Stochastic Simulation of Grover’s Algorithm

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Abstract

We simulate Grover’s algorithm in a classical computer by means of a stochastic method using the Hubbard-Stratonovich decomposition of $n$-qubit gates into one-qubit gates integrated over auxiliary fields. The problem reduces to finding the fixed points of the associated system of Langevin differential equations. The equations are obtained automatically for any number of qubits by employing a computer algebra program. We present the numerical results of the simulation for a small search space.

1 Introduction

Grover’s and Shor’s algorithms [1 2] are landmarks in the development of Quantum Computation since the foundation of this area in the 1980’s [3 4 5]. Shor’s algorithm provides an exponential speed up over currently known classical factorization algorithms. Although a classical polynomial factorization algorithm might be found, it is very unlikely that its complexity would be as low as Shor’s $O(n^3)$. Compare with the polynomial $O(n^{12} \text{ poly}(\log n))$ algorithm for the much easier problem of primality test recently developed by
Agrawal, Kayal, and Saxena [6]. Therefore, it is unlikely that a polynomial factorization algorithm, if it exists, would have complexity under $O(n^{12})$.

Shor’s algorithm is the best candidate to be simulated in classical computers, since the price paid by the simulation may still be low compared to the exponential timing of classical algorithms. Unfortunately, the techniques used in this paper do not seem to be suitable for Shor’s algorithm [7].

Grover’s algorithm plays an important role in Quantum Computation, since it provides a proof that quantum computers are faster than classical ones for unstructured database searching. It has complexity $O(\sqrt{N})$ while the best classical algorithm has complexity $O(N)$, where $N$ is the database size. Grover’s algorithm is optimal using oracle searching [8, 9], therefore the quadratic speed up is the best one can achieve in this case. The hope in simulating it in classical computers with a better efficiency compared to the classical algorithm is very low. Despite this fact, Grover’s algorithm provides a laboratory to test simulation techniques that might shed new light in distinguishing the way classical and quantum computers work.

In a seminal paper, Feynman [4] argues that classical computers can simulate quantum ones only with an exponential slow down. It is easy to see that an exact simulation uses either an exponential amount of memory or takes an exponential time to accomplish generic tasks that could be done by a quantum computer. A generic quantum state of $n$ qubits has $2^n$ complex amplitudes which must be taken into account by the classical computer. An alternative option is a stochastic simulation by some “non-deterministic computer”. The central issue is the local nature of classical computers. A classical computer of the same physical size of a quantum computer working under local classical physical laws does obey the Bell inequality [10] and cannot reproduce the same results of a computer which follows the quantum mechanical laws.

Feynman’s arguments, on the other hand, are not quantitative. The question is: what is exactly the loss introduced by the stochastic simulation, in such a way that the result given by the quantum computer is still reproduced?

An interesting stochastic simulation technique in the quantum computation context was introduced by Cerf and Koonin [7]. The quantum computer is viewed as a many-body dynamics which can be reduced to the time evolution of single qubits integrated in auxiliary fields. They used the Hubbard-Stratonovich [11, 12] representation to obtain an expression for two-qubit gates in terms of two one-qubit gates with two auxiliary fields. They used a Monte Carlo Method [13, 14] (in fact the Langevin equations with equivalent
solutions [15, 16]) to reduce the exponential size of the associated Hilbert space to an equivalent coupled system of differential equations with a polynomial number of auxiliary fields.

It is known that a general quantum circuit can be decomposed in terms of one and two-qubit gates, called universal gates [17, 18]. On the other hand, it is also known that this decomposition may use an exponentially large number of universal gates [18] (and auxiliary fields). In that case, the gain provided by the stochastic method would be lost in the decomposition in terms of the universal gates.

In this paper, we generalize Cerf and Koonin’s method to general \( n \)-qubit gates, avoiding the decomposition of \( n \)-qubit gates into universal gates. The generalization is straightforward and welcome in simulating Grover’s algorithm for a general number of qubits. We apply the method for Grover’s algorithm, and make use of a Maple program that generates automatically the associated system of Langevin equations. The equations are solved numerically (in Maple and in C) giving the relaxation values of the auxiliary fields which correspond to the fixed points of the Langevin dynamics. We present the numerical results for the simplest case of Grover’s algorithm and discuss some problems we are facing with the method.

