circ}t_k$  that transforms the information stored in its input places (i.e. Hilbert  
 and  $V$  vectors) and sets the new token (i.e.  $|\psi\rangle$  and  $V$  vectors) in its output place  $p_v \in t_k^{\circ}$   
 according to:

$$|\psi_v\rangle = map\Psi_k^v(|\psi_i\rangle, |\psi_j\rangle); p_i, p_j \in {}^{\circ}t_k \quad (11)$$

or its counterpart

$$V_v = mapV_k^v(V_i, V_j); \quad (12)$$

272 When one of them is missing, the formulas (5) are used for transformation.

273 A transition is enabled for the execution of its assigned  $mapV$  and/or  $map\Psi$  mappings  
 274 if and only if it has in its input places the corresponding  $V/\Psi$  tokens respectively.

275 The execution of an enabled transition mapping involves the atomic logical extraction  
 276 of the tokens from its input places and the injection of the tokens in its output places.  
 277 When a  $mapV$  mapping is executed, it is followed by the conversion and set of the  
 278  $|\psi\rangle = \mathcal{T}(V)$  tokens in the output places if the  $map\Psi$  mapping is not available or allowed.

279 An enabled transition  $t_k$  is executed at a moment in the time interval  $(0, d_k)$  with 0  
 280 and  $d_k$  real numbers; where  $d_k$  is a very short estimated (specified) moment of time.

281 The start and the end of a quantum program involve:

- *init* a method that initializes the places with quantum vectors with amplitudes from the matrix  $CS^0$

$$QS^0 = \text{init}(CS^0) \quad (13)$$

282 with  $CS^0$  an environment matrix of QS size and complex elements fulfilling the  
 283 Hilbert space condition;

- *end* a method that stops the quantum process by collapsing the current QS, extracts the information from places (i.e. the final state  $QS^f$ ) and sets it to an environment matrix  $CS^f$

$$CS^f = \text{end}(QS^f) \quad (14)$$

284 where  $CS^f$  is a matrix of  $g \cdot m$  size with the elements in  $\{0, 1\}$ .

## 285 2.6. Definition of QPNs

The definition of QPN is:

$$QPN = (N, D, G, Map, QM^0, \text{init}, \text{end}, QM^f) \quad (15)$$

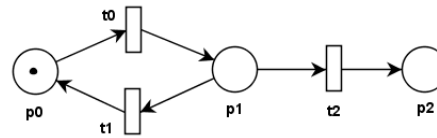
286 where:

- 287 •  $N = (P, T, F)$  is a net;
- 288 •  $D = [d_1, d_2, \dots, d_n]$  is a vector containing the maximum estimated delays assigned to transitions;
- 289 •  $G = [g_1, g_2, \dots, g_m]$  is a vector containing the sizes of the vectors  $(V_i, i = 1, 2, \dots, m)$  set in the corresponding places;
- 290 •  $Map$  is the set of mappings (i.e. pair  $(map\Psi_k^v(), mapV_k^v())$ ) assigned to arcs linking the transitions with places; when one of them is missing, it is denoted by *null*,
- 291 •  $QM^0$  is a matrix with initialized values (i.e. the initial quantum superposed states);
- 292 • *init* is the initialization method;
- 293 • *end* is the stop method;
- 294 •  $QM^f$  is a matrix storing the values of the final quantum superposed state (i.e. the result matrix).

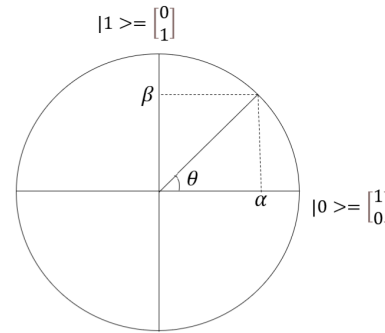
295 There are some differences concerning the QPNs related to classical PN:

- 296 • The same token set in a place can be used for enabling and execution of more than one transition.
- 297 • There are non-reversible transitions (that correspond to non-reversible quantum logic circuit) and reversible transitions (see Figure 5) that correspond to reversible quantum logic gates.
- 298 • Once a non-reversible transition is executed (it extracts the tokens from its input place set) no further transition can be enabled with the extracted tokens.
- 299 • The transition assessment is performed in iterations that have no duration.
- 300 • When some transitions are enabled, they are executed even if the tokens from their input place sets have already disappeared.
- 301 • If more than one transition set tokens concurrently (simultaneously) in a place, this situation leads to conflict and it has to be avoided.





**Figure 4.** QPN model of a while loop.



**Figure 5.** Qubit representation on circle.

### 312 2.7. Analysis and Verification of QPN Models

313 The need of the analysis and the verification of the quantum programs behaviors is  
 314 obviously in the development process as it is known from many procedures. The Petri  
 315 nets can sustain these by some popular methods. In the current approach Petri Nets  
 316 based language and the reachability graphs are used.

#### 317 2.7.1. Petri Net based Language

318 Using the notations: '\*' for sequence, '+' for alternative, '&' for concurrence and '#'  
 319 for closing a loop, the behavior of a PN can be described. For example:

- 320 •  $t_1 * t_2$  describes the sequential execution of the transitions  $t_1$  and  $t_2$ ;
- 321 •  $t_1 + t_2$  describes the alternative for execution the transition  $t_1$  or  $t_2$ ;
- 322 •  $t_1 \& t_2 = t_1 * t_2 + t_2 * t_1$  describes the concurrent execution;
- 323 •  $(t_1 * t_2) \# t_3$  describes a loop  $\sigma = (t_1 * t_2 * t_3) * \sigma$ .

324 Details of their use are provided in [3].

#### 325 2.7.2. Reachability Graphs

326 In [3] were used the reachability graphs that include the states and the transitions  
 327 that lead to them. Some transitions are concurrently executed changing the system states  
 328 simultaneously. Some examples of their use are provided further.

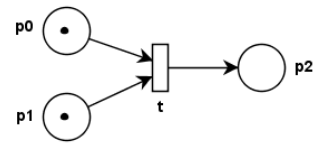
### 329 2.8. QPN Model Examples

#### 330 2.8.1. Qubit rotations and While Loops

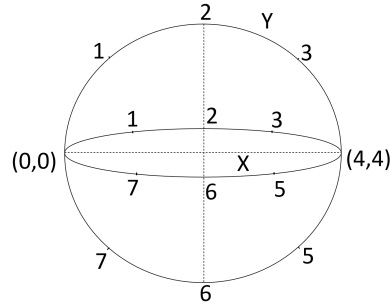
The QPN shown in Figure 4 describes the rotation of the qubit  $|q_0\rangle$  stored in the place  $p_0$  by the mapping assigned to  $t_0$ . The rotation with an angle  $\theta$  can be determined using the circle representation displayed on Figure 5. Supposing that the rotation angle is given by a qubit  $|q\rangle = \alpha|0\rangle + \beta|1\rangle$ , the angle  $\theta$  is given by  $\theta = \arcsin(\beta) = \arccos(\alpha)$ . Performing this calculus offline, the mapping assigned to  $t_0$  that achieves the rotation is:

$$A_1(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \quad (16)$$

331 The repetition of the loop until a specified state is achieved, is a more difficult  
 332 task. In the current proposal the method introduced by [5] is considered to be used. As  
 333 consequence, it is supposed that a loop can be admittedly executed with a specified



**Figure 6.** QPN model of a qubit rotation depending of another one.



**Figure 7.** QDRW movement space.

robustness. The measurement performed at each iteration for predicate condition of exiting the loop diminishes the qubits state with a value smaller than a specified and accepted one.

The QPN example displayed in Figure 6 corresponds to a mapping that rotates the qubit  $|q_o\rangle = \alpha_o|0\rangle + \beta_o|1\rangle$  store in the place  $p0$  with an angle given by the control qubit  $|q_c\rangle = \alpha_c|0\rangle + \beta_c|1\rangle$  stored in the place  $p1$ , resulting the qubit  $|q_r\rangle = \alpha_r|0\rangle + \beta_r|1\rangle$  injected in the place  $p2$ . This requires the synthesis of a QLC that performs the unitary transformation  $(\alpha_r, \beta_r) = \text{map}((\alpha_o, \beta_o), (\alpha_c, \beta_c))$ .

The problem can be extended for the case when the previous places model vectors of qubits. If  $A_1(\theta_0)$  and  $A_1(\theta_1)$  perform the rotations of two independent qubits, the matrix:

$$A_2(\theta_0, \theta_1) = \begin{bmatrix} A_1(\theta_0) & \mathbf{0} \\ \mathbf{0} & A_1(\theta_1) \end{bmatrix} \quad (17)$$

achieves the rotation of quantum vector (i.e. register) of two qubits.

### 2.8.2. Quantum Discrete Random Walker on a Circle

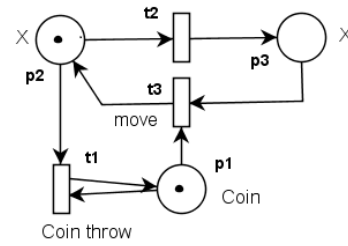
The chosen examples concern the Quantum Discrete Random Walker (QDRW) that moves on a circle or on a sphere (see Figure 7). They can be oriented or un-oriented. The specified 8 discrete positions on the circle can be coded with three qubits composing a vector  $V = [(\alpha_0, \beta_0)(\alpha_1, \beta_1)(\alpha_2, \beta_2)]$  or by referring to the quantum states for each position  $|\psi_X\rangle = \sum_{k=0}^7 c_k^x |q_k\rangle$ .

The usual walker random moves are decided by throwing a coin that can be modeled by Hadamard matrix (eq. 6).

The un-oriented QDRW model on a circle can be described in the Hilbert space  $\mathcal{H} = \mathcal{H}_X^8$  by the equation:

$$|\psi_x(\tau + 1)\rangle = SH(H \otimes I \cdot |\psi_x(\tau)\rangle) \quad (18)$$

where  $SH(\dots)$  denotes the shift operator applied to its argument and  $\tau$  is the clock tick.  $SH$  moves the walker to the right if the decision operator (i.e. the coin) provides "+" and to the left if the result is negative.  $SH$  is implemented by a permutation matrix (that has only '1' on each column or line) that performs the walker evolution.  $SH^+$



**Figure 8.** QPN of un-oriented QDRW on a circle.

358 achieves a positive move (i.e increase the position), while  $SH^-$  determines a negative  
359 move (decreasing the position value).

360 Denoting by  $q = \frac{1}{\sqrt{2}}$ , the application of  $H$  to a qubit provides:

$$H \cdot |q_0\rangle = q|0\rangle + q|1\rangle$$

$$H \cdot |q_1\rangle = q|0\rangle - q|1\rangle$$

361 Denoting the coin state with  $K(\tau) = [k_0(\tau), k_1(\tau)]^T$ , that leads to the coin evolution  
362 relation  $[k_0(\tau+1), k_1(\tau+1)]^T = H \cdot [k_0(\tau), k_1(\tau)]^T$ .

363 The repeated throwing of the coin provides the sequence:  $K(0) = [k_0(0), k_1(0)]^T =$   
364  $[1, 0]^T$ ,  $K(1) = [q, q]^T, \dots$ ;  $K(j) = [q, q]^T$  if  $j$  is odd and  $K(j) = [2q^2, 0]^T$  if  $j$  is even.

365 Figure 8 shows the QPN model of the un-oriented QDRW on a circle.

366 The model executes the sequence:  $\sigma = (t1 \& t2) * t3 * \sigma$ . The implementation requires  
367 three qubits for walker's position and one qubit for the coin.

