UNIVERSITÀ DI TRENTO

DEPARTMENT OF PHYSICS

MASTER DEGREE IN PHYSICS

The Hubbard-Stratonovich transformation in quantum computing applications

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Contents

Abstract

The standard Implementation of multi-qubit gates on quantum computers normally consists of decomposing them in a sequence of one- and two-qubit gates, that are part of a certain so-called *standard set*, applied on parts of the full system. This kind of expansion is guaranteed to converge less then exponentially by the Solovay-Kitaev theorem. However, on physical machines, two-qubit gates have in general a much worse fidelity (i.e. have a behavior further from ideal) with respect to the first ones. This thesis was initially inspired by the search of an alternative method for the implementation of certain multi-qubit gates by means of a combination of only one-qubit gates relying on the *Hubbard-Stratonovich* transformation (HST).

After a brief recap of the basic elements of quantum computing and the notion of entangled states in chapters 1 and 2 respectively, in chapter 3 this exact transformation is introduced along with the methods that can be used to implement it in terms of a quantum gate, and including some examples.

In chapter 4, several aspects of the implementations are presented and explicitly discussed. Among them, different possible ways of classically performing the integral, and a procedure to implement non-unitary gates on a quantum computer by introducing ancillas in the system are presented.

The results of a number of different simulations (both classical and quantum) are shown in chapter 5. Such simulations are aimed to test the validity of the HST method and to compare different implementations techniques.

Finally, chapter 6 is dedicated to one of the most intriguing aspects that emerged in the analysis of the HST used in the context of quantum computation, that is its apparent formal analogy to the local hidden-variable theories. In the chapter, a short introduction to local hidden-variable theories is given, and possible similarities and contrasts

between these and the HST are briefly discussed. An in-depth analysis of this topic, which could bare substantial fundamental implications about the technique presented in this thesis, will be carried out in a future follow-up work.

A conclusion is given in chapter 7, summing up all the arguments discussed in the thesis and outlining some of the perspectives that are pointed out by this work.

Chapter 1

Quantum Computing Overview [1]

1 Classical and quantum computers

At present time it is hard to find someone not knowledgeable about what a computer is: a very simple definition could be that such a computer is a machine which is able to memorize and do operations on some set of data.

The most fundamental information unit in a classic computer is the *bit*, which can be seen as a variable that can be found in only one of two possible states, usually labelled by 0 and 1. A classical operation g on a certain number N of bits is a function, called *gate*, which takes the values of the N bits as inputs and produces another binary value as output: $g : \{0,1\}^N \to \{0,1\}$.

Since 1980s, however, people began to think about a different kind of machines: *quantum computers*. In particular, the idea of a computer based on quantum elements and of its eventual advantages can be dated back to 1981, when Richard Feynman during a conference gave a speech about "Simulating Physics with computers" [2] [3].

Feynman main point was that classical computers are not suited for simulating physical systems, since these last have an intrinsic quantum nature which can be fully described in classical terms only at the cost of an exponential amount of resources. Feynman argued that instead the resources needed in a useful simulation should be only proportional to the volume occupied by the considered system. Consequently, he suggested the idea of simulating such systems directly with other quantum systems, i.e. to substitute the classical computers with a different kind of computers, which he referred to as quantum computers.

The main difference between a classical and a quantum computer consists of the fact that in the latter the most fundamental unit of memory is a two-states quantum system called *qubit*, onto which such a computer is able to perform transformations as defined in quantum mechanics, called *quantum gates*.
Consequently, the state $|\psi\rangle$ of a qubit can be at any time an arbitrary complex linear combination with constant norm (conventionally assumed to be unitary) of the two possible system levels (these last corresponding to the two classical bit states). The space of all these possible states $|\psi\rangle$ is the Hilbert space $\mathscr{H}$ of the qubit:

$$\mathscr{H} \ni |\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \quad \text{with} \quad |\alpha|^2 + |\beta|^2 = 1, \quad \alpha, \beta \in \mathbb{C}.$$

A convenient way to express the state of a qubit can be that of parametrizing it as a point on the surface of a sphere of unitary radius, which requires only two angles θ and ϕ:

$$\cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}\,|1\rangle$$

Such representation is called the *Bloch sphere*, and is illustrated in Fig. 1.1.

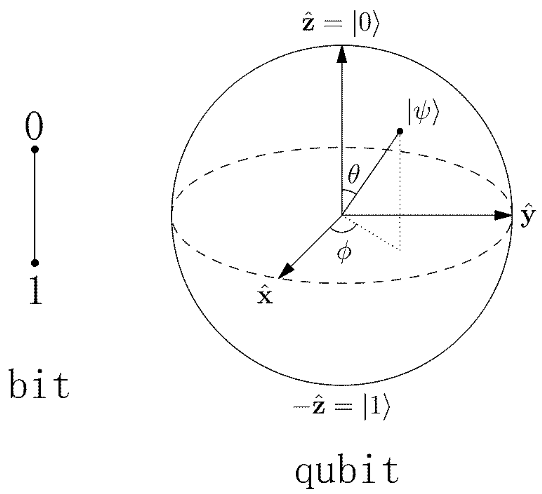


Figure 1.1: visual representation of the difference among possible states for a classical bit, that can assume values mapped on two points, and a qubit, that can span the whole surface of the Bloch sphere [4]

2 Quantum gates

Quantum gates, similarly to the classical ones, can be seen as unitary operators (since the norm must be conserved) acting onto one or more qubits. However, their effect is always that of changing the state of the full quantum system (i.e. the one describing all the i input qubits), not to produce a string of qubits each in a certain state (as it would be in a straightforward classical analogy). Indicating the gate as $\hat{G}$, this is defined as:

$$\begin{aligned} \hat{G} : \mathscr{H} &\to \mathscr{H} \qquad\qquad \text{where} \qquad \mathscr{H} = \bigotimes_i \mathscr{H}_i \\ |\psi\rangle &\to |\psi'\rangle = \hat{G}\,|\psi\rangle \end{aligned}$$

Quantum gates can be distinguished in two classes according to their action on the states of a multipartite system: the *entangling gates* and the non-entangling ones (rarely *separable gates*). A similar classification in fact exists also for the states, which can be either entangled or not-entangled (i.e. separable): separable states are those states $|\psi\rangle$ of a multipartite system which can be factorized in M other states, each one associated to a single different part of the system, while all the other states are the entangled ones. Separable states are then the only ones which can be written in the following form

$$|\psi\rangle = \bigotimes_{i=1}^{M} |\psi_i\rangle$$

Accordingly, entangling gates are defined as those operators which produce an entangled state when applied on a separable one.

This arguments will be discussed in further detail in Chap. 2.

2.1 Implementation

The standard way to implement a gate $\hat{G}$ in quantum computers, i.e. to transform the state $|\psi\rangle$ of a system of N qubits into a new state $|\psi'\rangle = \hat{G}\,|\psi\rangle$, is to rely on the natural time evolution $\hat{T}_H$ of the system itself. In general the operator $\hat{T}_H$ can be expressed as a *propagator* relative to some Hamiltonian $\hat{H}$ which does not necessarily coincide with the Hamiltonian describing the physical realization of the qubit. Then, the state $|\psi\rangle$

of a quantum system naturally changes over time according to the following formula:

$$|\psi'\rangle = \hat{T}_H |\psi\rangle = e^{-\frac{i}{\hbar}\hat{H}t} |\psi\rangle$$

Since the Hamiltonian $\hat{H}$ includes a time dependent external potential $V(t)$ (sometime called *driving term*), which can be classically controlled, one could in principle apply any gate $\hat{G}$ to the system: it would be sufficient to apply a potential $\tilde{V}(t)$ corresponding to the Hamiltonian $\hat{\tilde{H}}$ such that $\hat{G} = \hat{T}_{\tilde{H}}$, making the system evolve under such interaction for the required time period.

Controlled transformations $\hat{T}_H$ only produce unitary gates $\hat{G}_u$. While this is more than enough in order to implement a minimal set of quantum gates that can be used as a basis to build other arbitrary unitary transformations, in some applications one might want to access controlled non-unitary operations. Several methods have been proposed to implement such non-unitary gates. For example, this could be achieved by extending the Hilbert space of the system adding some extra qubits called *ancillas* and acting on the full Hilbert space (system + ancillas) with unitary gates in the standard way [5] (see Chap. 4 Sec. 3).

2.2 Universality

As it was just discussed above, it is possible in principle to create arbitrary gates by finding the Hamiltonian that evolves the quantum machine to the wanted state over a certain time T. However, finding such Hamiltonian is in general exponentially expensive. The question then rises whether it is possible to implement any unitary transformation as a composition of some limited set, and how many of them would in general be necessary.

A very important result (Solovay-Kitaev theorem [6] [7]) is that any possible quantum gate acting on any number of qubits can be efficiently approximated by a finite sequence of gates (called *quantum circuit*) belonging to a finite universal set, which can be chosen to consist of only one- and two-qubit gates (i.e. quantum gates acting only on one or at most two qubits) [8] [9] [10]: this means that in principle a universal quantum computer (i.e. a quantum computer which can do any possible operation on its qubits) can be built as a machine which is able to act on its qubits only with one- or two-qubit operators. Moreover, given ϵ a target distance in the Hilbert space between the required operator and its approximation, the number of gates needed grows as $\log^{\alpha}(1/\epsilon)$, with $3 < \alpha < 4$. For this very reason, one- and two-qubit gates play an

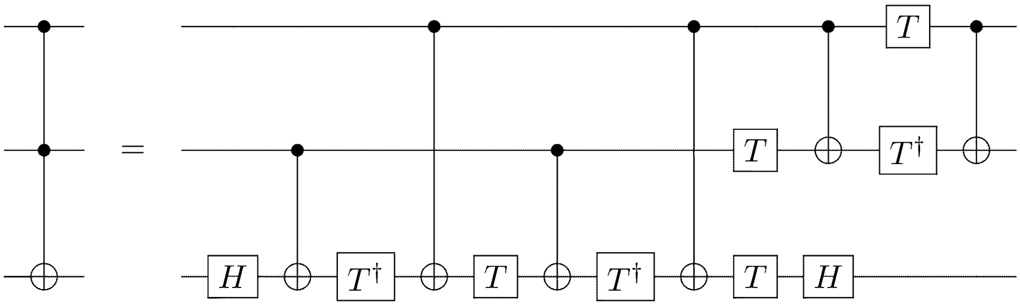


Figure 1.2: Quantum circuit showing the decomposition of a Toffoli gate (a three qubits gate) using only one qubit gates and CNOT gates (each of which is a two qubit gate) [11]

important role in quantum computing with respect to general quantum gates. There is a lot of interest in optimizing the performances of such gates in quantum machines, since a satisfactory approximation of a generic unitary transformations usually requires a large number of them.