2 Decomposition in terms of one-qubit gates

Consider a quantum circuit of \( g \) gates \((U_k, k = 1, \ldots, g)\) in a \( n \)-qubit quantum computer. Each gate \( U_k \) acts on two or more qubits \((j_k^{(1)}, j_k^{(2)}, \ldots, j_k^{(n_k)})\). The qubit indices within a gate \( U_k \) are put in parentheses. They do not coincide necessarily with the overall qubit indices, which will be denoted in square brackets.

In order to clarify the notation consider the following example: if \( U_k \) is a two-qubit gate acting on the third and fifth qubits, then \( n_k = 2, j_k^{(1)} = 3, \) and \( j_k^{(2)} = 5 \). The index \( s \) of \( j_k^{(s)} \) runs from 1 to \( n_k \). The actual values of \( j_k^{(s)} \) are in increasing order but not necessarily consecutive with respect to the overall qubits, as shown in the example. One-qubit gates will be trivially introduced in the next section, so they will not be considered for a while.

The computation as a whole is performed by the unitary operator \( U \) given
by
\[
U = \prod_{k=g}^{1} U_k = U_g \ldots U_1
\]  (1)
where the product is in reverse order, so the operators act in ascending order from left to right on input kets. \( U_k \) is a general \( n_k \)-qubit gate, with \( 2 \leq n_k \leq n \). We assume that \( U_k \) can be decomposed as an exponential of a tensor product of one-qubit gates, in the form
\[
U_k = e^{-i\alpha_k A_k^{(1)} \otimes A_k^{(2)} \otimes \ldots \otimes A_k^{(n_k)}},
\]  (2)
where \( A_k^{(s)} \) acts only on qubit \( j_k^{(s)} \). This equation generalizes eq.(2) of Cerf and Koonin’s paper [7].

The Hubbard-Stratonovich decomposition [11, 12] for a \( n_k \)-qubit gate follows from
\[
e^{-i\alpha_k A_k^{(1)} \otimes \ldots \otimes A_k^{(n_k)}} = \int_{-\infty}^{\infty} d\sigma_k^{(s)} e^{-i\alpha_k A_k^{(1)} \otimes \ldots \otimes \sigma_k^{(s)} I_k^{(s)}} \times \\
\delta(I_k^{(1)} \otimes \ldots \otimes I_k^{(s-1)} \otimes (A_k^{(s)} - \sigma_k^{(s)} I_k^{(s)})), \]  (3)
where \( I_k^{(s)} \) is the identity matrix acting on the qubit \( j_k^{(s)} \), and from the following representation for the Dirac delta function
\[
\delta(I_k^{(1)} \otimes \ldots \otimes I_k^{(s-1)} \otimes (A_k^{(s)} - \sigma_k^{(s)} I_k^{(s)})) = \\
\frac{1}{2\pi} \int_{-\infty}^{\infty} d\tau_k^{(s)} e^{-i\alpha_k \tau_k^{(s)} I_k^{(1)} \otimes \ldots \otimes I_k^{(s-1)} \otimes (A_k^{(s)} - \sigma_k^{(s)} I_k^{(s)})).} \]  (4)
Applying decomposition (3) and (4) recursively \( n_k - 1 \) times in eq.(2), we introduce real auxiliary fields \( \sigma_k^{(s)} \) and \( \tau_k^{(s)}, 2 \leq s \leq n_k \). For simplicity, we will drop the identity matrices from now on. The result is the following expression:
\[
U_k = \int_{-\infty}^{\infty} d\sigma_k^{(2)} d\tau_k^{(2)} \ldots d\sigma_k^{(n_k)} d\tau_k^{(n_k)} \left( \frac{\alpha_k}{2\pi} \right)^{n_k-1} e^{-i\alpha_k \sigma_k^{(2)} \ldots \sigma_k^{(n_k)} A_k^{(1)}} \times \\
e^{-i\alpha_k \tau_k^{(2)} (A_k^{(2)} - \sigma_k^{(2)} \ldots \ldots - \sigma_k^{(n_k)} A_k^{(n_k)} - \sigma_k^{(n_k)} \ldots \sigma_k^{(2)})}. \]  (5)
Substituting \( U_k \) into eq.(1) yields
\[
U = \int_{-\infty}^{\infty} \prod_{k=g}^{1} \left\{ d\sigma_k^{(2)} d\tau_k^{(2)} \ldots d\sigma_k^{(n_k)} d\tau_k^{(n_k)} \left( \frac{\alpha_k}{2\pi} \right)^{n_k-1} e^{i\alpha_k \sum_{s=2}^{n_k} \sigma_k^{(s)} \tau_k^{(s)}} \right\} V_k^{(1)}(\sigma_k) V_k^{(2)}(\tau_k) \ldots V_k^{(n_k)}(\tau_k), \]  (6)
where