368 The mappings assigned to transitions are:

- 369 •  $t1: K(\tau+1) = H \cdot K(\tau)$
- 370 •  $t2: X'(\tau+1) = X(\tau)$
- 371 •  $t3: X(\tau+1) = SH^+(k_0(\tau+1)X'(\tau+1)) + SH^-(k_1(\tau+1)X'(\tau+1))$

372 Figure 9 shows the evolution of the probabilities of the walker to be in each position.  
373 Horizontal axis  $X$  corresponds to positions, the vertical axis  $Z$  displays the probabilities  
374 and the elevated axis shows the ticks.

375 The probability of the QDRW to be in the position  $x = k$ , ( $0 \leq k \leq 7$ ) at a moment  
376  $\tau$  is  $\pi_k(\tau) = |c_k(\tau)|^2$ .

377 The probability that QDRW follows a trajectory described by the sequence  $\sigma =$   
378  $i * j * k$  is  $\Pi_\sigma = \pi_i(\tau) * \pi_j(\tau+1) * \pi_k(\tau+2)$ .

379 The probability that QDRW hits a target  $x = k$  during a discrete time interval  
380  $\theta = [a, b]$  is given by  $\Pi_{x=k;\theta} = \sum_{\tau=a}^b |c_k(\tau)|^2$ .

The oriented Quantum Discrete Random Walker (QDRW) QPN model is represented in Figure 10. Its state  $W = (O, X)$  is described in the Hilbert space  $\mathcal{H} = \mathcal{H}_K \otimes \mathcal{H}_O \otimes \mathcal{H}_X^8$  by the equation:

$$|\psi_w(\tau)\rangle = (\alpha(\tau)|0\rangle + \beta(\tau)|1\rangle) \otimes \sum_{k=0}^7 c_k(\tau)|q_k\rangle \quad (19)$$

381 with  $\alpha(\tau)$  and  $\beta(\tau)$  the complex coefficients needed for orientation fulfilling the Hilbert  
382 condition, and  $c_k, i = 0, \dots, r$  complex numbers from the set  $\mathbb{C}$  fulfilling the relation:  
383  $\sum_{k=0}^r (|\alpha(\tau)c_k(\tau)|^2 + |\beta(\tau)c_k(\tau)|^2) = 1$  in any moment  $\tau$ .

384 The place  $p2$  models the QDRW oriented toward increasing the position (i.e. state  
385  $X_0$ , while the place  $p5$  corresponds to its orientation toward decreasing the position  
386 (i. e.  $X_1$ ). Throwing the coin (i. e. applying the operator  $H$ ) determines the change of  
387 orientations that affect the moves performed by shift operators. The QDRW dynamics is  
388 achieved by the mappings assigned to transitions.

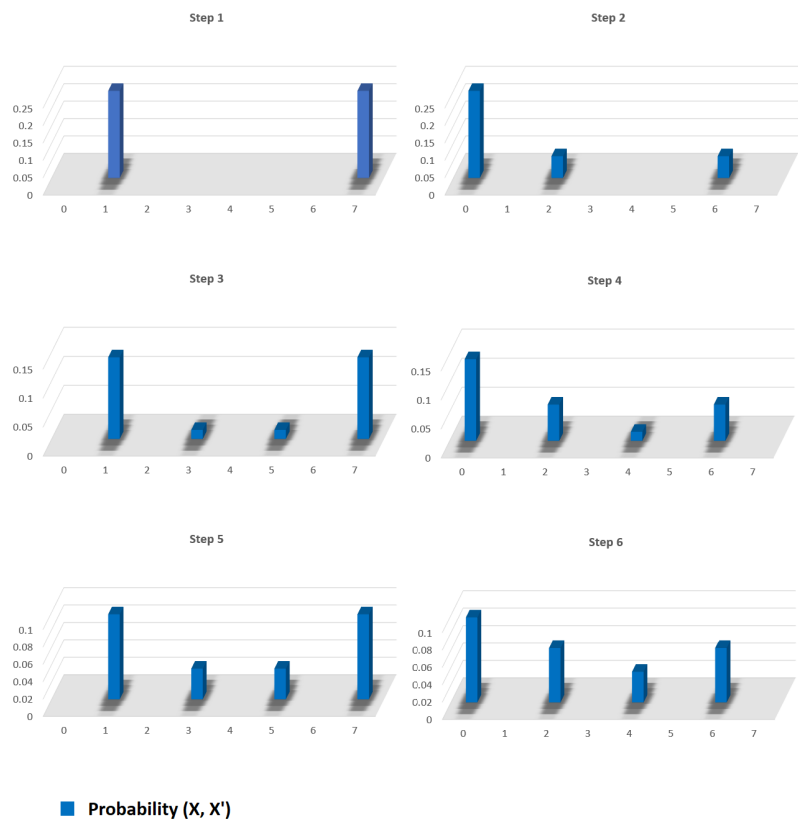


Figure 9. Probabilities of un-oriented QDRW on a circle.

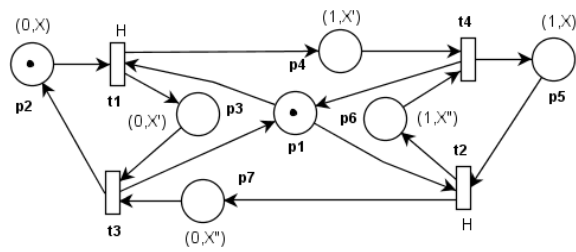
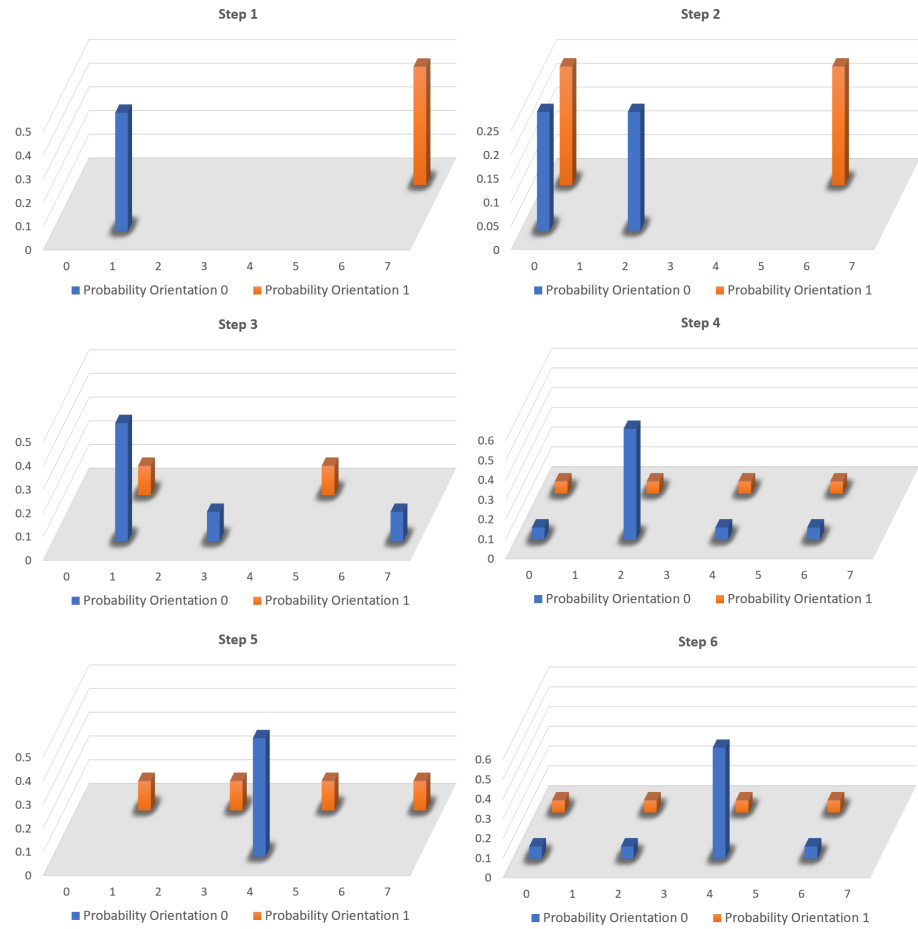


Figure 10. QPN of oriented QDRW on a circle.



**Figure 11.** Probabilities of oriented QDRW on a circle.

The model executes the sequence:  $\sigma = ((t1\&t2) * (t3\&t4))^k$ . The implementation requires three qubits for walker's position, one for orientation and another one for the coin.

The mappings assigned to transitions are:

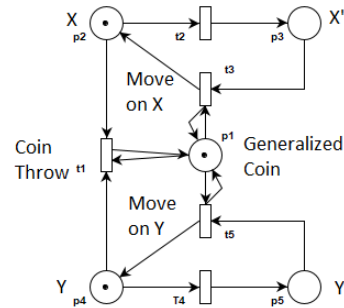
- $t_{1,3} : X'_0(\tau + 1) = \varrho \cdot X_0(\tau)$
- $t_{1,4} : X'_1(\tau + 1) = \varrho \cdot X_0(\tau)$
- $t_{2,6} : X''_1(\tau + 1) = -\varrho \cdot X_1(\tau)$
- $t_{2,7} : X''_0(\tau + 1) = \varrho \cdot X_1(\tau)$
- $t_3 : X_0(\tau + 1) = SH^+(X'_0(\tau + 1) + X''_0(\tau + 1))$
- $t_4 : X_1(\tau + 1) = SH^-(X'_1(\tau + 1) + X''_1(\tau + 1))$

The probability that QDRW be in a specified position at a time moment is given by the sum of the values stored in the places  $p2$  and  $p5$ . These probabilities are displayed in Figure 11.

For the QPN analysis of oriented QDRW on a circle its reachability graph is constructed as can be seen in Table 1. Instead of the quantum state, QRS is used here.

y7								
y6								
y5								
y4								
y3								
y2								
y1								
y0	(1,1)							
	x0	x1	x2	x3	x4	x5	x6	x7

**Figure 12.** Sphere surface deployment on two dimensions.



**Figure 13.** QPN model of un-oriented QDRW on a sphere.

**Table 1.** Reachability graph of QPN from Figure 10.

$p_1$	$p_2$	$p_3$	$p_4$	$p_5$	$p_6$	$p_7$	Transition
*	$X_0$	$\phi$	$\phi$	$\phi$	$\phi$	$\phi$	$t_1$
$\phi$	$\phi$	$X'_0$	$X'_1$	$\phi$	$\phi$	$\phi$	$t_3 \& t_4$
*	$X_0$	$\phi$	$\phi$	$X_1$	$\phi$	$\phi$	$t_1 \& t_2$
$\phi$	$\phi$	$X'_0$	$X'_1$	$\phi$	$X''_1$	$X''_0$	$t_3 \& t_4$
...	...	...	...	...	...	...	...

### 2.8.3. Quantum Random Walker on a Sphere

Figure 12 shows the surface of the sphere displayed on two dimensions. The walker initial position is  $(x_0, y_0)$ .

The system composed of *un-oriented QDRW moving on a sphere* and the coins that determine its move is described in the Hilbert space:

$$\mathcal{H} = \mathcal{H}_K^4 \otimes \mathcal{H}_X^8 \otimes \mathcal{H}_Y^8 \quad (20)$$

with the vectors  $|\psi_X\rangle = \sum_{k=0}^7 c_k^x \cdot |q_k\rangle$  and  $|\psi_Y\rangle = \sum_{k=0}^7 c_k^y \cdot |q_k\rangle$  describing the position on axes X and Y respectively. The generalized coin vector is:  $|\psi_K\rangle = \sum_{k=0}^3 c_k^K \cdot |q_k\rangle$  provided by the matrix  $G = H \otimes I$  that leads to:

$$G = \varrho \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \quad (21)$$

For the *un-oriented QDRW* on the sphere the QPN model is conceived and displayed in Figure 13.