2.3 Coherence and fidelity

One of the most severe drawbacks of quantum computation is that qubits maintain their state for a limited amount of time called *coherence time*. Since gates do not act in an instantaneous way, but need a finite amount of time to be applied (depending among other parameters also on the efficiency of the gate implementation), the number of possible operations which can be done on a qubit during a calculation is in turn limited.

While one-qubit gates are usually fast, in the sense that their implementation time is at the very least one order of magnitude shorter then the qubit coherence time, the true bottleneck is represented by two-qubit gates, which can be applied only a few times before the qubit completely looses its coherence.

Finite qubit coherence times together with non-ideal gate implementations translate in the fact that even if in theory it could be possible to exactly prepare an arbitrary desired state, the physical application of gates in an actual quantum machine would still produce a state which would be partly different from the expected one. The measured distance in the Hilbert space of the system between the actual final state and the ideal one is called the *gate fidelity*, and measures how close the physical gate is to the ideal one [12].

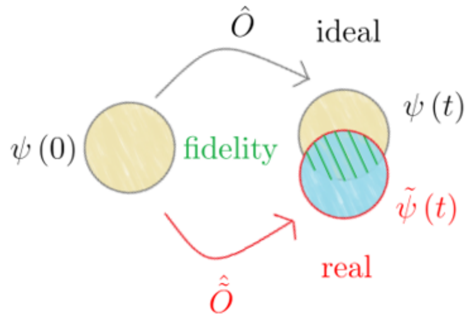


Figure 1.3: Pictorial representation of gate fidelity, which is the distance between the real state produced by the implemented gate and the ideal one

Since in principle the gate fidelity could depend on the chosen initial state, it could be useful to average over all the possible states: the computed quantity in this case is called *average gate fidelity*.

In the rest of this work I will discuss a possible method for implementing certain two-qubit gates by means of a classical combination of only one-qubit gates, where this combination is the Hubbard-Stratonovich transformation which I will discuss in further detail later.

Chapter 2

Entangled States [13]

1 Introduction

As anticipated in Chap. 1 Sec. 1, a general state $|\psi\rangle$ of a multi-qubit system could be any element with unitary norm of the full Hilbert space $\mathscr{H}$ of the system, where $\mathscr{H}$ is the tensor product of all the smaller Hilbert spaces $\mathscr{H}_i$ associated to each single qubit in the system.

In general, only the state of the full multi-qubit system will be well defined, while it won't be so for the subsystems constituted by subsets of all the qubits. If however there exist a certain number M of distinct portions of the full system which have a well defined state (calling $\{\psi_i\}_{i=1,\ldots,M}$ all such states), then $|\psi\rangle$ is said to be a *separable state* and can be written in the following form:

$$|\psi\rangle = \bigotimes_{i=1}^{M} |\psi_i\rangle \tag{2.1}$$

Moreover, if each single qubit is in a precise state, i.e. if M coincides with the number of qubits in the system, then the state is called *completely separable* or, equivalently, a *product state*.

An example of a state of this kind describing a bipartite system is the following, where the vector notation $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ is used:

$$|01\rangle = |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}.$$

All the other states that cannot be represented in the form of Eq. (2.1) are instead called *entangled states* and must be represented as normalized linear combinations of completely separable states. An example of such states describing once again a bipartite system is the following (*singlet state*):

$$|-\rangle \doteq \frac{1}{\sqrt{2}} (|01\rangle - |01\rangle) = \frac{1}{\sqrt{2}} \left(\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}.$$

From these definitions it can be shown that entangled states present correlations among different parts of the full system which have a completely quantum nature, i.e. correlations that have no classic counterpart. The full system is in a well defined and completely known state, although it is not possible to provide measurements to determine the state of a single part of it independent from the rest of the system.

Separable states on the other hand do not show this behaviour. If one measures the observable $\hat{A} \otimes \hat{B}$ on a bipartite system in a separable state $|\phi_A \phi_B\rangle \equiv |\phi_A\rangle \otimes |\phi_B\rangle$, where $\hat{A}$ is an operator acting only on the first part (which is in state $|\phi_A\rangle$) while $\hat{B}$ acts only on the second (this being in state $|\phi_B\rangle$), the result would be the following:

$$\begin{aligned} \langle \hat{A} \otimes \hat{B} \rangle_{AB} &\equiv \langle \phi_A \phi_B | \hat{A} \otimes \hat{B} | \phi_A \phi_B \rangle = (\langle \phi_A | \otimes \langle \phi_B |) \left(\hat{A} \otimes \hat{B} \right) (|\phi_A\rangle \otimes |\phi_B\rangle) = \\ &= \langle \phi_A | \hat{A} | \phi_A \rangle \langle \phi_B | \hat{B} | \phi_B \rangle \equiv \langle \hat{A} \rangle_A \langle \hat{B} \rangle_B \end{aligned}$$

This result shows that the *connected correlator* of the observable $\hat{A} \otimes \hat{B}$ over the separable state $|\phi_A \phi_B\rangle$ is 0, $\langle \hat{A} \otimes \hat{B} \rangle_{AB} - \langle \hat{A} \rangle_A \langle \hat{B} \rangle_B = 0$. In case the system was in an entangled state instead, such quantity would be non-zero, because the first term could not be separated in terms related each one to single parts of the system.

2 Density matrices and von Neumann entropy

The definitions given in the previous section are rather simple: they are "yes or no" definitions, i.e. they only allow to verify if a given state is entangled or not, but do not say anything about how to "quantify" entanglement.

In order to be able to introduce a measure for the entanglement of a state, it is first necessary to introduce the concept of *density matrix*. A density matrix is an alternate way to represent a state of a quantum system even when this is a *mixed state*, i.e. when the system can only be found with a certain probability in a given *pure state*, where a pure state is any element of the Hilbert space $\mathscr{H}$ of the system.

By choosing an orthonormal basis $\{\psi_i\}_{i=1,\dots,N}$ of $\mathscr{H}$ (with N the dimension of $\mathscr{H}$) one can represent the density matrix $\hat{\rho}$ of a system in the following way:

$$\hat{\rho} = \sum_{i=1}^{N} p_i \left|\psi_i\right\rangle \left\langle\psi_i\right| , \tag{2.2}$$

where p_i is the probability of finding the system in the pure state $|\psi_i\rangle$.

The trace of the density matrix squared gives the purity of a state: if a system is in a state characterized by a density matrix $\hat{\rho}$ such that $Tr(\hat{\rho}^2) = 1$, then the state will be pure, otherwise if $Tr(\hat{\rho}^2) < 1$ then the state will be mixed.

Furthermore, if the considered system is constituted of two different subsystems A and B having respectively Hilbert spaces $\mathscr{H}_A$ and $\mathscr{H}_B$ (such that $\mathscr{H} = \mathscr{H}_A \otimes \mathscr{H}_B$), by choosing an orthogonal basis for each of these spaces ($\{\psi_\alpha^{(A)}\}_{\alpha=1,\dots,N_A}$ and $\{\psi_\beta^{(B)}\}_{\beta=1,\dots,N_B}$, with $N_A + N_B = N$) it is possible to recast Eq. (2.2) in the following form:

$$\begin{aligned}\hat{\rho} &= \sum_{\alpha=1}^{N_A}\sum_{\beta=1}^{N_B} \left|\psi_\alpha^{(A)}\psi_\beta^{(B)}\right\rangle \left\langle\psi_\alpha^{(A)}\psi_\beta^{(B)}\right| \hat{\rho} \sum_{\alpha'=1}^{N_A}\sum_{\beta'=1}^{N_B} \left|\psi_{\alpha'}^{(A)}\psi_{\beta'}^{(B)}\right\rangle \left\langle\psi_{\alpha'}^{(A)}\psi_{\beta'}^{(B)}\right| = \\ &= \sum_{\substack{\alpha,\beta,\\ \alpha',\beta'}} \left\langle\psi_\alpha^{(A)}\psi_\beta^{(B)}\right| \hat{\rho} \left|\psi_{\alpha'}^{(A)}\psi_{\beta'}^{(B)}\right\rangle \left|\psi_\alpha^{(A)}\psi_\beta^{(B)}\right\rangle \left\langle\psi_{\alpha'}^{(A)}\psi_{\beta'}^{(B)}\right|\end{aligned}$$

At this point one can obtain the *reduced density matrix* relative to one of the two subsystems (for instance A) by tracing the last expression over the basis of the other subsystem:

$$\hat{\rho}_A \doteq Tr_B(\hat{\rho}) = \sum_{\alpha,\alpha'=1}^{N_A} \sum_{\beta=1}^{N_B} \left\langle \psi_\alpha^{(A)} \psi_\beta^{(B)} \right| \hat{\rho} \left| \psi_{\alpha'}^{(A)} \psi_\beta^{(B)} \right\rangle \left| \psi_\alpha^{(A)} \right\rangle \left\langle \psi_{\alpha'}^{(A)} \right| .$$

One can finally introduce the *von Neumann entropy* of a given density matrix $\hat{\rho}$, defined as:

$$S_{vN}(\hat{\rho}) = -Tr(\hat{\rho} \ln(\hat{\rho})).$$

Thanks to this quantity one finally obtains a correct measure for the entanglement of a state[1]: if a bipartite system is divided into two subsystems A and B and is found in a state defined by the density matrix $\hat{\rho}$, then the entanglement of such state can be quantified by the von Neumann entropy evaluated on the reduced density matrices relative to either of the two subsystems. If $\hat{\rho}$ describes a separable state than I will have that $S_{vN}(\hat{\rho}_A) = S_{vN}(\hat{\rho}_B) = 0$, otherwise both this quantities will have a positive value.