\[
V_{k}(1) = V_{k}(1)(\sigma_{k}, \ldots, \sigma_{nk}) = e^{-i\alpha_{k}\sigma_{k}^{(2)} \cdots \sigma_{k}^{(nk)} A_{k}^{(1)}}
\]

\[
V_{k}^{(s)}(\tau_{k}^{(s)}) = e^{-i\alpha_{k}\tau_{k}^{(s)} A_{k}^{(s)}}, \quad 2 \leq m \leq n_{k}.
\]

(7)

\(\sigma_{k}\) denotes all the \(\sigma_{k}^{(s)}\) for a given \(k\), and the superscript \((s)\) indicates in which qubit \(A_{k}^{(s)}\) acts.

Up to this point, we have been considering \(U\) as a composition of \(g\) gates. Using the Hubbard-Stratonovich representation, each gate was decomposed into one-qubit gates, paying the price of introducing \(2(n_{k} - 1)\) scalar fields and respective integrals. Now we focus on the world line of each qubit and multiply (horizontally) all one-qubit gates acting on that qubit. We end up with \(n\) one-qubit gates which are tensored out and integrated on the auxiliary fields, yielding the following expression for \(U\)

\[
U = \int D\sigma D\tau e^{i\sum_{k=1}^{g} \alpha_{k} \sum_{s=2}^{n_{k}} \sigma_{k}^{(s)} \tau_{k}^{(s)} \prod_{l=1}^{n} U[l](\sigma, \tau)}
\]

(8)

where square brackets denote an overall qubit label (as opposed to internal gate labels \(j_{k}^{(s)}\)), with

\[
U[l](\sigma, \tau) = \prod_{k=g}^{1} U[l]_{k}(\sigma, \tau),
\]

(9)

(here \(\sigma\) and \(\tau\) denote all of them) and

\[
U[l]_{k}(\sigma_{k}, \tau_{k}) = \left\{
\begin{array}{ll}
V_{k}(1)(\sigma_{k}) & \text{if } l = j_{1} \\
V_{k}(2)(\tau_{k}) & \text{if } l = j_{2} \\
\vdots & \vdots \\
V_{k}(n_{k})(\tau_{k}) & \text{if } l = j_{n_{k}} \\
I[l]_{k} & \text{otherwise.}
\end{array}
\right.
\]

(10)

In the remaining of this section, we follow closely Cerf and Koonin’s approach [7]. The last step of the computation is the measurement of the first \(m\) qubits, \(m \leq n\). We assume that the observable is the direct product of \(m\) one-qubit observables,

\[
O = \bigotimes_{l=1}^{m} O[l].
\]

(11)
From the remaining qubits, \( p \leq n - m \) have prescribed values \( \pi_1, \pi_2, \ldots, \pi_p \), so we define the projector \( \mathcal{P} \) as

\[
\mathcal{P} = \prod_{k=1}^{p} \mathcal{P}_k,
\]

where \( \mathcal{P}_k = |\pi_k\rangle \langle \pi_k| \). The expectation value of the observable \( \mathcal{O} \) is given by

\[
\langle \mathcal{O} \rangle = \frac{\langle 0 \ldots 0_n | U^\dagger \mathcal{O} P U | 0 \ldots 0_n \rangle}{\langle 0 \ldots 0_n | U^\dagger P U | 0 \ldots 0_n \rangle}
\]