The places  $p_2$  and  $p_4$  store the position on X and Y respectively, while the place  $p_1$  stores the generalized coin K value. The initial values are:  $K(0) = [\varrho, 0, \varrho, 0]^T$ ,



411  $X(0) = [(q, q), (0, 0), (0, 0), (0, 0)]^T$  and  $Y = [(q, q), (0, 0), (0, 0), (0, 0)]^T$ . The transitions  
412 have assigned the mappings:

- 413 •  $t_1 : K(\tau + 1) = G \cdot K(\tau)$
- 414 •  $t_2 : X'(\tau) = X(\tau)$
- 415 •  $t_3 : X(\tau + 1) = SH^+(c_0^K \cdot X'(\tau)) + SH^-(c_1^K(\tau) \cdot X'(\tau))$
- 416 •  $t_4 : Y'(\tau) = Y(\tau)$
- 417 •  $t_5 : Y(\tau + 1) = SH^+(c_2^K \cdot Y'(\tau)) - SH^-(c_3^K \cdot Y'(\tau))$

418 The model executes the sequence:  $\sigma = ((t_1 \& t_2 \& t_4) * (t_3 \& t_5))^k$ . The implementa-  
419 tion requires three qubits for X walker's position, another three qubits for Y and two  
420 qubits for the generalized coin.

421 For the QPN analysis of un-oriented QDRW on a sphere its reachability graph is  
422 constructed as can be seen in Table 2.

**Table 2.** Reachability graph of QPN from Figure 13.

$p_1$	$p_2$	$p_3$	$p_4$	$p_5$	Transition
$K$	$X$	$\phi$	$Y$	$\phi$	$t_1 \& t_2 \& t_4$
$\phi$	$\phi$	$X'$	$\phi$	$Y'$	$t_3 \& t_5$
$K$	$X$	$\phi$	$Y$	$\phi$	$t_1 \& t_2 \& t_4$
$\phi$	$\phi$	$X'_0$	$\phi$	$Y'$	$t_3 \& t_5$
...	...	...	...	...	...

423 The probability of the un-oriented QDRW to be at the moment  $\tau$  in the position  
424  $X = x_i$  and  $Y = y_j$  is given by the coefficients of the vectors  $\psi_X(\tau)$  and  $\psi_Y(\tau)$  at the  
425 moment  $\tau$ , i.e.  $\pi_X(\tau; i) = (c_i^X(\tau))^2$ ;  $\pi_Y(\tau; j) = (c_j^Y(\tau))^2$ . The probability of the walker  
426 to be in a position  $(i, j)$  at a moment  $\tau$  is given by  $\pi_{xy}(\tau; i, j) = \pi_X(\tau; i) \cdot \pi_Y(\tau; j) =$   
427  $(c_i^X(\tau; i))^2 \cdot (c_j^Y(\tau))^2$ . The needed information required for these calculations is available  
428 in the places  $p_2$  and  $p_4$ .

429 Figure 14 displays the simulation results of the un-oriented QDRW probabilities to  
430 be in different positions at different steps.

The oriented QDRW on a sphere is moving in the Hilbert space:

$$\mathcal{H} = \mathcal{H}_O^4 \otimes \mathcal{H}_X^8 \otimes \mathcal{H}_Y^8 \quad (22)$$

431 with the vectors  $|\psi_X\rangle = \sum_{k=0}^7 c_k^x \cdot |q_k\rangle$  and  $|\psi_Y\rangle = \sum_{k=0}^7 c_k^y \cdot |q_k\rangle$  describing the position  
432 on axes X and Y respectively. The walker state is extended with its orientation on the both  
433 axes:  $|\psi_X^O\rangle = (\alpha_0|0\rangle + \beta_0|1\rangle) \otimes \sum_{k=0}^7 c_k^x \cdot |q_k\rangle$  and  $|\psi_Y^O\rangle = (\alpha_1|0\rangle + \beta_1|1\rangle) \otimes \sum_{k=0}^7 c_k^y \cdot |q_k\rangle$ .

The generalized coin vector is:  $|\psi_K\rangle = \sum_{k=0}^3 c_k^C \cdot |q_k\rangle$  provided by the matrix G  
(according to J. Kempe [19]):

$$G = \frac{1}{2} \begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix} \quad (23)$$

The oriented QDRW movements are given by the formula:

$$[|\psi_X^O(\tau + 1)\rangle, |\psi_Y^O(\tau + 1)\rangle]^T = SH(G \cdot [|\psi_X^O(\tau)\rangle, |\psi_Y^O(\tau)\rangle]^T) \quad (24)$$

434 For this the QPN model is conceived and displayed in Figure 15. The places  $p_0, p_1, p_2$   
435 and  $p_3$  model walkers states  $((X^0, Y^0), (X^1, Y^1), (X^2, Y^2), (X^3, Y^3))$  oriented to the right,  
436 left, up and down respectively.

437 The place meanings are displayed in Table 3. The initial state is:  $X^0 = Y^0 =$   
438  $[(q, q), (0, 0), (0, 0), (0, 0), (0, 0), (0, 0), (0, 0), (0, 0)]$ .

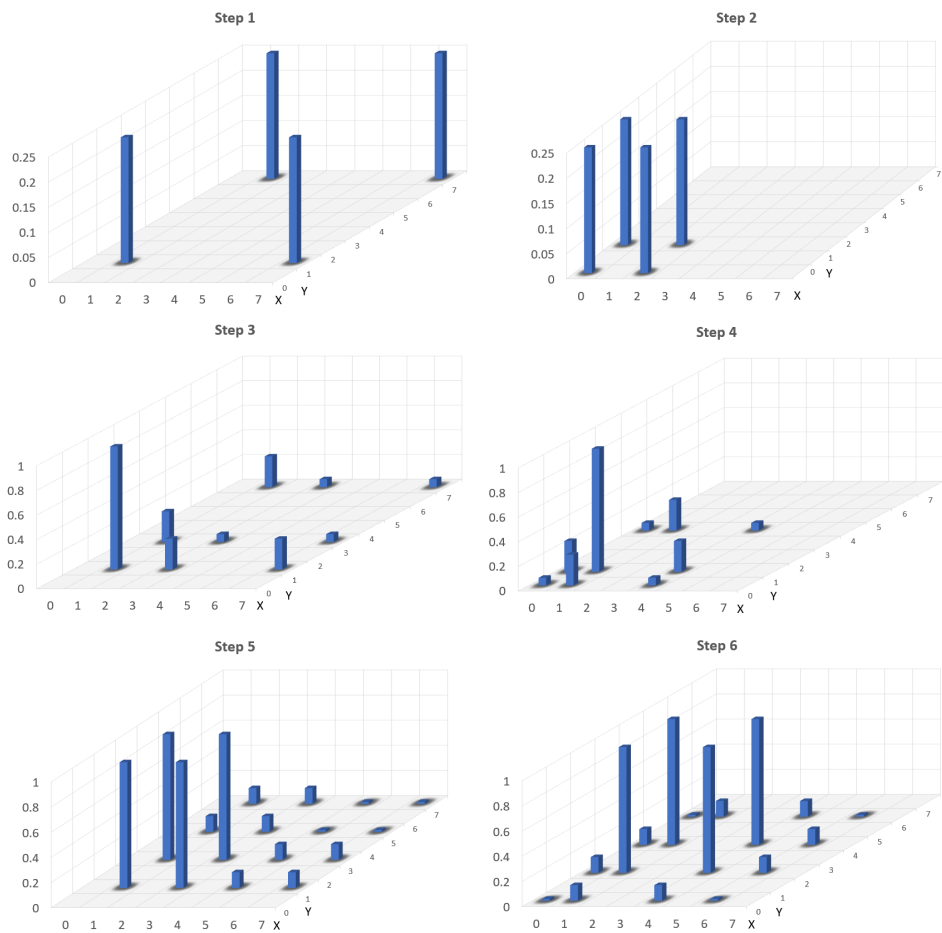


Figure 14. Probability representation of un-oriented QDRW moves on a sphere.

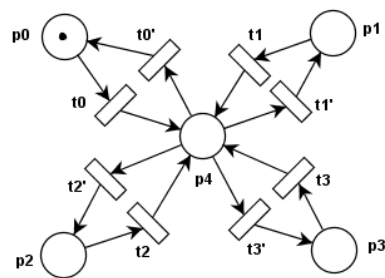


Figure 15. QPN model of oriented QDRW on a sphere.

Table 3. Place meanings of QPN from Figure 15.

$p0$	$p1$	$p2$	$p3$	Place Array $p4$
$(X^0, Y^0)$	$(X^1, Y^1)$	$(X^2, Y^2)$	$(X^3, Y^3)$	$(X_{00}, Y_{00}).(X_{01}, Y_{01}), \dots, (X_{33}, Y_{33})$

**Table 4.** Reachability graph of QPN from Figure 15.

$p0$	$p1$	$p2$	$p3$	$p4$	Transition
$(X^0, Y^0)$	$\phi$	$\phi$	$\phi$	$\phi$	$t0$
$\phi$	$\phi$	$\phi$	$\phi$	$(X_{00}, Y_{00}) \cdots (X_{03}, Y_{03})$	$t0' \& t1' \& t2' \& t3'$
$(X^0, Y^0)$	$(X^1, Y^1)$	$(X^2, Y^2)$	$(X^3, Y^3)$	$\phi$	$t0 \& t1 \& t2 \& t3$
$\phi$	$\phi$	$\phi$	$\phi$	$(X_{00}, Y_{00}) \cdots (X_{33}, Y_{33})$	$t0' \& t1' \& t2' \& t3'$
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$

The model executes the sequence:  $\sigma = t0 * ((t0' \& t1' \& t2' \& t3') * (t0 \& t1 \& t2 \& t3))^k$ .  
 The implementation requires three qubits for X walker's position, another three qubits Y and two qubits for the walker orientations on X and Y.

The mappings assigned to transitions are:

- $t0 : X_{00} = -\frac{1}{2}X^0; Y_{00} = -\frac{1}{2}Y^0; X_{01} = \frac{1}{2}X^0; Y_{01} = \frac{1}{2}Y^0; \dots; X_{03} = \frac{1}{2}X^0; Y_{03} = \frac{1}{2}Y^0;$
- $t1 : X_{10} = \frac{1}{2}X^1; Y_{10} = \frac{1}{2}Y^1; X_{11} = -\frac{1}{2}X^1; Y_{11} = -\frac{1}{2}Y^1; \dots; X_{13} = \frac{1}{2}X^1; Y_{13} = \frac{1}{2}Y^0;$
- $t2 : X_{20} = \frac{1}{2}X^2; Y_{20} = \frac{1}{2}Y^2; X_{21} = \frac{1}{2}X^2; Y_{21} = \frac{1}{2}Y^2; \dots; X_{23} = \frac{1}{2}X^2; Y_{23} = \frac{1}{2}Y^2;$
- $t3 : X_{30} = \frac{1}{2}X^3; Y_{30} = \frac{1}{2}Y^3; X_{31} = \frac{1}{2}X^3; Y_{31} = \frac{1}{2}Y^3; \dots; X_{33} = -\frac{1}{2}X^3; Y_{33} = -\frac{1}{2}Y^3;$
- $t0' : X^0 = SH^+(X_{00} + X_{10} + X_{20} + X_{30}); Y^0 = SH^+(Y_{00} + Y_{10} + Y_{20} + Y_{30});$
- $t1' : X^1 = SH^-(X_{01} + X_{11} + X_{21} + X_{31}); Y^1 = SH^+(Y_{01} + Y_{11} + Y_{21} + Y_{31});$
- $t2' : X^2 = SH^+(X_{02} + X_{12} + X_{22} + X_{32}); Y^2 = SH^-(Y_{02} + Y_{12} + Y_{22} + Y_{32});$
- $t3' : X^3 = SH^-(X_{03} + X_{13} + X_{23} + X_{33}); Y^3 = SH^-(Y_{03} + Y_{13} + Y_{23} + Y_{33});$

For the QPN analysis of oriented QDRW on a sphere its reachability graph is constructed and displayed in Table 4.