The von Neumann entropy has also a maximum value, which corresponds to the natural logarithm of the dimension of its argument: if a system is in a pure state defined by $\hat{\rho}$ such that the von Neumann entropy of the reduced density matrices are maximum, then the state corresponding to $\hat{\rho}$ is unique (up to local unitary operations) and said to be *maximally entangled* (often this state is also called *Bell state*).

As an example, I will now present three different pure states for a system of 2 qubits: the first is separable, the second is partly entangled and the last one is a Bell state, i.e. maximally entangled

[1]This definition works fine only for pure states, but in this work I will totally focus on these and I will ignore mixed states

$\vert\psi\rangle$	$\hat{\boldsymbol{\rho}}_{\boldsymbol{A}}$	$\boldsymbol{S_{vN}(\hat{\rho}_A)}$
$\vert 11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$	$\vert 1\rangle\langle 1\vert$	0
$\sqrt{0.9}\,\vert 11\rangle + \sqrt{0.1}\,\vert 00\rangle = \begin{pmatrix} \sqrt{0.9} \\ 0 \\ 0 \\ \sqrt{0.1} \end{pmatrix}$	$0.9\,\vert 1\rangle\langle 1\vert + 0.1\,\vert 0\rangle\langle 0\vert$	$\ln(10) - \frac{9}{10}\ln(9) \approx 0.325$
$\frac{1}{\sqrt{2}}(\vert 11\rangle + \vert 00\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$	$\frac{1}{2}\,\vert 1\rangle\langle 1\vert + \frac{1}{2}\,\vert 0\rangle\langle 0\vert$	$\ln(2) \approx 0.693$

Besides the von Neumann entropy there are several other quantities which can be used in order to measure the entanglement of a state (entanglement as a resource, distillable entanglement, entanglement cost, ...), some of which also works for mixed states: different quantities may order differently certain states, however separable and Bell states will always be such according to any entanglement measure.

Chapter 3

Hubbard-Stratonovich Transformation

1 Overview

I recall that in Chap. 1 I have shown that in quantum computers usually a unitary gate $\hat{G}_u$ is implemented as a real time evolution operator, i.e. an operator having the following form

$$\hat{G}_u = e^{-\frac{i}{\hbar}\hat{H}t_r} \tag{3.1}$$

where $\hat{H}$ is a precise Hamiltonian applied to the system of qubits onto which the gate $\hat{G}_u$ is acting.

It was also anticipated that several methods exist which allow for the implementation of non-unitary gates $\hat{G}_{nu}$. Such non-unitary gates can always be written in the following form, i.e. as if they were obtained by an imaginary time evolution of the system onto which they act:

$$\hat{G}_{nu} = e^{-\frac{1}{\hbar}\hat{H}t_i} \tag{3.2}$$

From Eq. (3.1) and Eq. (3.2) it follows that it is possible to represent any (unitary or non-unitary) gate $\hat{G}$ as if it was obtained by the evolution of the system onto which it acts for a complex time $\tilde{t} \doteq -it \doteq t_r - it_i$ under a given Hamiltonian $\hat{H}$:

$$\hat{G} = e^{-\frac{i}{\hbar}\hat{H}\tilde{t}} = e^{-\frac{1}{\hbar}\hat{H}t}. \tag{3.3}$$

One can now introduce the Hubbard-Stratonovich transformation [14] [15], which is defined as the following exact mathematical relation:

$$e^{-\frac{ax^2}{2}} = \int dy \frac{1}{\sqrt{2\pi a}} e^{-\frac{y^2}{2a} - ixy}. \tag{3.4}$$

This transformation introduces a classical field y that makes it possible to reduce the exponent of the left hand side (LHS) of (3.4) from quadratic in x to linear in the operator, though coupled with the auxiliary classical field y. In one of the next chapters we will discuss when this feature turns out to be useful.

For the moment we limit ourselves to note that the LHS of (3.4) is very similar to the form (3.3) in which we have written any operator $\hat{G}$ which can act on an arbitrary number of qubits in a quantum computer. In fact, any Hamiltonian $\hat{H}$ can always be written as the square of its square root $\hat{H} = \sqrt{\hat{H}}\sqrt{\hat{H}} = \left(\sqrt{\hat{H}}\right)^2$. It is then possible to recast (3.3) in the following way:

$$\hat{G} = e^{-\frac{1}{\hbar}\hat{H}t} = e^{-\frac{1}{\hbar}\left(\sqrt{\hat{H}}\right)^2 t} = e^{-\frac{\left(\sqrt{2\frac{t}{\hbar}\hat{H}}\right)^2}{2}} \doteq e^{-\frac{\left(\sqrt{t\hat{H}'}\right)^2}{2}}, \tag{3.5}$$

where we defined $\hat{H}' \doteq \frac{2\hat{H}}{\hbar}$ for a clearer comparison: it is in fact now immediate to identify the RHS of (3.5) with the LHS of (3.4) by setting $a = 1$ and $x = \sqrt{t\hat{H}'}$. Substituting these identities in (3.4) one obtains:

$$e^{-\frac{\hat{H}'}{2}t} = \int dy \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} e^{-iy\sqrt{t}\sqrt{\hat{H}'}}. \tag{3.6}$$

2 First Example

I will now show explicitly how to use the Hubbard-Stratonovich formalism in order to rewrite a simple operator.

One can start by choosing a time independent gate $\hat{O} = e^{-i\frac{\hat{H}}{2}}$ acting on a two-qubit system. This operator can be represented by means of a 4x4 matrix. In particular, let us choose the following operator:

$$\hat{O} = e^{-i\frac{\hat{H}}{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \end{pmatrix}, \tag{3.7}$$

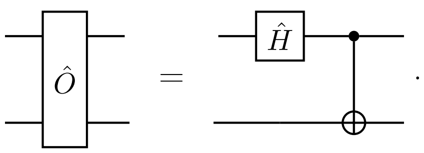
which is easy to demonstrate to be unitary. The operator $\hat{H}$ is also Hermitean and such that one of its square roots is the following:

$$\sqrt{\hat{H}} = \frac{i\sqrt{\pi}}{4\sqrt{2}}\begin{pmatrix} 3-\sqrt{2}+i & 1-\sqrt{2}-i & -1-\sqrt{2}-i & 1-\sqrt{2}+i \\ 1-\sqrt{2}-i & 3-\sqrt{2}+i & 1-\sqrt{2}+i & -1-\sqrt{2}-i \\ 1-\sqrt{2}+i & -1-\sqrt{2}-i & 3+\sqrt{2}+i & 1+\sqrt{2}-i \\ -1-\sqrt{2}-i & 1-\sqrt{2}+i & 1+\sqrt{2}-i & 3+\sqrt{2}+i \end{pmatrix}.$$

Using the matrix Kronecker product it is possible to show that $\hat{O}$ can be decomposed in the following sequence of operators, each one acting on one or both the qubits in the system:

$$\hat{O} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = C\hat{NOT} \cdot \hat{H} \otimes \hat{\mathbb{1}},$$

where $\hat{H}$ is the Hadamard gate, $C\hat{NOT}$ the controlled not gate and $\hat{\mathbb{1}}$ the two dimensional identity, acting on a single qubit.
This means that $\hat{O}$ can also be represented graphically by the following circuit, which is the easiest circuit used to generate an entangled state of two qubits:



Acting with this gate $\hat{O}$ on the system state $|00\rangle \doteq |0\rangle \otimes |0\rangle$, in fact, transforms it into the Bell state $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, i.e. one of the four possible maximally entangled states for a two qubit system:

$$\hat{O}\,|00\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle\right)$$

Now, Eq. (3.6) with unitary real time t_r and null imaginary time t_i can be used to recast $\hat{O}$ through its definition by means of the Hermitean operator $\hat{H}$ as an integral of an infinite set of operators $\hat{O}_x$, parametrized by an auxiliary real field x:

$$\hat{O} = e^{-i\frac{\hat{H}}{2}} = \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \hat{O}_x, \tag{3.8}$$

with $\hat{O}_x \doteq e^{-ix\sqrt{i\hat{H}}}$.

Knowing $\hat{H}$, one can explicitly compute the form of operators $\hat{O}_x$:

$$\hat{O}_x \doteq e^{-ix\sqrt{i\hat{H}}} = \frac{1}{4} \begin{pmatrix} a & b & c & d \\ b & a & d & c \\ d & c & e & f \\ c & d & f & e \end{pmatrix},$$

with:

$$\begin{aligned}
a &= \frac{\sqrt{2}-1}{\sqrt{2}} e^{-\sqrt{\pi}(1+i)x} + 2e^{-i\frac{\sqrt{\pi}}{2}x} \cosh\left(\frac{\sqrt{\pi}}{2}x\right) + \frac{\sqrt{2}+1}{\sqrt{2}} \\
b &= \frac{\sqrt{2}-1}{\sqrt{2}} e^{-\sqrt{\pi}(1+i)x} - 2e^{-i\frac{\sqrt{\pi}}{2}x} \cosh\left(\frac{\sqrt{\pi}}{2}x\right) + \frac{\sqrt{2}+1}{\sqrt{2}} \\
c &= -\frac{1}{\sqrt{2}} e^{-\sqrt{\pi}(1+i)x} + 2ie^{-i\frac{\sqrt{\pi}}{2}x} \sinh\left(\frac{\sqrt{\pi}}{2}x\right) + \frac{1}{\sqrt{2}} \\
d &= -\frac{1}{\sqrt{2}} e^{-\sqrt{\pi}(1+i)x} - 2ie^{-i\frac{\sqrt{\pi}}{2}x} \sinh\left(\frac{\sqrt{\pi}}{2}x\right) + \frac{1}{\sqrt{2}} \\
e &= \frac{\sqrt{2}+1}{\sqrt{2}} e^{-\sqrt{\pi}(1+i)x} + 2e^{-i\frac{\sqrt{\pi}}{2}x} \cosh\left(\frac{\sqrt{\pi}}{2}x\right) + \frac{\sqrt{2}-1}{\sqrt{2}} \\
f &= \frac{\sqrt{2}+1}{\sqrt{2}} e^{-\sqrt{\pi}(1+i)x} - 2e^{-i\frac{\sqrt{\pi}}{2}x} \cosh\left(\frac{\sqrt{\pi}}{2}x\right) + \frac{\sqrt{2}-1}{\sqrt{2}}
\end{aligned} \quad .$$

Substituting now this matrix in Eq. (3.8) one explicitly obtains the formulation of $\hat{O}$ by means of the Hubbard-Stratonovich transformation: performing the integrals of each element one recovers exactly the matrix in Eq. (3.7).