Using eqs. (8), (12) and (16) we get

\[
\langle \mathcal{O} \rangle \approx \frac{1}{T} \int_{t}^{t+T} dt \mathcal{O}(\sigma(t), \sigma'(t))
\]

where \( \mathcal{O}(\sigma, \tau, \sigma', \tau') = \prod_{l=1}^{n} \frac{\langle 0_l | U^\dagger[l](\sigma', \tau') | \mathcal{O}[l] P[l] U^\dagger[l](\sigma, \tau) | 0_l \rangle}{\langle 0_l | U^\dagger[l](\sigma', \tau') P[l] U^\dagger[l](\sigma, \tau) | 0_l \rangle} \)

The most promising method to calculate \( \langle \mathcal{O} \rangle \) is by using the associated Langevin equations given by

\[
\frac{d\sigma_k^{(s)}}{dt} = -\frac{i}{2} \frac{\partial S}{\partial \sigma_k^{(s)}} + \eta_k^{(s)}(t)
\]

where \( t \) is a simulation time, \( \eta_k^{(s)} \) is a real Gaussian white noise and the scalar fields have been extended to the complex plane. The stochastic estimate of \( \langle \mathcal{O} \rangle \) is

\[
\langle \mathcal{O} \rangle \approx \frac{1}{T} \int_{t}^{t+T} dt \mathcal{O}(\sigma(t), \sigma'(t))
\]
where $\sigma$ and $\sigma'$ are solutions of eq.(17), and $T$ represents a sufficiently large simulation time. In the next section, we will obtain that $\sigma$ and $\sigma'$ converge to some final limiting value, so we will use the formula

$$\langle O \rangle \approx O(\sigma_{\text{final}}, \sigma'_{\text{final}}).$$

(19)

3 Simulation of Grover's algorithm

Grover's algorithm [1] allows us to search an element in an unstructured database with $N$ elements (suppose that $N = 2^n$) using $O(\sqrt{N})$ steps. The best classical algorithm uses $O(N)$ steps. This quadratic speed-up is one of the greatest successes of quantum computation so far.

Grover's algorithm has two registers, the first one with $n$ qubits and the second one with one qubit. It starts by preparing a superposition of all computational basis states with same amplitude. An oracle is used to probe the database (a quantum memory is assumed to exist in some form), and it changes the sign of the amplitude of the state which corresponds to the numerical index of the searched element. In order to simulate the oracle action, we use a $n + 1$ qubits generalized Toffoli gate, which marks the state $|N - 1\rangle$ (we are assuming that $N - 1$ is the searched element).

The state $|N - 1\rangle$ has $n$ ones in binary notation, and that is why the oracle just changes the sign of the amplitude of that state. Any other state of the computational basis could be marked as well, introducing two $X$ gates in the oracle, for each zero in the binary representation of the state’s label. The $X$ gates are placed symmetrically with respect to the generalized Toffoli gate, in the qubits corresponding to the zeroes in the binary representation.

Fig. 1 shows the Grover operator in terms of two generalized Toffoli gates and one-qubit gates. This decomposition is enough to apply the method of the previous section. Note that the method used in [7] would require the decomposition of the generalized Toffoli gate into two- and one-qubit gates. This would introduce more scalar fields ($\sigma$’s and $\tau$’s) and lead to cumbersome calculations. For example, for $N = 4$, the method of Cerf and Koonin would use 28 scalar fields, while ours uses 12.