The probability of the oriented QDRW to be at the moment  $\tau$  in the position  $X = x_i$  and  $Y = y_j$  is given by the coefficients of the vectors  $\psi_X(\tau)$  and  $\psi_Y(\tau)$  at the moment  $\tau$ , i.e.  $\pi_X(\tau; i) = (c_i^X(\tau))^2; \pi_Y(\tau; j) = (c_j^Y(\tau))^2$ . The needed information required for these calculations is stored in the places  $p0, p1, p2$  and  $p3$ . They can be seen in Figure 16.

## 2.9. Quantum Discrete Controlled Walker (QDCW)

The previous oriented walker's randomness (given by the generalized coin) is replaced by a matrix denoted by  $\Gamma$  that influences its move direction. The QDCW move equation becomes:

$$[|\psi_X^O(\tau+1)\rangle, |\psi_Y^O(\tau+1)\rangle] = SH(G \cdot \Gamma(\tau)[|\psi_X^O(\tau)\rangle, |\psi_Y^O(\tau)\rangle]) \quad (25)$$

with

$$\Gamma(\tau) = A(\theta_1, \theta_2) \quad (26)$$

and  $G$  the previous diffusion matrix. The angles  $\theta_1$  and  $\theta_2$  determine the move directions. Again, the shift operator  $SH$  determines the QDCW moves toward these angles.

The control problem consists of the application of  $\Gamma$  that leads the QDCW from a given initial state (i.e. position and orientation) to some specified target points or region.

## 2.10. Classic and Quantum Computers Connection

The quantum algorithms are not executed independently, but in collaboration with classic implemented algorithms. Figure 17 shows a composition of an OETPN model that interacts with a QPN model. OETPN receives demands from operator through the classic place  $cp2$  and interacts with QPN through the interface (classic-quantum place)  $cqp$ . This provides the information used for the first steps of the quantum program. OETPN receives the quantum computation results through the interface (quantum-classic place)  $qcp$ .

According to [34] a qubit  $|x\rangle = \alpha|0\rangle + \beta|1\rangle$  observation or measurement can be modeled by the wave function collapse as:

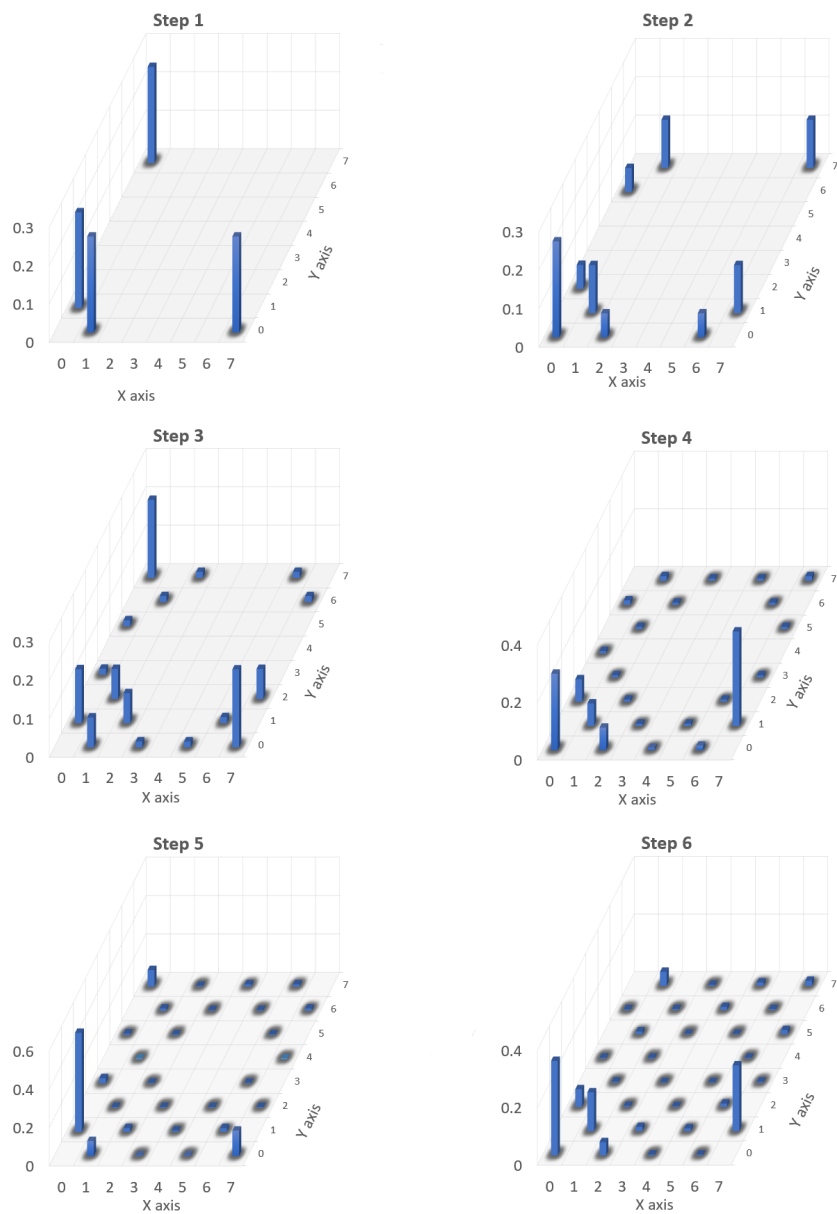


Figure 16. Probability representation of oriented QDRW moves on a sphere.

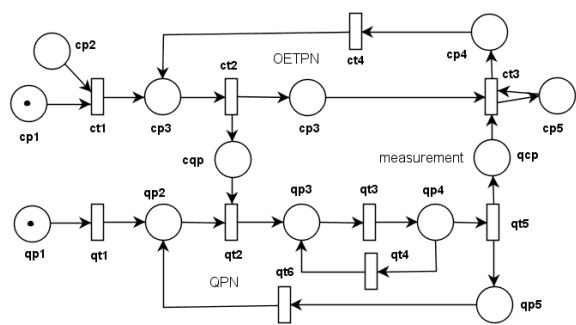


Figure 17. Classic-quantum application structure.

$$\begin{cases} x = 0, & \text{if } |\alpha|^2 \leq pr(x'), \\ x = 1, & \text{if } |\alpha|^2 > pr(x'), \end{cases} \quad (27)$$

where  $pr(x')$  is a random number in the range  $[0, 1)$  used for the assessing of  $x$ .

QPN is initialized by the transition  $qt1$  in the pure state  $|00 \dots 0\rangle$  that is switched by  $qt2$  in the desired initial state  $V$  or  $|\psi\rangle$  state in  $qp3$  using the information provided by  $cqp$ . The mapping(s) of  $qt3$  applies the QLC operations. If the exit condition is not fulfilled, the quantum calculations are repeated after the reaching of the  $qp3$  inserted by the transition  $qt4$ . When the exit condition is reached, the transition  $qt5$  sets the measured value of  $qp4$  by collapsing on specified axis.

Approximately  $1/\epsilon^2$  measurements are required to get the results with the precision  $\epsilon$ . This means to repeat the quantum process with the same initialization values. OETPN can request to repeat the QPN execution by reloading the initial condition, until the expected statistical results are obtained.

The QPN places do not necessarily represent independently the quantum processor qubits that are described by the entire QPN marking. The QPN places describe the quantum program state. All the transitions' mappings are implemented at the lower level by QLCs.

### 2.11. Quantum Evolutionary Systems (QES)

The extension of classical ES to Quantum Evolutionary Systems (QES) concerns the replacing of the genes of classical genomes with qubits. This makes possible the description of an infinite number of individuals in the same instantiation of the model. The classical genetic operators have to be adapted to the new form of information encryption.

The individual evaluation, which in the classical computation requires the separate simulation of each of them, can be performed simultaneously. The read of evaluations performed with different parameters can extract the information for individual selection and further on for their improvement.

Quantum control is an effective tool to drive the quantum system to a given target state and thus manipulate the dynamics of a quantum system. [Zeng(2020)] [59]; The center of the first control strategy is to control a multilevel system from an initial state to a given target state. This can solve problems related to quantum control strategies based on supervised machine learning to suppress the quantum noise in an open quantum system.

Quantum approach can be used in GA by:

- Quantum Inspired Genetic Algorithms (QIGA) where the simulation and improvement are implemented on classical computers;
- Hybrid Classic Quantum GA (HCQGA) where the simulations are performed by QC, but the improvements are determined by task implemented on classical computer;
- CQGA (Complete Quantum Genetic Algorithm) where the individual simulations and improvements are performed by tasks implemented completely on QC.

### 2.12. Quantum Genetic Algorithms

Genetic Algorithms contain:

- Genome specification that is followed by this template filling obtaining the genotypes that contain the necessary information used for individual construction.
- Individual evaluation that consists of modeling the individual behaviors and assessing their performances.
- Individual selection for reproduction.
- The individual improvements are performed randomly based on the previous generation performance and using some genetic operators.

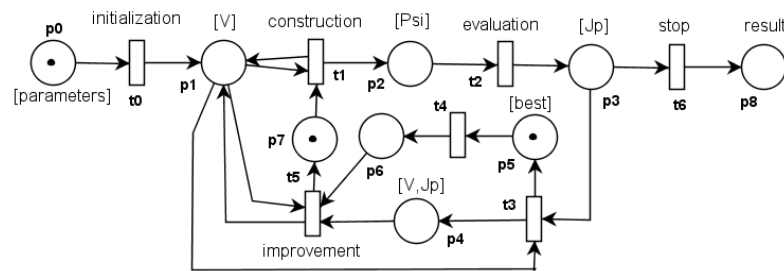


Figure 18. OETPN model of an evolutionary process.

- The stopping criteria use either a number of tested generations, the reaching of performances over a desired threshold, or just the execution is exceeding a specified duration or a specified number of generations without relevant improvements,

Figure 18 shows the evolutionary process performed by a GA. It executes the sequence  $\sigma = t0 * (((t1 * t2) \& t4) \# (t3 * t5))^K * t6$  where  $K$  represents the number of iterations performed until the result is obtained.

Generally, the ESs need to properly solve the evaluations of individuals and their improvement. Both of them should be adapted to the problems otherwise the targets are not reached. Due to the problem complexities there are no clear and proved rules for the general construction of fitness functions and individual evolution operators. There are two main approaches for individual evolution (i. e. improvement) of QGAs: one uses only the mutation and the other uses the crossover before performing the mutation. The first approach uses the best individual from the previous generation as target for random genotype improvement, while the second selects the individuals for evolution according to their performances and randomly interchanges the two individual genotypes.

QGA achieves the solution using a set of genetic operators as can be found in the above mentioned references. For example, in [35] the authors propose a QGA implementation that does not need the crossover involving two individuals. The justification is that all the individuals are simulated simultaneously. More recently, [64] includes and justifies the use of crossover.