3 Developing separability

The previously discussed example is not a very useful application of the Hubbard-Stratonovich transformation to the decomposition of a quantum gate, at least not in the optics of rephrasing the latter in a form more easily implementable on a quantum computer. The problem has in fact moved from the implementation of a single two-qubit gate $\hat{O}$ to that of many two-qubit gates $\hat{O}_x$ (each of which in principle could even be harder to implement than the original one), with the additional nuisance of having to deal with a classical integration step (which will definitely require a certain amount of resources).

It is however possible to show that there exist particular cases in which this Hubbard-Stratonovich formulation of gates allows for a simplification of the problem, at least in some aspects.

Let us consider, for example, a system with N qubits whose Hamiltonian takes the form of the square of a sum of N terms, each one of them being an operator acting on a single, different qubit of the system:

$$\hat{H} = \frac{1}{2} \left(\sum_{i=1}^{N} \hat{O}_i \right)^2 . \tag{3.9}$$

Formally, each of the $\hat{O}_i$ is still an N-qubit operator, which could be written in terms of the corresponding one-qubit operator $\hat{\hat{O}}_i$ in the following way:

$$\hat{O}_i = \bigotimes_{j=1}^{N} \hat{\mathbb{1}}_j^{(2)} + \left(\hat{\hat{O}}_j - \hat{\mathbb{1}}_j^{(2)} \right) \delta_{ij},$$

where $\hat{\mathbb{1}}_i^{(2)}$ is the two dimensional identity operator acting on qubit i and δ_{ij} is the Kronecker delta, equal to 1 if $i = j$ and to 0 otherwise.

The important thing is that since each $\hat{O}_i$ operator acts on a different qubit, all of them will commute one with the other: the complex time evolution operator associated to such an Hamiltonian, which will be in general an N-qubit operator acting on all the qubits in the system, could then be decomposed by means of the Hubbard-Stratonovich transformation (see Eq. (3.6)) in a combination of just one-qubit operators:

$$\begin{aligned}\hat{T}_H &= e^{-\hat{H}t} = e^{-\frac{1}{2}\left(\sqrt{t}\sum_{i=1}^{N}\hat{O}_i\right)^2} = \int dy \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} e^{-iy\sqrt{t}\sum_{i=1}^{N}\hat{O}_i} = \\ &= \int dy \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} \prod_{i=1}^{N} e^{-iy\sqrt{t}\hat{O}_i} = \int dy \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} e^{-iy\sqrt{t}\bigoplus_{i=1}^{N}\hat{\hat{O}}_i} = \\ &= \int dy \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} \bigotimes_{i=1}^{N} e^{-iy\sqrt{t}\hat{\hat{O}}_i},\end{aligned} \tag{3.10}$$

with $t = it_r + t_i$ the complex evolution time (t_r and t_i being respectively the real and imaginary evolution times), $\oplus$ the Kronecker sum of operators (i.e. the application such that $\hat{A} \oplus \hat{B} = \hat{A} \otimes \hat{\mathbb{1}} + \hat{\mathbb{1}} \otimes \hat{B}$) and where in the fourth identity the already discussed property that $\left[\hat{O}_i, \hat{O}_j\right] = 0 \quad \forall\ i \neq j$ is used, while in the last step one exploits $e^{N \oplus M} = e^N \otimes e^M$ (see for example [16]).

This result is now potentially very useful: if it is possible to write a multi-qubit gate $\hat{G}$, to be used in a certain calculation, in the form of $\hat{T}_H$, i.e. as the (in general complex) time evolution operator of the system under an Hamiltonian of the kind of Eq. (3.9), then it will be possible to implement on the machine such operator $\hat{G}$ using exclusively a classical combination of one-qubit gates, having a much better fidelity than the two-qubit ones (as it has already been discussed in Chap. 1 Sec. 2.3).

4 Second Example

Let us now consider another explicit example of a realistic situation in which the Hubbard-Stratonovich transformation can be use to formulate a multi-qubit gate. In this case the HST leads to the possibility of applying the latter by means of one-qubit gates only.

The starting point consists of considering a two-qubit system subject to the following Hamiltonian (a case which is extremely common in physics):

$$\hat{H} = \hat{\vec{\sigma}}^{(1)} \cdot \hat{\vec{\sigma}}^{(2)} = \hat{\sigma}_x^{(1)}\hat{\sigma}_x^{(2)} + \hat{\sigma}_y^{(1)}\hat{\sigma}_y^{(2)} + \hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)}, \tag{3.11}$$

with $\hat{\vec{\sigma}}^{(i)}$ being the Pauli vector $(\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ acting, for instance, on the spinor of some spin 1/2 Fermion of index i.

This Hamiltonian can be recast in a different form by using the following identities:

$$\hat{\sigma}_i^{(a)}\hat{\sigma}_i^{(b)} = \frac{\left(\hat{\sigma}_i^{(a)} + \hat{\sigma}_i^{(b)}\right)^2 - \hat{\sigma}_i^{2(a)} - \hat{\sigma}_i^{2(b)}}{2} = \frac{\left(\hat{\sigma}_i^{(a)} + \hat{\sigma}_i^{(b)}\right)^2}{2} - 1 \qquad \forall \quad i \in \{x, y, z\}.$$

By inserting this result in the previous formula it becomes evident that the following holds:

$$\hat{H} = \hat{\vec{\sigma}}^{(1)} \cdot \hat{\vec{\sigma}}^{(2)} = \frac{\left(\hat{\vec{\sigma}}^{(1)} + \hat{\vec{\sigma}}^{(2)}\right)^2}{2} - 3 = \frac{\sum_{i=x,y,z}\left(\hat{\sigma}_i^{(1)} + \hat{\sigma}_i^{(2)}\right)^2}{2} - 3.$$

Besides a constant "offset" factor (which commutes with any of the other terms) this Hamiltonian is now written exactly in the form of Eq. (3.9). Given what was discussed in the last section, it is already known that the time evolution operator $\hat{T}_H$ associated to $\hat{H}$ can be expressed as an integral of the Kronecker product of only one-qubit operators. Let us then consider such operator, that we call $\hat{T}_H$ (with $\tilde{t} = t_r - it_i$ as in Chap. 3 Sec. 1):

$$\hat{T}_H = e^{-i\hat{\vec{\sigma}}^{(1)}\cdot\hat{\vec{\sigma}}^{(2)}\tilde{t}} = e^{3i\tilde{t}}e^{-i\frac{\left(\hat{\vec{\sigma}}^{(1)}+\hat{\vec{\sigma}}^{(2)}\right)^2}{2}\tilde{t}} = e^{3i\tilde{t}}e^{-i\frac{\left(\hat{\sigma}_x^{(1)}+\hat{\sigma}_x^{(2)}\right)^2}{2}\tilde{t}}e^{-i\frac{\left(\hat{\sigma}_y^{(1)}+\hat{\sigma}_y^{(2)}\right)^2}{2}\tilde{t}}e^{-i\frac{\left(\hat{\sigma}_z^{(1)}+\hat{\sigma}_z^{(2)}\right)^2}{2}\tilde{t}},$$

and where in the last identity the fact that $\left[\left(\hat{\sigma}_i^{(1)} + \hat{\sigma}_i^{(2)}\right)^2, \left(\hat{\sigma}_j^{(1)} + \hat{\sigma}_j^{(2)}\right)^2\right] = 0 \quad \forall\, i, j \in \{x, y, z\}$ was used, together with the factorization of the constant commuting term.
All the last three exponential factors are now in the form of Eq. (3.10), which means that one can write any of them in the following form thanks to the Hubbard-Stratonovich transformation

$$e^{-i\frac{\left(\hat{\sigma}_i^{(1)}+\hat{\sigma}_i^{(2)}\right)^2}{2}\tilde{t}} = \int dy \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} e^{\frac{1-i}{\sqrt{2}}y\sqrt{\tilde{t}}\hat{\sigma}_i^{(1)}} \otimes e^{\frac{1-i}{\sqrt{2}}y\sqrt{\tilde{t}}\hat{\sigma}_i^{(2)}}.$$

We will later discuss how the implementation of such integrals can be actually performed. However, the important fact is that now any decomposition of the integrand can be expressed as the tensor product of two one-qubit operators only. This means that the evaluation of any of the terms contributing to the integrand requires to act with single one-qubit gates only on each of the two qubits in the system.
Since the combination of all the terms needed to get the final result will be performed

classically, the full quantum action of the original two-qubit gate on the two-qubit system can now be obtained simply by repeating several times, one for each needed term making up the integrand, the application of a single one-qubit gate to each qubit. Any of these gates will then in general have a better fidelity then that of the original two-qubit gate, which means that if the combination of each contribute into the integral is efficient enough, there are good chances that the final result will be better then the bare application of the original gate.

4.1 Entanglement from one-qubit operators

There is a detail of the example that was just discussed that was not pointed out yet, which nonetheless bares fundamental implications and looks quite puzzling. Let us go a bit deeper in the previous analysis.