A non-trivial part of our procedure is the calculation of the decomposition (2) for a general $n$-qubit gate. Fortunately, it is easy to obtain the
decomposition of the generalized Toffoli gate:

\[
\begin{pmatrix}
1 & 1 & \cdots & 1 \\
1 & 1 & \cdots & 1 \\
& & 1 & 1 \\
& & 0 & 1 \\
& & 1 & 0 \\
\end{pmatrix}
= e^{-i\alpha A^{(1)} \otimes \cdots \otimes A^{(n+1)}},
\]  

(20)

where

\[
\alpha = \frac{\pi}{2},
\]

\[
A^{(1)} = \cdots = A^{(n)} = \frac{1 - \sigma_z}{2} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},
\]

\[
A^{(n+1)} = 1 - \sigma_x = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.
\]

The next step is the calculation of \(U^{[l]}(\sigma, \tau)\) given by eq. (9) for \(l = 1, \ldots, n_k\). Recall that \(U^{[l]}(\sigma, \tau)\) is the ordered composition of all one-qubit gates for the qubit \(l\), including the two gates that come from the decomposition (20), one for each generalized Toffoli gate of Fig. 2.
Since the Grover operator $G$ must be applied $k_0$ times, we have
\[
U^{[l]}(\sigma, \tau) = \begin{cases} 
\left( \prod_{k=k_0}^l U_k^{[l]}(\sigma, \tau) \right) H & \text{for } l = 1, 2, \ldots, n \\
XH \left( \prod_{k=k_0}^{l+1} U_k^{[l+1]}(\sigma, \tau) \right) HX & \text{for } l = n + 1.
\end{cases}
\]

(22)

Examining Fig. 2 we see that there are four distinct kinds of $U^{[l]}(\sigma, \tau)$, which we address now. For $l = 1$, $U^{[l]}(\sigma, \tau)$ must be treated separately, since from eq. (10) we see that for $l = j_1$ (here $j_1 = 1$) $V_k^{(1)}$ depends only on the $\sigma$ fields while $V_k^{(s)}$ depends on $\tau_k^{(s)}$. So
\[
U_k^{[1]} = HX \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\alpha \sigma^{(2)}_{2k} \ldots \sigma^{(n)}_{2k}} \end{pmatrix} \cdot XH \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\alpha \sigma^{(2)}_{2k-1} \ldots \sigma^{(n+1)}_{2k-1}} \end{pmatrix}.
\]

(23)

For $l = 2, \ldots, n - 1$ the gate configuration is similar, then
\[
U_k^{[l]} = HX \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\alpha \tau^{(l)}_{2k}} \end{pmatrix} \cdot XH \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\alpha \tau^{(l)}_{2k-1}} \end{pmatrix}.
\]

(24)

For $l = n$, Grover operator has two extra Hadamard and a $X$ gate. Then
\[
U_k^{[n]} = \frac{1}{2} HXH \begin{pmatrix} 1 + e^{-2i\alpha \tau^{(n)}_{2k}} & 1 - e^{-2i\alpha \tau^{(n)}_{2k}} \\ 1 - e^{-2i\alpha \tau^{(n)}_{2k}} & 1 + e^{-2i\alpha \tau^{(n)}_{2k}} \end{pmatrix} \cdot HXH \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\alpha \tau^{(n)}_{2k-1}} \end{pmatrix}.
\]

(25)

Finally, for $l = n + 1,$
\[
U_k^{[n+1]} = \frac{1}{2} \begin{pmatrix} 1 + e^{-2i\alpha \tau^{(n+1)}_{2k-1}} & 1 - e^{-2i\alpha \tau^{(n+1)}_{2k-1}} \\ 1 - e^{-2i\alpha \tau^{(n+1)}_{2k}} & 1 + e^{-2i\alpha \tau^{(n+1)}_{2k-1}} \end{pmatrix}.
\]

(26)
Next we can insert the latter results in eq. (24) and obtain $U^{[l]}$. We note that in eq. (16), $|0_i\rangle$ is represented as \[ \begin{bmatrix} 1 \\ 0 \end{bmatrix}. \] So we get for example, for observable $O_{00} = (|0_1\rangle \langle 0_1|) \otimes (|0_2\rangle \langle 0_2|)$,

$$O_{00}(\sigma, \tau, \sigma', \tau') = \prod_{i=1}^{n} \frac{U^{[l]}_{1,1}(\sigma', \tau')U^{[l]}_{1,1}(\sigma, \tau)}{U^{[l]}_{1,1}(\sigma', \tau')U^{[l]}_{1,1}(\sigma, \tau) + U^{[l]}_{1,2}(\sigma', \tau')U^{[l]}_{1,2}(\sigma, \tau)}. \tag{27}$$

Similarly, in each observable we choose to test, we need to calculate only the relevant elements of $U^{[l]}$.