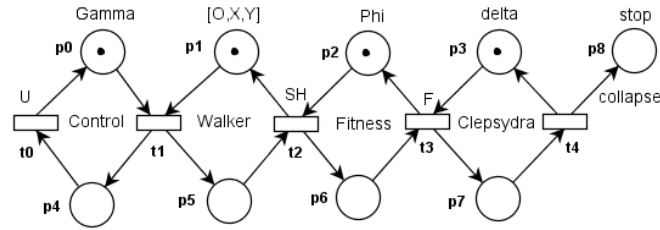
The current approach concerns the control of the Quantum Discrete Walker with the model shown in Figure 15. The individuals of GA determine the mappings assigned to transitions  $t0, t1, t2, t3, t'0, t'1, t'2$ , and  $t'3$ . The Classic GA (CGA) problem usually involves the finding in each intersection (node and/or time) of the walker directions such that it reaches the targets avoiding the traps. Due to the fact that the walker can start from different initial points, the search should be repeated from all of them.

For the QDCW, the problem can be defined in two manners: one solves only the change of direction and the other performs the move length (i.e.  $0, 1, 2, \dots$ ) in the chosen direction.

The efficiency of QGA is significantly better than the conventional genetic algorithm [53]. Classic Genetic Algorithm (CGA) has to execute (simulate) many individuals for their assessment one by one. QC (quantum computing) has the advantage that it can simulate simultaneously a large number of individuals. QC uses quantum variables that can cover by superposition the entire search domain. QGAs (Quantum Genetic Algorithms) have to represent the individuals by quantum vectors. The individual modifications fulfill the Hilbert condition by using mappings involving unitary matrices.

The transition  $t0$  of the model shown in Figure 18 creates in the place  $p1$  the genotypes pool using the initial information stored in the place  $p0$ . The genotype  $V$  is used for the construction of the individual  $\psi$ . For the walker control problem the solution is obtained by replacing the previous  $G$  matrix (eq. 21) with a unitary





**Figure 19.** Quantum individual evaluation.

matrix  $\Gamma = [\gamma_{j,k}]_{j,k=0,1,2,3}$  that acts on the vectors in the space  $\mathcal{H}^2$ . The genes are  $|\gamma_0\rangle = \alpha_0|q_0\rangle + \beta_0|q_1\rangle$  and  $|\gamma_1\rangle = \alpha_1|q_0\rangle + \beta_1|q_1\rangle$  that, for implementation reasons, are changed in the vector  $V_j = [(\alpha_0^j, \beta_0^j), (\alpha_1^j, \beta_1^j)]$  describing the quantum individual genotype.

The execution of the mapping assigned to transition  $t2$  evaluates the individuals using the model displayed in Figure 15. The walkers described by  $[\psi^o, \psi^x, \psi^y]$  are equally initialized  $V_0^w = [(q, q) \cdots (q, q)]$  to occupy the entire walker's space:

$$\mathcal{H} = \mathcal{H}_O^4 \otimes \mathcal{H}_X^8 \otimes \mathcal{H}_Y^8 \quad (28)$$

The individual performances are set in the place  $p3$ . The transition  $t3$  selects the individuals for evolution setting them in  $p4$ , linking their genotypes with the performances. For improvement, the best individuals from the previous generation are stored in  $p5$ . The transition  $t5$  performs the individual improvement (i.e. population evolution). The evolution continues until a stop condition is fulfilled and then the transition  $t6$  is executed providing the final results in the place  $p8$ .

In conclusion, all the possible initial states of the controlled system are evaluated simultaneously based on the walkers superposition. The transitions  $t1, t2, t3$  and  $t5$  can perform their activities in parallel for the current population.

Problems of optimal control of the QDCW can be defined in two manners. One consists of application of control signals at each tick for direction modification and the other one involves the syntheses of an environment that leads to a kind of deflectors set in each intersection. The deflectors direct the QDCW towards the desired targets avoiding the undesired traps. The current approach concerns the first manner.

The QPN model of the QDCW that solves the first approach is shown in Figure 19. As can be seen, the parallel simulations of QDCW, the controller (replacing in each moment of time the former  $\Gamma$ ) and the individual evaluation (i. e. fitness) is governed by the Clepsydra ticks that will stop the execution when the experiment duration expires.

QDCW can discretely move on a sphere with the above presented structure. It has to reach some target points  $T_g = \{(x_g^a, y_g^a), (x_g^b, y_g^b), \dots\}$  avoiding some trap points  $T_p = \{(x_p^a, y_p^a), (x_p^b, y_p^b), \dots\}$ .

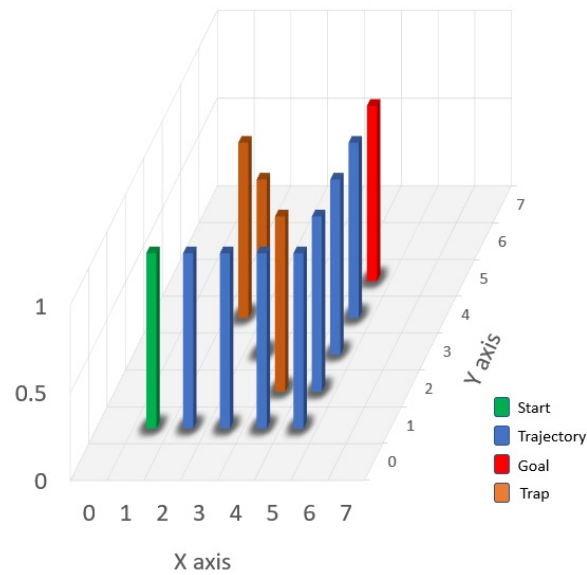
Figure 20 shows the QDCW problem with initial walker state  $(1, 1)$ ,  $T_g = \{(5, 5)\}$  and  $T_p = \{(2, 4), (3, 3), (4, 2)\}$ . The sequence  $0 * 1 * 2 * 3 * 4 * 5 * 6 * 7$  represents an obtained (by CGA) optimal trajectory.

The walker state is described by superposition of the composed vectors

$$[|\psi_o(\tau)\rangle, |\psi_x(\tau)\rangle, |\psi_y(\tau)\rangle] \quad (29)$$

QDCW move for 12 clock ticks is represented by the sequence:

$$\sigma = [|\psi_o(0)\rangle, |\psi_x(0)\rangle, |\psi_y(0)\rangle] * [|\psi_o(1)\rangle, |\psi_x(1)\rangle, |\psi_y(1)\rangle] * \dots * [|\psi_o(11)\rangle, |\psi_x(11)\rangle, |\psi_y(11)\rangle] \quad (30)$$



**Figure 20.** Representation of the targets and traps of the QDCW problem solved by a classic GA.

#### 588 2.12.1. Fitness Functions

For the classic GA an efficient *fitness function* is constructed based on assessing the trajectory cost on each point. When QDCW reaches a point  $(i, j)$  with the probability  $\pi_{ij}$ , the cost to be in that position is:

$$Cost(i, j, \tau) = \begin{cases} 20 \cdot \pi_{ij}, & \text{if } (i, j) \in T_g, \\ -20 \cdot \pi_{ij}, & \text{if } (i, j) \in T_p, \\ \pi_{ij}, & \text{otherwise.} \end{cases} \quad (31)$$

The cost of the QDCW at a moment of time  $\tau$  is:

$$Cost(|\psi_x(\tau)\rangle, |\psi_y(\tau), \tau\rangle) = \sum_{0 \leq i \leq 7} \sum_{0 \leq j \leq 7} Cost(i, j, \tau) \quad (32)$$

The move performance is assessed with the formula:

$$J_p = \sum_{\substack{\exists \tau \leq 15; [q_k^X, q_k^Y] \in T_g; |c_k^X(\tau)|^2 \geq \eta; |c_k^Y(\tau)|^2 \geq \eta; \\ \forall [|\psi_o(\tau)\rangle, |\psi_x(\tau)\rangle, |\psi_y(\tau)\rangle] \in \sigma}} Cost(|\psi_x(\tau)\rangle, |\psi_y(\tau), \tau\rangle) \quad (33)$$

589 with  $\eta$  a specified real value considered acceptable for walker to be in a target point.

As a consequence, if the sequence  $\sigma$  includes points  $[|\psi_x(\tau_i)\rangle, |\psi_y(\tau_i)\rangle] \in T_g$  and  $[|\psi_x(\tau_i)\rangle, |\psi_y(\tau_j)\rangle] \in T_p$  such that  $\tau_i < \tau_j$  (i.e.  $\tau_i$  is precedent to  $\tau_j$ ) then

$$Cost([|\psi_x(\tau_i)\rangle, |\psi_y(\tau_i)\rangle]) = 0. \quad (34)$$

590 More over, when the walker hits a target point with a probability greater than  $\eta$  its move  
591 is not assessed further.

592 For a quantum approach of QGA the current research used the following *quantum*  
593 *fitness function*. Let  $\psi_{xy} = |\psi_x\rangle \otimes |\psi_y\rangle$  be the composed vector providing the information  
594 related to the walker's position (i.e. the amplitude to be there) and  $\Psi_{xy} = |\psi_{xy}\rangle\langle\psi_{xy}|$   
595 its density matrix. The diagonal elements of this matrix  $\Psi_{xy}[k, k] = c_i^X(\tau)^2 c_j^Y(\tau)^2; k =$   
596  $0, \dots, 15; i = 0, \dots, 7; j = 0, \dots, 7$ ; provide the probability of the walker to be in the  
597 position  $(i, j)$ .

The set  $T_n$  is used to denote the positions when the walker is not on  $T_g$  or  $T_p$ , while  $T_d$  (meaning degenerated) denotes the case when the positions are simultaneously target and trap.

Let the values  $\Psi^n(\tau)$ ,  $\Psi^g(\tau)$ ,  $\Psi^p(\tau)$  and  $\Psi^d(\tau)$  be calculated by the formulas:

$$\Psi^n(\tau) = \sum_{(i,j) \in T_n} \Psi_{xy}[i, j] \quad (35)$$

$$\Psi^g(\tau) = \sum_{(i,j) \in T_g} \Psi_{xy}[i, j] \quad (36)$$

$$\Psi^p(\tau) = \sum_{(i,j) \in T_p} \Psi_{xy}[i, j] \quad (37)$$

$$\Psi^d(\tau) = \sum_{(i,j) \in T_d} \Psi_{xy}[i, j] \quad (38)$$

They will be used to assess the probabilities of QDCW to be in the mentioned partition. Obviously  $\Psi^n(\tau) + \Psi^g(\tau) + \Psi^p(\tau) + \Psi^d(\tau) = 1$  evaluates the probability of QDCW to be in the current moment of time in the mentioned partition, but the individual evaluation needs the assessment of its entire trajectory. The evaluation is given by a dynamic quantum fitness function  $\Phi$  composed of two parts ( $\Phi^0, \Phi^1$ ) moving toward positive and negative (respectively) depending of the superposition of QDCW.  $\Phi$  has orientation (stored by one qubit) and position (stored by 16 qubits).

The orientation is given by:

$$|O^\Phi(\tau + 1)\rangle = A_1(\theta) \cdot H \cdot |O^\Phi(\tau)\rangle \quad (39)$$

where  $A_1(\theta)$  is given by the relation (16),  $\theta = \arcsin(\Psi^g - \Psi^p)$  and  $H$  is the Hadamard matrix.