We have so far considered the Hamiltonian reported in Eq. 3.11, $\hat{H} = \hat{\vec{\sigma}}^{(1)} \cdot \hat{\vec{\sigma}}^{(2)}$, which has three degenerate eigenstates called *triplet states* plus a fourth one with a different eigenvalue, the *singlet state*:

$$\begin{array}{lclcl} \hat{\vec{\sigma}}^{(1)} \cdot \hat{\vec{\sigma}}^{(2)} \begin{cases} |00\rangle \\ |+\rangle \\ |11\rangle \end{cases} & = & 1 \begin{cases} |00\rangle \\ |+\rangle \\ |11\rangle \end{cases} & & \text{TRIPLET STATES} \\ \hat{\vec{\sigma}}^{(1)} \cdot \hat{\vec{\sigma}}^{(2)} \quad |-\rangle & = -3 & |-\rangle & & \text{SINGLET STATE,} \end{array}$$

where I used the following definition:

$$|\pm\rangle = \frac{1}{\sqrt{2}} \left(|01\rangle \pm |10\rangle \right).$$

From these considerations it follows that the separable state $|01\rangle$ *is not* an eigenstate of $\hat{H}$. It can in fact be written in the following way as a function of two of the previously shown eigenstates:

$$|01\rangle = \frac{1}{\sqrt{2}} \left(|+\rangle + |-\rangle \right).$$

The implications of this fact, together with the results of the last section, are nearly astounding: it seems that one could first prepare the two-qubit system in a separable state $|01\rangle$, and then let it evolve under the operator $\hat{T}_H = e^{-i\hat{H}\tilde{t}}$ (with $\tilde{t} = t_r - it_i$ as in section 1), which would eventually produce the following time dependent final state:

$$\begin{aligned}\hat{T}_H |01\rangle &= e^{-i\hat{\vec{\sigma}}^{(1)}\cdot\hat{\vec{\sigma}}^{(2)}\tilde{t}} |01\rangle = e^{-i\hat{\vec{\sigma}}^{(1)}\cdot\hat{\vec{\sigma}}^{(2)}\tilde{t}} \frac{1}{\sqrt{2}} (|+\rangle + |-\rangle) = \\ &= \frac{1}{\sqrt{2}} \left(e^{-i\tilde{t}} \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) + e^{3i\tilde{t}} \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle) \right) = \\ &= \frac{1}{2} \left(e^{-i\tilde{t}} + e^{3i\tilde{t}} \right) |01\rangle + \frac{1}{2} \left(e^{-i\tilde{t}} - e^{3i\tilde{t}} \right) |10\rangle = \\ &= e^{i\tilde{t}} \left(\cos(2\tilde{t}) |01\rangle - i \sin(2\tilde{t}) |10\rangle \right).\end{aligned} \tag{3.12}$$

It is evident that the evolution will bring the system in a non separable state and that in some instants it will even be in a maximally entangled state (*Bell state*). This is however creating some tension with our understanding, since we know from the previous discussion that $\hat{T}_H$ can be implemented by using one-qubit gates only.

This would mean that, with the only additional ingredient of the classical integration, one seems to be able to generate entanglement in an originally separable system only by working on the single qubits (or at least to recover the same measurements results that I would expect to find on such an entangled system). This looks contradictory at first sight, since entanglement explicitly implies the presence of correlations among different parts of a system which do not have a classical counterpart.

These considerations will be further discussed at the end of the thesis. For the moment let us stop by at acknowledging this implication of the Hubbard-Stratonovich formalism.

5 Bilinear forms

The Hubbard-Stratonovich formulation of quantum gates turns out to be useful in an even more general set of cases, thanks to the results presented in the following (see e.g. Ref. [17]).

Let us consider a system of N qubits with an Hamiltonian $\hat{H}$ which is a general bilinear form of M operators $\{\hat{O}_i^{(n_i)}\}_{i=1,\ldots,M}$, each one acting on a single qubit[1]. Such

[1] $\hat{O}_i^{(n_i)}$ will act on the n_i-th qubit, however it is still represented by an NxN matrix

Hamiltonian can be rewritten in the following form:

$$\hat{H} = \frac{1}{2} \sum_{i,j=1}^{M} \hat{O}_i^{(n_i)} A_{ij} \hat{O}_j^{(n_j)}, \tag{3.13}$$

where A_{ij} is a real and symmetric matrix of coefficients and $\hat{O}_i^{(n_i)} = \bigotimes_{m=1}^{N} \hat{\mathbb{1}}^{(m)} + \left(\hat{\hat{O}}_i^{(n_i)} - \hat{\mathbb{1}}^{(m)}\right) \delta_{mn_i}$ $\forall\, i \in (1, M)$, with $\hat{\hat{O}}_i^{(n_i)}$ a one-qubit operator acting on qubit n_i and $\hat{\mathbb{1}}^{(m)}$ the 2-dimensional identity operator acting on qubit m.

Now one can recast $\hat{H}$ in a form more suitable for the application of the Hubbard-Stratonovich formalism. In fact, the matrix A_{ij} can be diagonalized finding its M eigenstates $\left|\psi^{[k]}\right\rangle = \{\psi_i^{[k]}\}_{i=0,\dots,M}$ and corresponding eigenvalues λ_k, which by definition will be such that the following holds:

$$\begin{aligned} &\sum_{j=1}^{M} A_{ij} \psi_j^{[k]} = \lambda_k \psi_i^{[k]} \qquad && \forall \quad i \in [1, M] \\ &\sum_{j=1}^{M} \psi_j^{[k]} \psi_j^{[l]} = \delta_{kl} && \forall \quad k, l \in [1, M] \end{aligned}$$

.

With these tools it is possible to write A_{ij} in the following way:

$$A_{ij} = \sum_{k=1}^{M} \psi_i^{[k]} \lambda_k \psi_j^{[k]}.$$

Substituting this expression in Eq. (3.13) yields:

$$\hat{H} = \frac{1}{2} \sum_{i,j=1}^{M} \hat{O}_i^{(n_i)} \left(\sum_{k=1}^{M} \psi_i^{[k]} \lambda_k \psi_j^{[k]} \right) \hat{O}_j^{(n_j)} = \frac{1}{2} \sum_{k=1}^{M} \lambda_k \left(\sum_{i=1}^{M} \psi_i^{[k]} \hat{O}_i^{(n_i)} \right) \left(\sum_{j=1}^{M} \psi_j^{[k]} \hat{O}_j^{(n_j)} \right) =$$
$$= \frac{1}{2} \sum_{k=1}^{M} \lambda_k \hat{\mathcal{O}}_k^2,$$

where $\hat{\mathcal{O}}_k \doteq \sum_{i=1}^{M} \psi_i^{[k]} \hat{O}_i^{(n_i)}$.

Since sums of one-qubit operators acting on the same qubit are still one-qubit operators acting on such qubit, one can also define $\hat{\hat{O}}_m^{[k]} \doteq \sum_{i=1}^{M} \psi_i^{[k]} \hat{O}_i^{(n_i)} \delta_{mn_i}$ which acts only on qubit m, so that $\hat{\mathcal{O}}_k = \sum_{m=1}^{N} \hat{\hat{O}}_m^{[k]}$.

At this point one can proceed by defining $\hat{H}_k \doteq \frac{1}{2}\lambda_k \hat{\mathcal{O}}_k^2$ so that $\hat{H} = \sum_{k=1}^{M} \hat{H}_k$. It becomes evident that by this definition each $\hat{H}_k$ is written in the form of Eq. (3.9), meaning that the (complex) time evolution operator $\hat{T}_{H_k}$ associated to any of the various $\hat{H}_k$ can always be implemented on a quantum computer by means of only one-qubit gates (see Chap 3 Sec. 3).

If operators $\hat{\mathcal{O}}_k$ are such that they satisfy the following property:

$$\left[\hat{\mathcal{O}}_k^2, \hat{\mathcal{O}}_l^2\right] = 0 \qquad \forall k, l \in [1, M],$$

then $[\hat{H}_k, \hat{H}_l] = 0 \ \ \forall k, l \in [1, M]$ would also hold, so that one could write the (complex) time evolution operator $\hat{T}_H$ associated to the full Hamiltonian $\hat{H}$ as the product of all the various $\hat{T}_{H_k}$:

$$\hat{T}_H = e^{-\hat{H}t} = e^{-\sum_{k=1}^{M} \hat{H}_k t} = \prod_{k=1}^{M} e^{-\hat{H}_k t} = \prod_{k=1}^{M} \hat{T}_{H_k}, \tag{3.14}$$

with the complex time $t = t_i + it_r$ as defined in Chap. 3 Sec. 1.

This last result implies that one can also implement $\hat{T}_H$, the time evolution operator associated to the original general bilinear form in Eq. (3.13), with only one-qubit gates by using the Hubbard-Stratonovich procedure for all the $\hat{T}_{H_k}$ and taking their product.

Operators $\hat{\mathcal{O}}_k^2$ may also not commute with each other, though. In that case the decomposition in Eq. (3.14) would not hold, since one would have to add a term proportional to the commutator of the exponents appearing in such formula.

Since each operator always commutes with itself, however, the evolution operator can always be decomposed in consecutive evolutions for smaller times in the following way:

$$\hat{T}_H = e^{-\hat{H}t} = e^{-\hat{H}\frac{t}{n}n} = \left(e^{-\hat{H}dt}\right)^n = \prod_{j=1}^{n} e^{-\hat{H}dt} = \prod_{j=1}^{n} e^{-\sum_{k=1}^{M} \hat{H}_k dt},$$

with $dt \doteq \frac{t}{n}$ constant for each j and n chosen at will (actually, for the last identity n must be a positive integer).