In the Appendix, we describe a Maple\textsuperscript{1} program that calculates the physical quantities of this section starting from this point. Given $n$, the program uses eqs. (23) to (26) to calculate $U^{[l]}(\sigma, \tau)$ and $U^{[l]}(\sigma', \tau')$, and then obtains $O(\sigma, \tau, \sigma', \tau')$ for a given observable constructed similarly to the above. Using eqs. (15) and (17), the program obtains the Langevin equations for the simulation of Grover’s algorithm with an arbitrary number of qubits.

The simplest case is a search space of $N = 4$ elements, for which the auxiliary fields are $\sigma_2^{(2)}, \sigma_1^{(2)}, \sigma_1^{(3)}, \tau_2^{(2)}, \tau_1^{(2)}, \tau_1^{(3)}$, and the respective primed versions. We give below the first Langevin equation for this case. The other equations of the system of partial differential equations have a format similar to this one:

$$\frac{d\sigma_1^{(2)}}{dt} = \frac{\pi}{4} \tau_1^{(2)} + \eta(t) - \frac{\pi}{4} \sigma_1^{(3)} \left( e^{-\frac{i\pi}{2}}(-\sigma_1^{(2)} + \sigma_1^{(2)} + \sigma_1^{(3)}) + e^{-\frac{i\pi}{2}}(-\sigma_1^{(2)} + \sigma_1^{(2)} + \sigma_1^{(3)}) + e^{-\frac{i\pi}{2}}(-\sigma_1^{(2)} + \sigma_1^{(2)} + \sigma_1^{(3)}) + e^{-\frac{i\pi}{2}}(-\sigma_1^{(2)} + \sigma_1^{(2)} + \sigma_1^{(3)}) + e^{-\frac{i\pi}{2}}(-\sigma_1^{(2)} + \sigma_1^{(2)} + \sigma_1^{(3)}) + e^{-\frac{i\pi}{2}}(-\sigma_1^{(2)} + \sigma_1^{(2)} + \sigma_1^{(3)}) + e^{-\frac{i\pi}{2}}(-\sigma_1^{(2)} + \sigma_1^{(2)} + \sigma_1^{(3)}) \right). \tag{28}$$

This system of equations is discretized and solved numerically. After trying different values for the discretization parameter and initial conditions, we plot each scalar field $\sigma_k^{(s)}$ as a function of $t$ in order to determine the convergence.

\textsuperscript{1}Maple Waterloo Software, Inc. See http://www.maplesoft.com
value, to be substituted in the previously obtained formula (27), for the observable \( \langle O_{00} \rangle \) and in the equivalent formulas for \( \langle O_{01} \rangle, \langle O_{10} \rangle \) and \( \langle O_{11} \rangle \), corresponding to the observables

\[ O_{ij} = |ij\rangle \langle ij| \] (29)

for \( i, j = 0, 1 \). Since we have chosen the oracle that changes the sign of the state \( |11\rangle |-\rangle \), we expect to obtain \( \langle O_{11} \rangle \) close to 1, and the remaining ones close to 0.

Unfortunately, we are faced with technical difficulties. First, there are some fields that do not converge to a definite value, at least to the extent of our simulation. In our case, this issue was circumvented by imposing the constraint that total probability equals one, but in the general case the use of such an artifact would not be desired. The second problem are fields that seem to have a logarithmic behaviour. We have tried to solve this by fitting the logarithmic behaviour by a log function, then inserting it in the expressions and taking the limit as \( t \to \infty \). Even then, contrary to our expectation, we get the following results

\[
\begin{align*}
\langle O_{00} \rangle &= .28 \\
\langle O_{01} \rangle &= .24 \\
\langle O_{10} \rangle &= .24 \\
\langle O_{11} \rangle &= .21
\end{align*}
\] (30)

It is not clear to us whether we are making some mistake or this result shows that the method does not work with Grover’s algorithm. Any comment on this issue is very welcome.