Denoting by  $a_0 = \rho(\cos(\theta) - \sin(\theta))$  and  $a_1 = \rho(\cos(\theta) + \sin(\theta))$ , the quantum fitness function is calculated by:

$$\Phi^0(\tau + 1) = SH^+(a_0 \cdot \Phi^0(\tau) + a_1 \cdot \Phi^1(\tau)) \quad (40)$$

$$\Phi^1(\tau + 1) = SH^-(a_1 \cdot \Phi^0(\tau) - a_0 \cdot \Phi^1(\tau)) \quad (41)$$

It can be seen that:

- if  $\Psi^g = \Psi^p$ ,  $\Phi$  moves equally toward positive and negative,
- if  $\Psi^g > \Psi^p$ ,  $\Phi$  moves more toward positive than negative and
- if  $\Psi^g < \Psi^p$ ,  $\Phi$  moves more toward negative than positive.

The performance is given by:

$$|\Phi^0(16)\rangle = \sum_{k=0}^{16} c_k^{\Phi^0} \cdot |q_k\rangle$$

$$J_p = [c_0^{\Phi^0}, c_1^{\Phi^0}, \dots, c_{16}^{\Phi^0}] \quad (42)$$

with  $c_k^{\Phi^0}$  ( $k = 0, 1, \dots, 16$ ) the amplitudes of  $\Phi^0$ .

All the individuals and their assessments are simulated simultaneously during the specified time horizon (see the model represented in Figure 19). It continues with Grover's algorithm that provides the best individual and its fitness.

### 621 2.12.2. Controller Genome

Regarding Figure 19, the first manner has to find the value of  $\Gamma(0)$  and the unitary matrix  $U$  that modify the control signals according to the formula:

$$\Gamma(\tau + 1) = U \cdot \Gamma(\tau) \quad (43)$$

622 The matrix  $U = A_2(\theta_0^u, \theta_1^u)$  is constructed based on the relation (17).

623 The controller's genome is:  $[|qb_0^u\rangle, |qb_1^u\rangle, |qb_0^\gamma\rangle, |qb_1^\gamma\rangle]$  where the vectors  $|qb_0^\gamma\rangle$  and  
624  $|qb_1^\gamma\rangle$  correspond to the value of  $\Gamma(0)$ .

$\Gamma$  changes the QDCW orientation according to the relation:

$$|\psi_o(\tau + 1)\rangle = G \cdot \Gamma(\tau) \cdot |\psi_o(\tau)\rangle \quad (44)$$

In conclusion, the GA has the task of finding the angles  $\theta_0^\gamma, \theta_1^\gamma, \theta_0^u, \theta_1^u$  that lead to maximum performance. For the current problem an individual genome  $V_i$  is denoted by

$$V_i = (\theta_0^\gamma, \theta_1^\gamma, \theta_0^u, \theta_1^u)_i \quad (45)$$

The population  $\mathcal{P}^w$  of the generation  $w$  is:

$$\mathcal{P}^w = [V_i]_{i=0,1,\dots,pd-1} \quad (46)$$

625 where  $pd$  is the population dimension. The individual implementation requires  $2 + 2$   
626 qubits, so for the simultaneous simulation of the entire population  $4pd$  qubits are needed  
627 that are also needed to the 8 qubits implementing the QDCW.

### 628 2.12.3. Genetic Operators

629 The *individual (genotype) improvement* introduced in [53] is used for the purpose of  
630 avoiding the premature convergence problem that leads to lose of individual diversity  
631 in early generations. For the gene improvement the direction (i.e. positive or negative)  
632 and the amplitude should be found. The direction can be chosen by comparing the best  
633 performance from the previous generation with the current individual performance. The  
634 amplitude of the search in [53] is dynamically adapted by diminishing it at each new  
635 generation.

636 The rotation direction is chosen based on a determinant  $\mathcal{A}_k = \begin{vmatrix} \alpha_k^b & \alpha_k^j \\ \beta_k^b & \beta_k^j \end{vmatrix}$ , where  
637 the elements are provided by a qubit from the previous generation best individual  
638  $qb_k^b = (\alpha_k^b, \beta_k^b)$  and the current individual that has to be improved  $qb_k^j = (\alpha_k^j, \beta_k^j)$ . The  
639 direction of the rotation angle for improvement toward the best individual is given by  
640  $-sign(\mathcal{A}_k)$ . The direction is not determined if  $\mathcal{A}_k = 0$ .

641 Let  $V^b$  be the best individual from the previous generation and  $V_j$  an individual of  
642 the current generation. If their fitness functions are  $Jp^b$  and  $Jp_j$  respectively, the improve-  
643 ment of  $V_j$  consists of applying the rotation improvement vector  $\Theta = [\theta_0, \theta_1, \dots, \theta_{g-1}]$ .  
644 Let  $\theta_{max}$  and  $\theta_{min}$  be the maximum and minimum accepted rotation angle respectively.

645 If an adaptation of the rotation angle in the generation  $w$  of the maximum  $z$  genera-  
646 tions is used, the function for an individual improvement becomes:

647 *Function Improve*( $V_j, Jp_j, V^b, Jp^b, \theta_{max}, \theta_{min}, z, w$ ) :

648  $\Delta\theta_w = \theta_{max} - \frac{\theta_{max} - \theta_{min}}{z} \cdot w \cdot v$ ;

649 **for all**  $qb_k \in V_j$  **do**

650 **if** ( $Jp^b > Jp_j$ )  $\wedge$  ( $\mathcal{A}_k = \begin{vmatrix} \alpha_k^b & \alpha_k^j \\ \beta_k^b & \beta_k^j \end{vmatrix} \neq 0$ ) **then**

651  $\theta_k^j = -sign(\mathcal{A}_k) \cdot \Delta\theta_w$ ;

652 **else**

653  $\theta_k^j = (0.5 - random()) \cdot \Delta\theta_w$ ;

```

654     end if
655      $qb_k^j = A(\theta_k^j) \cdot qb_k^j;$ 
656   end for
657   return  $V_j$ .

```

658 The coefficient  $v$  was added for convergence adjustment.

659 The *quantum crossover* operator introduced in [64] was developed and applied in  
 660 the current research. It works simultaneously on the entire population  $\mathcal{P}^w$  of dimension  
 661  $pd$  (assumed even) at the generation  $w$ . It is split in two equal parts  $\mathcal{P}_0^w$  and  $\mathcal{P}_1^w$ . After  
 662 ordering  $\mathcal{P}^w$  according to the chosen fitness function,  $\mathcal{P}_0^w$  is randomly copied in  $\mathcal{P}_1^w$ .  
 663 The crossover operator (consisting of swapping the second parts of two individuals'  
 664 genotypes) is applied simultaneously to all the individuals and so the population  $\mathcal{P}^{w+1}$   
 665 results.

```

666   Function Crossover( $\mathcal{P}^w, pd$ ) :
667   *parallel  $Jp^w = simulate(\mathcal{P}^w);$ 
668   sort( $\mathcal{P}^w$ );
669   * randomly copy  $\mathcal{P}_0^w$  to  $\mathcal{P}_1^w$ ;
670   for all  $V_j \in \mathcal{P}_0^w$  do
671     * swap the last halves of  $V_j$  and  $V_{pd-1}$ ;
672   end for
673   return  $\mathcal{P}^{w+1} = \mathcal{P}_0^w \cup \mathcal{P}_1^w$ .

```

674 The classical mutation operator acts on a genotype randomly choosing a gene  
 675 and randomly switching its value. The *quantum mutation operator* acts on the entire  
 676 population simultaneously rotating all the qubits with random angles.

#### 677 2.12.4. Quantum Inspired Genetic Algorithms

QIGA needs a different kind of genome [52] that can be stored in the vector  $V$   
 according to formula (4). Usually all the individuals  $j; j = 0, 1, \dots, pd$  have the initial  
 genotypes:

$$V_j^0 = [(q, q), (q, q), \dots, (q, q)]^T \quad (47)$$

The individual genotype modification is performed by a unitary transformation  
 $A_1(\theta)$  (given by (16)) with  $\theta = random() \cdot 2\pi$ , where  $random() \in (0, 1)$  is a function that  
 generates random values. The transformation  $A_1(\theta)$  in an iteration  $k$  acts on a qubit  $qb_i$   
 of  $V$ :

$$qb_i^j = A_1(\theta_k) \cdot qb_i^{j-1}. \quad (48)$$

678 The individual's qubits can be rotated with the same  $\theta$  or using different rotation angle  
 679 for each qubit. The individual is obtained by a transformation  $\Gamma_j = \mathcal{T}(V_j)$ .

680 The individual assessment is performed by the simulation of the QPN model. Their  
 681 selection for reproduction is performed by the classical roulette wheel.

682 Based on Figure 18, the QIGA is constructed by detailing the mappings. The  
 683 following notations are used:

- 684 •  $z$  is the maximum accepted number of generation/iterations,
- 685 •  $w$  is the current iteration,
- 686 •  $(pd + 1)$  the population dimension,
- 687 •  $\mathcal{P}^w$  is the population in the generation  $w$ ,
- 688 •  $V^b, Jp^b$  are the best individual of the previous generation and its fitness function.

689 QIGA algorithm:

```

690   Input:  $pd, z, \theta_{max}, \theta_{min};$ 
691   Initialization:  $\mathcal{P}^0 = [V_j^0]_{j=0,1,\dots,pd-1}; (V^b, Jp^b);$ 
692    $w = 0;$ 
693   while ( $w \leq z$ ) do
694     for all  $V_j \in \mathcal{P}^w$  do
695        $Jp_j^w = simulate(QPN, V_j^w)$  (Figure 18);

```

```

696   end for;
697   for all  $V_j^w \in \mathcal{P}^w$  do
698      $V_j^{w+1} = \text{Improve}(V_j^w, Jp_j^w, V^b, Jp^b, \theta_{\max}, \theta_{\min}, z, w);$ 
699   end for;
700   Find  $(V^b, Jp^b) = \max_{Jp_i, V_i^w \in \mathcal{P}^w} \{(V_j^w, Jp_j^w)\};$ 
701    $w++;$ 
702   end while;
703   return  $V^b, Jp^b;$ 
704   END algorithm;

```

The crossover operation can lead the GA search to conserve a part of the path if and where some individuals perform better. [67]. This involves the modification of the previous algorithm by replacing *Improvement* with *Crossover* and *Mutation*.

#### 2.12.5. Hybrid Classic Quantum Genetic Algorithms (HCQGAs)

HCQGAs perform the individual improvement implemented in CC and the individual evaluations in QC using an architecture similar to those presented in Figure 17.

The algorithm implemented on CC constructs the population and sends it for the evaluation on QC. QC parallelly and simultaneously evaluates all the individuals and provides the best individual with its score.

The individuals evaluation is performed by partitioning the QDCW positions related to the partitions:  $T_n, T_g, T_p$  and  $T_d$  corresponding to the case when the positions  $(i, j)$  are neutral (i.e. neither on target or trap) zone, on target zone, on trap zone and on degenerated zone if it is on a target and a trap (simultaneously) zone respectively. The inclusions in these four sets can be coded by two qubits and the degree of walker inclusion is proposed to be assessed by three qubits. The QDCW simulation, its control (i.e.  $\Gamma$ ) and assessment (i. e.  $\Phi$ ) are run simultaneously.

The quantum system evolves in the Hilbert space:

$$\mathcal{H} = \mathcal{H}_T^4 \otimes \mathcal{H}_O^4 \otimes \mathcal{H}_X^8 \otimes \mathcal{H}_Y^8 \otimes \mathcal{H}_J^2 \otimes \mathcal{H}_\Phi^{12} \quad (49)$$

where  $\mathcal{H}_J^2$  provides the information related to the performance given by the current QDCW position. Similar to the walker state (i.e. orientation and position on X and Y), the individual assessment is given by the position inclusion in an assessment partition and the corresponding degrees.