Now, the commutators among the terms appearing in the exponent of the last identity is not zero because of what was just stated. However, the error due to omitting it for each single step will be proportional to dt^2, which can be made small at wish by choosing n to be sufficiently large. By making a suitable choice for n one can then very well approximate $\hat{T}_H$ in the following way (we will name this procedure *Trotterization*):

$$\hat{T}_H = \prod_{j=1}^{n} e^{-\sum_{k=1}^{M} \hat{H}_k dt} = \prod_{j=1}^{n} \prod_{k=1}^{M} e^{-\hat{H}_k dt} + O(dt^2) \approx \left(\prod_{k=1}^{M} d\hat{T}_{H_k} \right)^n ,$$

with $d\hat{T}_{H_k} \doteq e^{-\hat{H}_k dt}$, each of which that can again be implemented by using only one-qubit operators.

Chapter 4

Hubbard-Stratonovich Gate Implementation

In this chapter we will describe the procedure to practically implement the Hubbard-Stratonovich, in order to realize a given quantum gate.

First, let us recall Eq. (3.6) (setting $t = 1$ and renaming some other quantities):

$$e^{-\frac{\hat{H}}{2}} = \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} e^{-ix\sqrt{\hat{H}}}.$$

This is the Hubbard-Stratonovich transformation of the exponential quantum operator $\hat{O}(\hat{H}) \doteq e^{-\frac{\hat{H}}{2}}$, that can be recast in a more compact form by defining the operator $\hat{\tilde{O}}_x(\hat{H}) \doteq e^{-ix\sqrt{\hat{H}}}$:

$$\hat{O}(\hat{H}) = \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \hat{\tilde{O}}_x(\hat{H}). \tag{4.1}$$

We saw in the previous chapter that the situations in which this formulation turns out to be useful are those for which $\hat{\tilde{O}}_x(\hat{H})$ is, for any possible x, a product of operators each one acting on a different single qubit.

There is a straightforward interpretation of the last reported formula: it is possible to associate to any possible value of x a different operator $\hat{\tilde{O}}_x(\hat{H})$ such that by acting with the composition of them on the same initial state $|\psi_0\rangle$, weighting all the results with the appropriate Gaussian factor $\frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$ and summing together all the contributes, the action of the operator $\hat{O}(\hat{H})$ onto the state $|\psi_0\rangle$ is recovered.

The evident problem of this procedure is that the number of possible values for the x variable are infinite, so that in principle a correspondent infinite number of operators

$\hat{\tilde{O}}_x(\hat{H})$ should be applied on the initial state in order to obtain exactly the action of the original operator $\hat{O}(\hat{H})$.

The idea is that of performing this integral with any of the algorithm usually employed for numerical integration (see for example Ref. [18]), choosing a certain desired accuracy and consequently sampling the integrand only at a finite number N of points of the integration domain and weighting them for an appropriate factor.

$$\hat{O}(\hat{H}) \approx \sum_{i=1}^{N} w_i \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \hat{\tilde{O}}_{x_i}(\hat{H}).$$

Obviously this approximation would introduce an *intrinsic limitation of the fidelity* related to the degree at which the integral is approximated. We will discuss this aspect later. The action of taking the sample is the "quantum step", which is performed on the quantum computer. Each sample will be the element of the Hilbert space of the system obtained by applying a specific gate onto the considered initial state. Such element can be, as usual, represented by decomposing it onto a given basis of the Hilbert space in a certain set of amplitudes.

This step is followed by the "classical step". Amplitudes relative to the different samples (which are simply numbers) are firstly rescaled by the Gaussian weight (if needed, depending on the integration algorithm) and then summed together.

In case a better accuracy is needed, a straightforward way to achieve it could consist simply in increasing the number of samples. Alternatively, it is always possible to try a different algorithm which gives a more accurate result for the same number of samples. In this thesis work I considered two different algorithms (besides the vanilla Riemann sum described in Ref. [18]):

- *Gauss-Hermite quadrature*, a method which is particularly suitable for integrals with Gaussian factors and which samples the integrand at points chosen deterministically in function of their number;

- *Monte Carlo integration*, a method which works for any integrand written as a product of any function times a probability density and which samples the integrand in stochastically chosen points.

1 Gauss-Hermite quadrature

The Gauss-Hermite quadrature [18] is a method which allows to obtain the exact value of the following integral $I(f)$ by means of a finite sum of N terms, when $f(x)$ is a polynomial at most of order $2N-1$:

$$I(f) = \int_{-\infty}^{\infty} e^{-x^2} f(x) dx. \tag{4.2}$$

The idea consists in exploiting the properties of the Hermite polynomials $H_m(x)$, which have exact order m and are orthonormal over the interval $(-\infty, \infty)$ with respect to the weight e^{-x^2}:

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx = \delta_{mn}.$$

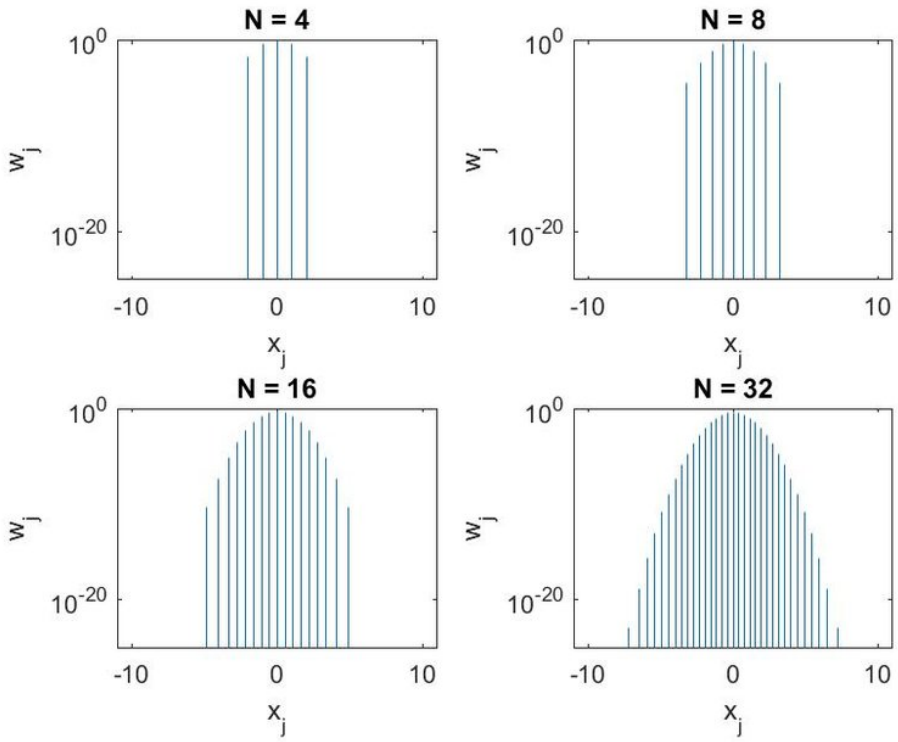


Figure 4.1: Zeros $\{x_j\}_{j=1,\dots,N}$ of the Hermite polynomials and corresponding positive constants $\{w_j\}_{j=1,\dots,N}$ for four different values of N. [19]

The method is implemented by finding the zeros $\{x_j\}_{j=1,\dots,N}$ of the Hermite polynomial of a certain order N, which can be used to uniquely identify those positive constants $\{w_j\}_{j=1,\dots,N}$ such that the following holds for any polynomial $p(x)$ of maximum order $2N-1$:

$$\int_{-\infty}^{\infty} e^{-x^2} p(x)dx = \sum_{j=1}^{N} w_j p(x_j).$$

Points $\{x_i\}_{i=1,\dots,N}$ and constants $\{w_j\}_{j=1,\dots,N}$ can then be used to approximate with the aforementioned sum the integral of any function with the previously considered weight.

This procedure turns out to be very useful in our case, since the integral in Eq. (4.1) is nearly identical to the one in Eq. (4.2). In order to recover the form of the second from the one of the first it is sufficient to change the integration variable from x to $y = \frac{x}{\sqrt{2}}$:

$$\hat{O}(\hat{H}) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \hat{\tilde{O}}_x(\hat{H})dx = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-y^2} \hat{\tilde{O}}_{\sqrt{2}y}(\hat{H})dy \approx \frac{1}{\sqrt{\pi}} \sum_{j=1}^{N} w_j \hat{\tilde{O}}_{\sqrt{2}x_j}(\hat{H}).$$

As an example, I applied this procedure in order to classically[1] simulate the problem illustrated in the first example of Chap. 2. I used different values of N and, for each of them I computed the fidelity F of the final state $|\psi_{f,true}\rangle$ with respect to the expected one $|\psi_{f,exp}\rangle$, where the fidelity is defined as $F = |\langle\psi_{f,exp}|\psi_{f,true}\rangle|^2$.

Results are summed up in Fig. 4.2, were I reported the modulus of the difference between each computed value of F and 1. The fidelity gradually improves by increasing the order N of the Hermite polynomial whose zeros are used in the simulation. Using polynomials of order 5 or greater already gives results which are exact within the uncertainty of the simulation (I considered amplitude values keeping the first six digits). There is no point in taking N too large [20]. As it can be seen in Fig. 4.1 the weights associated to the zeros of the Hermite polynomials decrease very fast, so that the contribution of many of them can quickly be safely neglected. Their magnitude is indeed much smaller than the precision of the machine, and in the limit $N \to \infty$ the fraction of the negligible weights and points approaches unity.