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Appendix

This appendix describes a Maple program for release 6 or higher that calculates the Langevin equations for the simulation of Grover’s algorithm, as described in Section 3. The number of qubits is fixed in the beginning of the session. The lines beginning with the prompt > are Maple commands. We make some comments about each group of commands.

1. Starting a new session, defining matrices $H$, $X$ and $Z$, and setting the number of qubits.

```maple
> restart;
> with(LinearAlgebra):
> H := 1/sqrt(2)*Matrix([[1,1],[1,-1]]):
> X := Matrix([[0,1],[1,0]]):
> Z := Matrix([[1,0],[0,-1]]):
> n := 2:
```

2. Function $k_0$ finds the number of times the Grover operator is applied.

```maple
> k0 := proc()
> local theta;
> theta := 2*evalf(arccos(sqrt(1-1/(2^n))));
> eval(round(Pi/(2*theta) - 1/2))
> end proc:
```

3. The next two procedures calculate $U^l(\sigma,\tau)$ given by eq.(22) and $U^l_k(\sigma_k,\tau_k)$ given by eqs.(23-26). They are not used directly, as we see ahead.

```maple
> Ul := proc(l)
> if l<n+1 then
> '\.'(seq(Ul_k(l,k0()-s),s=0..k0()-1)).H
> elif l=n+1 then
> X.H.'.'(seq(Ul_k(n+1,k0()-s),s=0..k0()-1)).H.X
> else error(‘expecting l<=n+1, got %1’,l)
> end if
> end proc:
>
> Ul_k := proc(l,k)
```

if l=1 then
H.X.Matrix1(mul(sigma[s,2*k][t],s=2..n)).X.H.
Matrix1(mul(sigma[s,2*k-1][t],s=2..n+1))
elif 1<l and l<n then
H.X.Matrix1(tau[l,2*k][t]).X.H.Matrix1(tau[l,2*k-1][t])
elif l=n then
Z.Matrix2(tau[n,2*k][t]).Z.Matrix1(tau[n,2*k-1][t])
elif l=n+1 then
Matrix2(tau[n+1,2*k-1][t])
end if
end proc:

4. The next two procedures are auxiliary functions for calculating the matrices of eqs.(23-26).

Matrix1 := proc(x)
Matrix([[1,0],[0,exp(-I*(Pi/2)*x)])
end proc:

Matrix2 := proc(x)
Matrix([[1/2+1/2*exp(-I*Pi*x), -1/2*exp(-I*Pi*x)+1/2],
[-1/2*exp(-I*Pi*x)+1/2, 1/2+1/2*exp(-I*Pi*x)])
end proc:

5. The next two functions calculate $U[l](\sigma,\tau)$ and its hermitian conjugate, automatically applying simplifying functions. An user should use these functions since they return the simplified result.

U := l -> Map(simplify,Ul(l)):
Udagger := l -> Map(simplify, subs(I=-I, sigma=sigma1,
tau=tau1, Transpose(Ul(l)))):

6. The next command calculates the action $S$ given by eq.(15), taking $|0\rangle$ as the input state for all qubits.

S := - (Pi/2)*add(
add(sigma[s,k][t]*tau[s,k][t] -
sigma1[s,k][t]*tau1[s,k][t], s=2..n+2*frac(k/2)),
k=1..k0()) +
I* add( ln( simplify( Udagger(l)[1,1]*U(l)[1,1]+
Udagger(l)[1,2]*U(l)[2,1] ) ),l=1..n+1):

13
7. The next commands calculate the Langevin equation given in eq. (17).

\[ dS := \text{map(factor,diff}(S,\sigma[2,1][t])): \]
\[ \text{Diff}(\sigma[2,1][t],t) = \text{map}(x->x*(-I/2),dS) + \eta(t); \]

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