The HCQGA is composed of two parts: Classic Component of GA and Quantum Component of GA. The algorithms they execute are presented below.

*Classic Component of GA algorithm:*

*Input:*  $pd, z, \theta_{\max}, w, \theta_{\min};$

*Initialization:*  $\mathcal{P}^0 = [V_j^0]_{j=0,1,\dots,pd-1};$

$w = 0;$

**while**  $(w \leq z)$  **do**

**set**  $(\mathcal{P}^w = [V_j^w]_{j=0,1,\dots,pd-1});$

**get**  $(\Phi^w, V^b, \Phi^b);$

$w++;$

**if**  $w < z$  **then**

**for all**  $V_j \in \mathcal{P}^w$  **do**

$V_j^w = \text{Improve}(V_j^{w-1}, \Phi_j^{w-1}, V^b, \Phi^b, \theta_{\max}, \theta_{\min}, z, w);$

**end for**

**end if;**

**end while;**

**return**  $V^b, \Phi^b;$

END algorithm;



744 *Quantum Component of GA algorithm:*

745 *Input:*  $\mathbf{o}(0), \mathbf{x}(0), \mathbf{y}(0), w, z$ ;

746  $w = 0$ ;

747 **while** ( $w \leq z$ ) **do**

748     **get**( $\mathcal{P}^w$ );

749     *Initialization:*  $\mathcal{P}^w, QDCW$ ;

750     **for all**  $V_j \in \mathcal{P}^w$  **do**

751          $\Phi_j^w = \text{simulate}(QDCW, V_j)$ ;

752     **end for**

753     *Find* ( $V^b, \Phi^b$ ) = *bubble\_Sorting*( $V_j, \Phi_j$ );

754     **set**( $\Phi^w = [\Phi_j]_{j=0,1,\dots,pd-1}, V^b, \Phi^b$ );

755      $w = w + 1$ ;

756 **end while**

757 *END algorithm;*

758     The methods **set** and **get** were used for the description of communication between  
759 classic and quantum computers.

760     For QDCW simulation another 3 qubits are required for the clepsydra.

761     The QLC has to be endowed with the necessary quantum gates for the mappings  
762 implementation.

763     The use of the quantum genetic operators *Crossover* and *Mutation* would lead to  
764 complete quantum genetic algorithm.

#### 765 2.12.6. Complete Quantum Genetic Algorithm (CQGA)

766     This is implemented completely on a quantum computer that executes:

767 *CQGA algorithm:*

768 *Input:*  $pd, z$ ;

769 *Initialization:*  $\mathcal{P}^0 = [V_j^0]_{j=0,1,\dots,pd-1}$ ;

770  $w = 0$ ;

771 **while** ( $w \leq z$ ) **do**

772      $\mathcal{P}^{w+1} = \text{Crossover}(\mathcal{P}^w, pd)$ ;

773      $\mathcal{P}^{w+1} = \text{Mutation}(\mathcal{P}^{w+1}, pd)$ ;

774      $w = w + 1$ ;

775 **end while**

776 **return** measure  $V_0$ ;

777 *END algorithm;*

### 778 3. Results

779     QDRW models were tested on a software company simulator, but all the genetic  
780 algorithms were tested by simulation using Java language. For QPN a framework can  
781 be found at "<https://github.com/dahliajanabi/QPN>".

782     For experimentation of the proposed methods, the previously presented QDRW  
783 was modified to the move control of a Quantum Discrete Controlled Walker (QDCW).

#### 784 3.1. Classic GA Solution of Walker Move Control

785     The quantum QDCW model is similar to the QPN displayed in Figure 15. The  
786 classic walker model has the same graph (Figure 15) but the guards and mappings  
787 have to be modified according to Object Enhanced Time Petri Nets (see reference [66]  
788 for details). For this case, the transitions  $t_0, t_1, t_2$  and  $t_3$  perform the rotations and  
789 the transitions  $t'_0, t'_1, t'_2$  and  $t'_3$  perform the move to the next positions. Unlike the  
790 quantum case, the classic walker can be in only one place  $p_0, p_1, p_2$  or  $p_3$ , because the  
791 superposition is not used in the classic computation.

**Table 5.** Search evolution of QIGA.

$w$	$Jp$	$\theta_0^\gamma$	$\theta_1^\gamma$	$\theta_0^\mu$	$\theta_1^\mu$	$\Psi^g$	$\Psi^p$
1	5.184191	1.970711	0.172057	5.517499	3.816113	0.327686	0.252499
20	6.151463	5.105799	2.803489	4.184666	5.264229	0.5896	0.173016
50	25.99559	0.098936	0.117976	5.426092	3.997787	0.73656	0.261046
100	26.98992	1.604711	0.136218	5.446864	3.971793	0.883818	0.094816
200	30.26643	1.622495	1.675234	0.00887	1.554262	0.948257	0.296517
400	30.40533	1.50628	1.515821	6.277452	1.575274	0.971144	0.26478

The classic computation deterministic walker has the model:

$$\begin{bmatrix} o_x(\tau + 1) \\ o_y(\tau + 1) \end{bmatrix} = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \cdot \begin{bmatrix} o_x(\tau) \\ o_y(\tau) \end{bmatrix}$$

(50)

$$\begin{bmatrix} x(\tau + 1) \\ y(\tau + 1) \end{bmatrix} = \begin{bmatrix} x(\tau) \\ y(\tau) \end{bmatrix} + \begin{bmatrix} o_x(\tau + 1) \\ o_y(\tau + 1) \end{bmatrix}$$

(51)

with  $o_x(\tau)$  and  $o_y(\tau)$  describing the orientation on axes  $X$  and  $Y$  respectively. The initial condition is  $[o_x(0), o_y(0), x(0), y(0)]^T$ . The control matrix has the argument  $\theta = \gamma(\tau) \cdot \pi/2$  with  $\gamma(\tau) \in \{0, 1, 2, 3\}$ .

The GA genome  $\Gamma$  is a vector of rotations  $\gamma(\tau)$  for  $0 \leq \tau < 15$ .

The usual mutation and crossover genetic operations were performed and the obtained results are presented in Figure 20 for the initial state  $[1, 1]$ , with orientation  $[0, 0]$ ,  $TargetPoint = \{(5, 5)\}$  and  $TrapPoints = \{(2, 4), (3, 3), (4, 2)\}$ . The best individual genotype is  $\Gamma = [2, 0, 0, 0, 1, 0, 0, 0, 0, -, -, -, -, -]$  and the resulting best trajectory is:  $(1, 1) * (2, 1) * (3, 1) * (4, 1) * (5, 1) * (5, 2) * (5, 3) * (5, 4) * (5, 5)$ .

3.2. Application of QIGA for QDCW

For QDCW model the mappings assigned to transitions  $t_0, t_1, t_2$  and  $t_3$  (that correspond to generalized coin throw) in the QDRW model have to be replaced with control values applied to qubit registers. The qubit register is composed of 2 qubits for orientation, 3 qubits for  $X$  and another 3 qubits for  $Y$ .

The probabilities of the best individual obtained by QIGA are represented in Figure 21.

The evolution of the solution search is given in Table 5. The maximum values  $\Psi^g$  and  $\Psi^p$  were obtained at different moments of time.

3.3. Application HQCGA for QDCW Control

The values provided by the quantum fitness function where transformed in classic values using the formula:

$$Jp = (\Phi_{10} - 2^{16}) \cdot 10^{-4}$$

(52)

where  $\Phi_{10}$  represents the conversion in the base 10 of  $\Phi$ .

The probabilities of the best individual obtained by HCQGA are represented in Figure 22.

The evolution of the solution search is given in Table 6.

3.4. Complete Implemented QGA for QDCW Control

The probabilities of the best individual obtained by CQGA are represented in Figure 23.

The evolution of the solution search is given in Table 7.

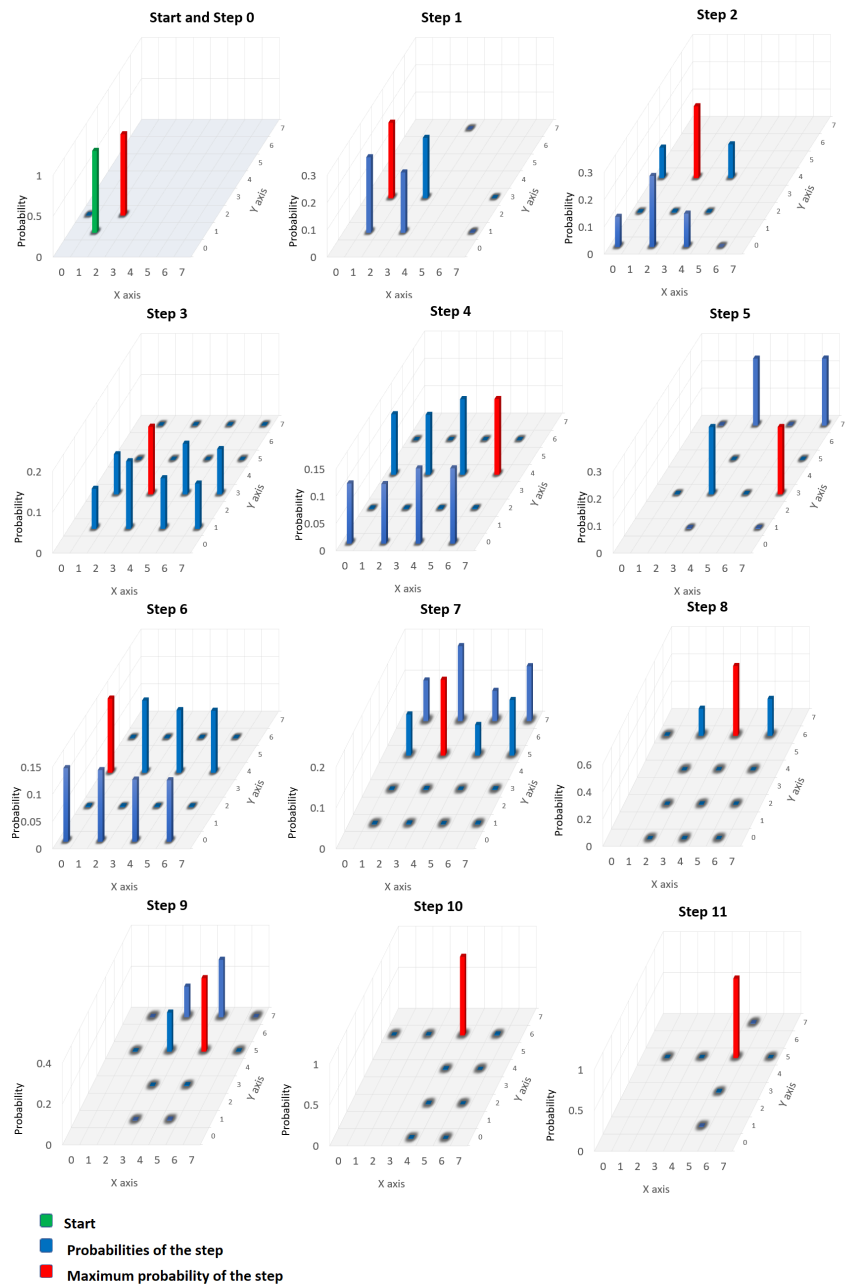


Figure 21. The representation of the probabilities of the best individual for QIGA.