[1]Classically here means that physical states are treated as complex vectors and quantum gates as complex matrices to be applied on them, producing a completely known new vector

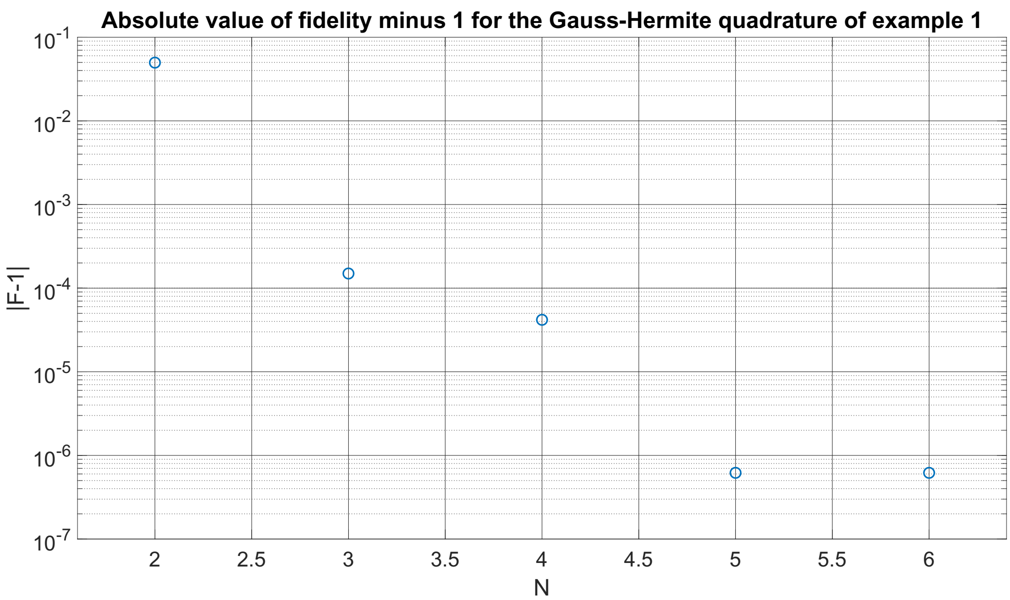


Figure 4.2: $|F-1|$ obtained from the classical simulation of the first example (Chap. 3 Sec. 2) using the Gauss-Hermite quadrature of different orders N.

2 Monte Carlo integration

The Monte Carlo integration procedure [17] allows for the estimation of any integral written in the following form:

$$\int p(x)f(x)dx,$$

with $p(x)$ a probability density (or distribution), i.e. a function satisfying the following conditions:

$$p(x) \geq 0 \quad \forall\ x$$
$$\int p(x)dx = 1.$$

The idea in this case consists of obtaining a sufficiently large number N of independent samples of the probability distribution $p(x)$, evaluating then the integrand $f(x)$ on such samples $\{x_i\}_{i=1,\ldots,N}$ and taking the average $S_N(f)$ of all the results.
Such average will have the following form:

$$S_N(f) = \frac{1}{N}\sum_{i=1}^{N} f(x_i),$$

and will itself be a stochastic variable with its own probability density $p(S_N)$, depending in general on N. If points x_i are indeed independent samples, the Central Limit Theorem states that in the limit of $N \to \infty$ the probability density $p(S_N)$ will be the following Gaussian:

$$\lim_{N\to\infty} p(S_N) = \frac{1}{\sqrt{2\pi\sigma_N^2(f)}} e^{-\frac{(S_N - \langle f\rangle)^2}{2\sigma_N^2(f)}},$$

with the definitions for expectations values and variance given hereafter:

$$\langle f\rangle = \int p(x) f(x) dx,$$
$$\langle f^2\rangle = \int p(x) f^2(x) dx,$$
$$\sigma_N^2(f) = \frac{1}{N}(\langle f^2\rangle - \langle f\rangle^2).$$

The integral represented by $\langle f\rangle$ could then be estimated for a finite number of samples N by $S_N(f)$, while the error on this estimate can in turn be estimated by

$$\sqrt{\frac{1}{N-1}\left(S_N(f^2) - S_N^2(f)\right)},$$

meaning that the error on the result decreases proportionally to $\sqrt{N}$ regardless of the dimensionality of the original integral.

Analogously to what it was done in the last section, I applied this method to the first example of Chap. 2 by doing a classical simulation of the application of the gate $C\hat{NOT} \cdot \hat{H} \otimes \hat{\mathbb{1}}$ to the state $|00\rangle$.

I chose a set of 11 different values for N, i.e. 11 different numbers of Monte Carlo samples and for each of them I repeated several times the computation: each time I computed as before the absolute value of the fidelity minus one, $|F-1|$, and I reported the results in Fig.4.3. Compared to the Gauss-Hermite quadrature, this method needs considerably more resources in order to achieve the same precision in this particular case, since the number of points to be evaluated is fairly larger.

It must be considered tough that this is just a toy example, and that in general the Monte Carlo procedure allows for a better control onto the error of the integral implementation and is also very useful in all those very frequent situations where the dimensionality of the integral is very high.

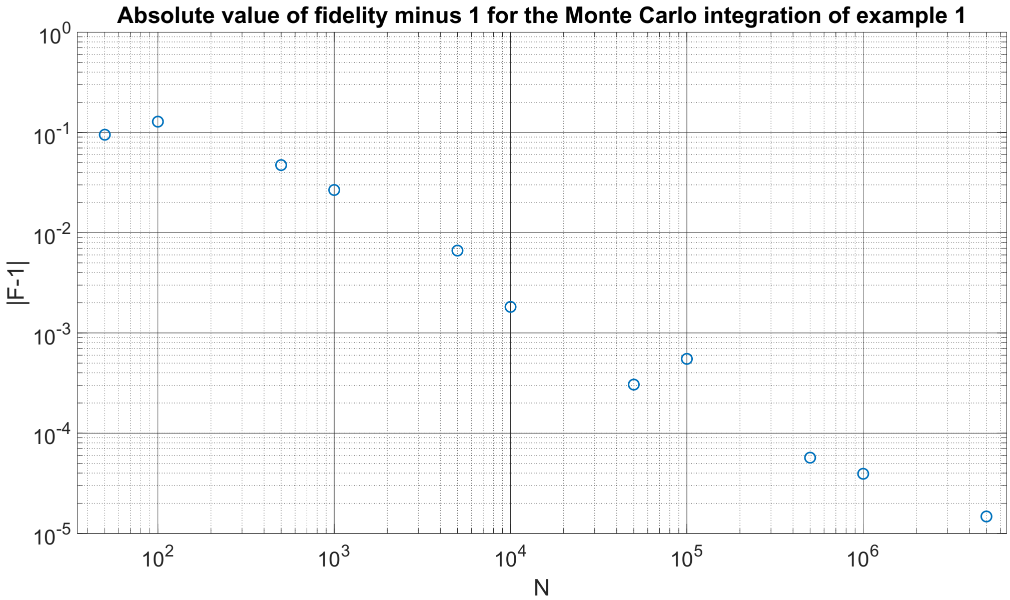


Figure 4.3: $|F-1|$ obtained from the classical simulation of the first example (Chap. 3 Sec. 2) using the Monte Carlo integration with different numbers of samples N

3 Sampling the quantum integrand

Let us go back to Eq. (4.1), i.e. to the Hubbard-Stratonovich decomposition of a general operator $\hat{O}(\hat{H}) \doteq e^{-\frac{\hat{H}}{2}}$ into a combination of operators $\hat{\tilde{O}}_x(\hat{H}) \doteq e^{-ix\sqrt{\hat{H}}}$. When the operator $\hat{O}(\hat{H})$ is a (generally complex) time evolution operator of a system of N qubits subject to an Hamiltonian that can be written as a bilinear form $\hat{H} = \frac{1}{2}\sum_{i,j=1}^{M} \hat{O}_i^{(n_i)} A_{ij} \hat{O}_j^{(n_j)}$ of M different N-dimensional operators $\{\hat{O}_j^{(n_j)}\}_{j=1,\ldots,M}$ acting each on the single qubit n_j, such equation can be approximated by the following expression:

$$
\begin{aligned}
\hat{O}(\hat{H}) = e^{-\hat{H}t} &= e^{-\frac{1}{2}\sum_{i,j=1}^{M}\hat{O}_i^{(n_i)}A_{ij}\hat{O}_j^{(n_j)}t} = \\
&= e^{-\frac{1}{2}\sum_{k=1}^{M}\lambda_k\hat{\mathcal{O}}_k^2 t} \simeq \left(\prod_{k=1}^{M} e^{-\frac{\lambda_k\hat{\mathcal{O}}_k^2}{2}\frac{t}{n}}\right)^n = \\
&= \left(\prod_{k=1}^{M}\int_{-\infty}^{\infty} dx\frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}}e^{-ix\sqrt{\lambda_k dt}\hat{\mathcal{O}}_k}\right)^n = \\
&= \left(\prod_{k=1}^{M}\int_{-\infty}^{\infty} dx\frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}}\prod_{m=1}^{N} e^{-ix\sqrt{\lambda_k dt}\hat{\hat{O}}_m^{[k]}}\right)^n = \\
&= \left(\prod_{k=1}^{M}\int_{-\infty}^{\infty} dx\frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}}\hat{\hat{O}}_{x,k}(\hat{H})\right)^n ,
\end{aligned}
\tag{4.3}
$$

with $\hat{\mathcal{O}}_k \doteq \sum_{i=1}^{M}\psi_i^{[k]}\hat{O}_i^{(n_i)}$, $dt \doteq \frac{t}{n}$, $\hat{\hat{O}}_m^{[k]} \doteq \sum_{i=1}^{M}\psi_i^{[k]}\hat{O}_i^{(n_i)}\delta_{mn_i}$ and λ_k, $\left|\psi^{[k]}\right\rangle \equiv \{\psi_i^{[k]}\}_{i=1,\ldots,N}$ being respectively the k-th eigenvalue and eigenvector of the matrix A_{ij}. In the last two sections the classical part of such decomposition was discussed, describing how to compute the integrals appearing in the previous formula for $\hat{O}(\hat{H})$ by assuming that one could sample several times the integrand $\hat{\hat{O}}_{x,n}(\hat{H})$: it remains now to clarify how such sampling can be achieved.

Looking at Eq. 4.3 it should be evident that this is not a straightforward task. The complex time t can in fact be written in general as $t = t_i + it_r$, where t_i is the imaginary time and t_r the real time (see Chap. 3 Sec. 1), which means that if $t_r \neq 0$ then $\hat{\hat{O}}_{x,k}(\hat{H})$ is not a unitary operator. The same also happens if λ_k, the real eigenvalues of matrix A_{ij}, are negative numbers.