Table 6. Search evolution of HCQGA.

$w$	$Jp$	$\theta_0^\gamma$	$\theta_1^\gamma$	$\theta_0^\mu$	$\theta_1^\mu$	$\Psi g$	$\Psi p$
1	-0.2591	4.327966	4.355129	4.691925	5.285935	0.32319	0.249785
20	0.9694	4.69221	0.926491	1.752213	4.315906	0.48180	0.201644
50	1.0063	5.785132	3.212869	3.069224	1.579819	0.59034	0.172353
100	1.1924	2.841270	4.073705	1.163401	2.024726	0.71703	0.205691
200	1.3248	1.533609	1.703517	4.7155721	0.047902	0.91005	0.2772
400	1.3426	1.533609	1.545308	4.715572	6.279499	0.9891	0.261999

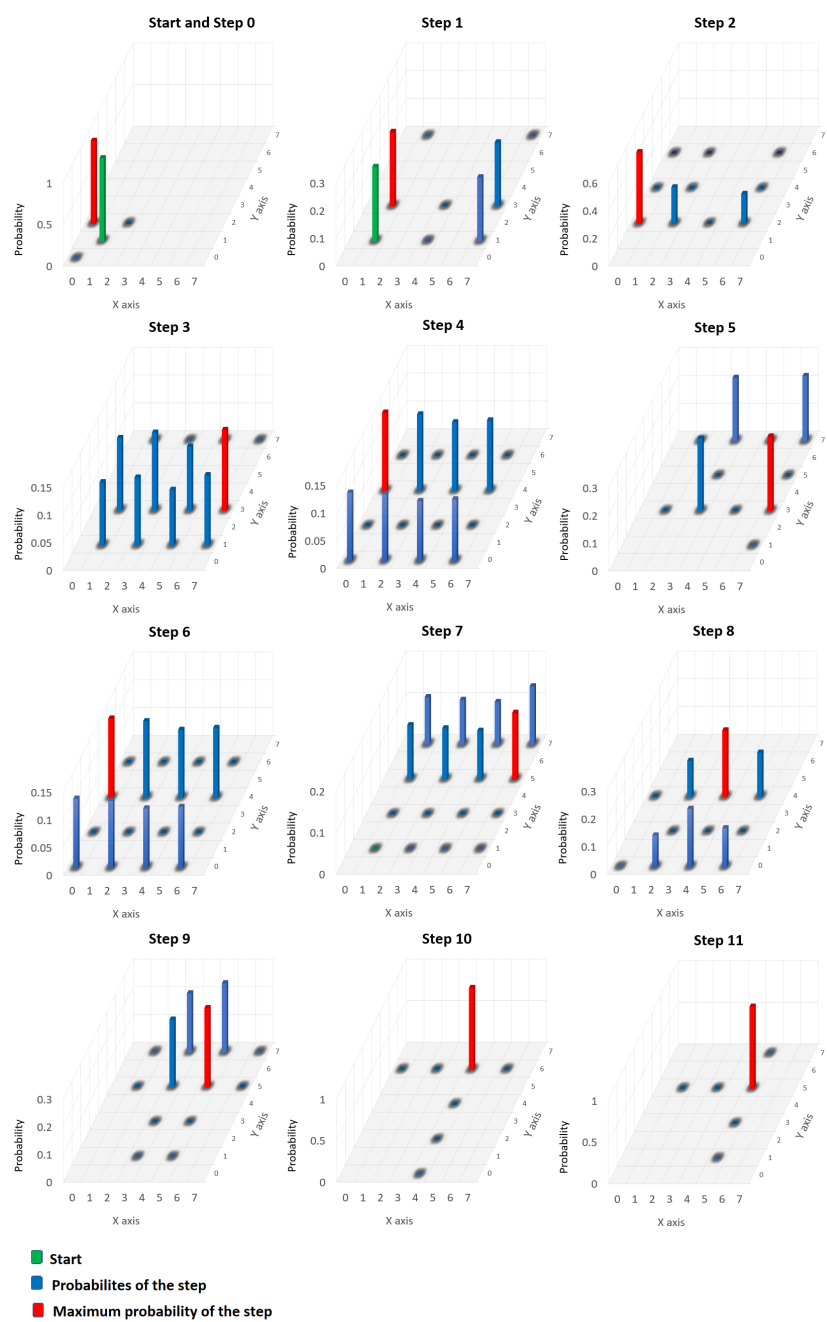


Figure 22. The representation of the probabilities of the best individual for HCQGA.

Table 7. Search evolution of CQGA.

$w$	$Jp$	$\theta_0^\gamma$	$\theta_1^\gamma$	$\theta_0^\mu$	$\theta_1^\mu$	$\Psi^g$	$\Psi^p$
1	-0.2169	4.718726	1.826285	0.868892	5.209561	0.372534	0.149553
20	1.0427	6.133167	1.175452	4.349668	5.18827	0.560429	0.1686
50	1.2230	6.133167	0.1142914	4.247011	5.18827	0.749876	0.178494
100	1.2408	6.133167	1.456658	0.868892	2.269625	0.859324	0.18782
200	1.2631	6.133167	1.456658	0.868892	2.25455	0.888608	0.198289
400	1.3220	6.231308	1.515613	0.855429	2.266428	0.930239	0.197465

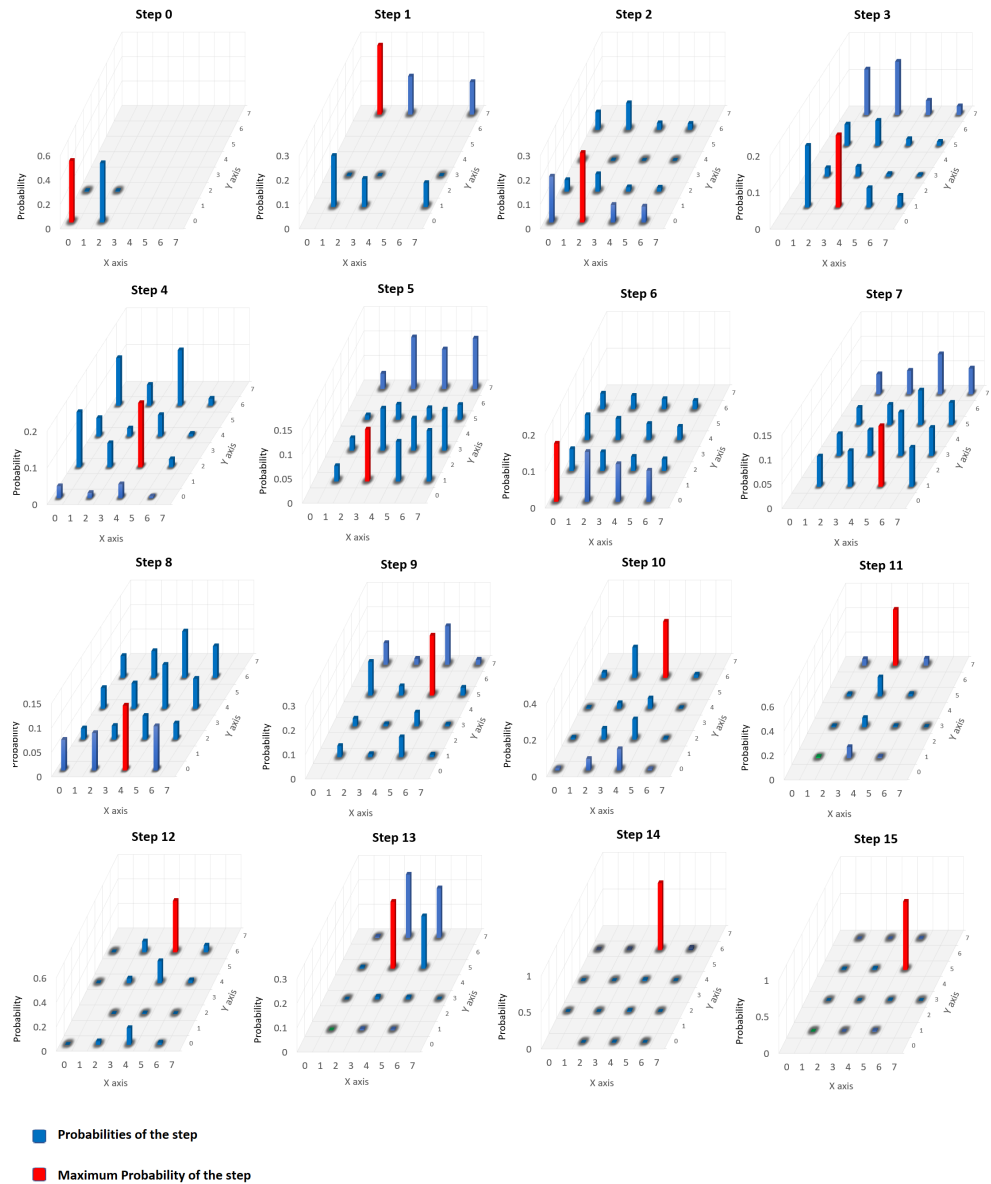


Figure 23. The representation of the probabilities of the best individual for CQGA.

819 **4. Discussion**

820 Modeling with QPNs can sustain all the phases of quantum software development.  
821 They help the understanding of the quantum complex problems and their use facilitate  
822 the quantum software conception. QPN can be used for description at the qubit level,  
823 or at a higher-level modeling complex mappings. The Petri net based language can be  
824 used for analysis of classic programs as well as quantum programs. Because quantum  
825 programs are expected to be used in tandem with classic programs, the Petri nets are  
826 useful for constructing a bridge between quantum computers and classic computers  
827 successfully showing their concurrent cooperation. The reachability graph can be used  
828 for the classic program and for quantum program as well. The development based  
829 on QPN provides the mappings that lead to the QLC structure required for quantum  
830 program implementation.

831 The current approach concerns the control of dynamic systems where statistic  
832 features are relevant. This kind of applications requires fitness functions assessing the  
833 temporal behaviors as they were introduced here.

834 The classic discrete walker has a deterministic behavior, so its optimal control led  
835 to a deterministic solution. QDCW has a stochastic behavior described by superposition  
836 and so its optimal control is described by superposition too. Both walkers are controlled  
837 by changing their orientations.

838 The classic controller genome is a time variable vector  $\Theta$ , while the quantum  
839 controller genome is composed of the initial orientation function  $\Gamma(0)$  and a matrix  $U$   
840 for this function correction.

841 QIGA and HCQGA use similar individual evolution algorithms (genotypes im-  
842 provement). Their results are closed to each other. CQGA uses quantum crossover and  
843 mutation and these led to a different solution, slightly with lower performance than the  
844 previous GAs.

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**Abbreviations**

The following abbreviations are used in this manuscript:

QC	Quantum Computation or Computer
CC	Classic Computation or Computer
PN	Petri Net
OETPN	Object Enhanced Time Petri Net
QPN	Quantum Petri Net
QDRW	Quantum Discrete Random Walker
ME	Mobile Entity
EA	Evolutinary Algorithm
QEA	Quantum Evolutionary Algorithm
PSO	Particle Swarm Optimization
QME	Quantum Mobile Entity
GA	Genetic Algorithm
CGA	Classic Genetic Algorithm
QGA	Quantum Genetic Algorithm
QIGA	Quantum Inspired Genetic Algorithm
HCQGA	Hybrid Classic Quantum Genetic Algorithm
CQGA	Complete Quantum Genetic Algorithm
QAOA	Quantum Approximate Optimization Algorithm
ES	Evolutionary System
QES	Quantum Evolutionary System

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