A possible solution for implementing a non unitary operator could be achieved by adding enough qubits (called *ancillas*) to the system and then by applying a unitary operator on the full Hilbert space (ancillas + system) that reduces to the desired non-unitary operator on the subspace associated to the system [5] [21] [22].

In particular, it can be shown [5] that the following operator acting on the Hilbert space of the system plus one ancilla is indeed unitary:

$$
\hat{\hat{O}}_{x,k}^{(\mathrm{tot})}(\hat{H}) \doteq \left[\hat{\mathbb{1}}_2 \otimes \frac{1}{\sqrt{\hat{\hat{O}}_{x,k}^2(\hat{H}) + \hat{\mathbb{1}}_{dim\left(\hat{\hat{O}}_{x,k}(\hat{H})\right)}}}\right]\begin{pmatrix} \hat{\hat{O}}_{x,k}(\hat{H}) & \hat{\mathbb{1}}_{dim\left(\hat{\hat{O}}_{x,k}(\hat{H})\right)} \\ \hat{\mathbb{1}}_{dim\left(\hat{\hat{O}}_{x,k}(\hat{H})\right)} & -\hat{\hat{O}}_{x,k}(\hat{H}) \end{pmatrix}, \tag{4.4}
$$

with $dim\left(\hat{O}\right)$ the dimension of operator $\hat{O}$ and $\hat{\mathbb{1}}_\alpha$ the identity operator of dimension α.

If the ancilla is prepared in the state $|0\rangle$ and the operator $\hat{\tilde{O}}^{(\text{tot})}_{x,k}$ is applied on the full complex (system + ancilla), one can show that the result on the system corresponds to the application on this latter of the operator $\hat{\tilde{O}}_{x,k}(\hat{H})$, whenever the ancilla is found to be still in $|0\rangle$.

At the end of the procedure one can measure the ancilla: if the eigenvalue corresponding to the $|0\rangle$ state is found and the system was initially in the state $|\psi_s\rangle$, the measure will have projected the system onto the ground state $|\psi'_s\rangle = \hat{\tilde{O}}_{x,k}(\hat{H})\,|\psi_s\rangle$ (up to a normalization factor):

$$
\begin{aligned}
&\hat{O}_M \hat{\tilde{O}}^{(\text{tot})}_{x,k}(\hat{H})\left[|0\rangle \otimes |\psi_s\rangle\right] = \\
&= \left[\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \hat{\mathbb{1}}_{dim\left(\hat{\tilde{O}}_{x,k}(\hat{H})\right)}\right]\left[\hat{\mathbb{1}}_2 \otimes \frac{1}{\sqrt{\hat{\tilde{O}}^2_{x,k}(\hat{H}) + \hat{\mathbb{1}}_{dim\left(\hat{\tilde{O}}_{x,k}(\hat{H})\right)}}}\right]\cdot \\
&\cdot \begin{pmatrix} \hat{\tilde{O}}_{x,k}(\hat{H}) & \hat{\mathbb{1}}_{dim\left(\hat{\tilde{O}}_{x,k}(\hat{H})\right)} \\ \hat{\mathbb{1}}_{dim\left(\hat{\tilde{O}}_{x,k}(\hat{H})\right)} & -\hat{\tilde{O}}_{x,k}(\hat{H}) \end{pmatrix}\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes |\psi_s\rangle\right] = \\
&= \left[\hat{\mathbb{1}}_2 \otimes \frac{1}{\sqrt{\hat{\tilde{O}}^2_{x,k}(\hat{H}) + \hat{\mathbb{1}}_{dim\left(\hat{\tilde{O}}_{x,k}(\hat{H})\right)}}}\right]\left[\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \hat{\mathbb{1}}_{dim\left(\hat{\tilde{O}}_{x,k}(\hat{H})\right)}\right]\cdot \\
&\cdot \left(\left[\hat{\sigma}_z \otimes \hat{\tilde{O}}_{x,k}(\hat{H})\right] + \left[\hat{\sigma}_x \otimes \hat{\mathbb{1}}_{dim\left(\hat{\tilde{O}}_{x,k}(\hat{H})\right)}\right]\right)\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes |\psi_s\rangle\right] = \\
&= \left[\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \frac{\hat{\tilde{O}}_{x,k}(\hat{H})}{\sqrt{\hat{\tilde{O}}^2_{x,k}(\hat{H}) + \hat{\mathbb{1}}_{dim\left(\hat{\tilde{O}}_{x,k}(\hat{H})\right)}}}\right]\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes |\psi_s\rangle\right] = \\
&= \left[\hat{\mathbb{1}}_2 \otimes \frac{\hat{\tilde{O}}_{x,k}(\hat{H})}{\sqrt{\hat{\tilde{O}}^2_{x,k}(\hat{H}) + \hat{\mathbb{1}}_{dim\left(\hat{\tilde{O}}_{x,k}(\hat{H})\right)}}}\right]\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes |\psi_s\rangle\right] = \\
&= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \frac{\hat{\tilde{O}}_{x,k}(\hat{H})}{\sqrt{\hat{\tilde{O}}^2_{x,k}(\hat{H}) + \hat{\mathbb{1}}_{dim\left(\hat{\tilde{O}}_{x,k}(\hat{H})\right)}}}\,|\psi_s\rangle
\end{aligned}
\tag{4.5}
$$

where the projective measurement operator onto the state $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ of the ancilla is defined as $\hat{O}_M \doteq \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \hat{\mathbb{1}}_{dim\left(\hat{\hat{O}}_{x,k}(\hat{H})\right)}$.

Actually, due to possible issues related to the normalization $\sqrt{\hat{\hat{O}}^2_{x,k}(\hat{H}) + \hat{\mathbb{1}}_{dim\left(\hat{\hat{O}}_{x,k}(\hat{H})\right)}}$, it would be better to add one ancilla for each qubit in the system and repeat the just discussed procedure once for each of them, substituting everywhere $\hat{\hat{O}}_{x,k}(\hat{H})$ with $\hat{\hat{O}}^{(m)}_{x,k}(\hat{H}) \doteq e^{-ix\sqrt{\lambda_k dt}\hat{\hat{O}}^{[k]}_m}$ and taking the product of all these terms.

Chapter 5

Simulations

In order to apply the arguments developed so far, several simulations were performed. In particular the situation described in Chap. 3 Sec. 4 (second example) was considered. This is the case of a two qubit system subject to the following Hamiltonian:

$$\hat{H} = \hat{\vec{\sigma}}^{(1)} \cdot \hat{\vec{\sigma}}^{(2)} = \frac{\sum_{i=x,y,z} \left(\hat{\sigma}_i^{(1)} + \hat{\sigma}_i^{(2)} \right)^2}{2} - 3.$$

The complex time evolution

$$\hat{O}(\hat{H}) = e^{-\hat{H}t} = e^{3t} \prod_{j=x,y,z} e^{-\frac{\left(\hat{\sigma}_j^{(1)} + \hat{\sigma}_j^{(2)}\right)^2}{2} t} \tag{5.1}$$

was simulated considering as initial state the $|01\rangle$ state, so that during the evolution the 2 qubits in the system become entangled (see discussion in Chap. 3 Sec. 4.1).
Both classical and quantum simulations were performed. By the former different algorithms implementing the Hubbard-Stratonovich integral were compared, while with the latter I tested the correctness of the procedure realizing the non-unitary gate by means of the ancillas.
Results are discussed in the following sections.

1 Real time evolution

At first I consider the evolution in real time, i.e. I choose $t = it_r$ (actually in this section I will still call t_r with t assuming this last to be real, for ease of notation):

$$\begin{aligned}\hat{O}(\hat{H}) &= e^{-i\hat{H}t} = e^{3it}\prod_{j=x,y,z} e^{-i\frac{\left(\hat{\sigma}_j^{(1)}+\hat{\sigma}_j^{(2)}\right)^2}{2}t} \\ &= e^{3it}\prod_{j=x,y,z}\int dy\frac{1}{\sqrt{2\pi}}e^{-\frac{y^2}{2}}e^{\frac{1-i}{\sqrt{2}}y\sqrt{t}\hat{\sigma}_j^{(1)}}\otimes e^{\frac{1-i}{\sqrt{2}}y\sqrt{t}\hat{\sigma}_j^{(2)}}\end{aligned} \tag{5.2}$$

Recalling the arguments presented in Chap. 3 Sec. 4.1, it is possible to see that the action of this operator onto the state $|01\rangle \equiv |0\rangle \otimes |1\rangle$ will be the following (with t real, as already mentioned):

$$\hat{O}(\hat{H})\,|01\rangle = e^{it}\left(\cos(2t)\,|01\rangle - i\sin(2t)\,|10\rangle\right). \tag{5.3}$$

This means that during the evolution the system will always be in a combination of states $|01\rangle$ and $|10\rangle$, oscillating between separable and completely entangled states.

1.1 Classical simulation

By representing the initial state as the Kronecker product of two 2-dimensional vectors and the operators $e^{\frac{1-i}{\sqrt{2}}y\sqrt{t}\hat{\sigma}_j^{(m)}}$ with 2x2 matrices, I implemented the RHS of Eq. (5.2) on a classical machine realising the integral both with the Gauss-Hermite and the Monte Carlo procedure. Results are summarized in Figs. 5.1, 5.2. In both figures the probabilities of finding the system in the states $|01\rangle$ or $|10\rangle$ and the difference between the phases of the two terms in Eq. (5.3) are reported, both obtained from the simulations and computed from such equation (probabilities are the squared modulus of each factor).

The Gauss-Hermite procedure was implemented choosing 4 samples for each time step evolution and using $5 \cdot 10^4$ steps, from $t = 0$ to $t = 5$.

The Monte Carlo procedure was implemented choosing 10^4 samples for each time step evolution and using $5 \cdot 10^3$ steps, from $t = 0$ to $t = 5$.

In both cases the predictions are well compatible with the simulation results, but once

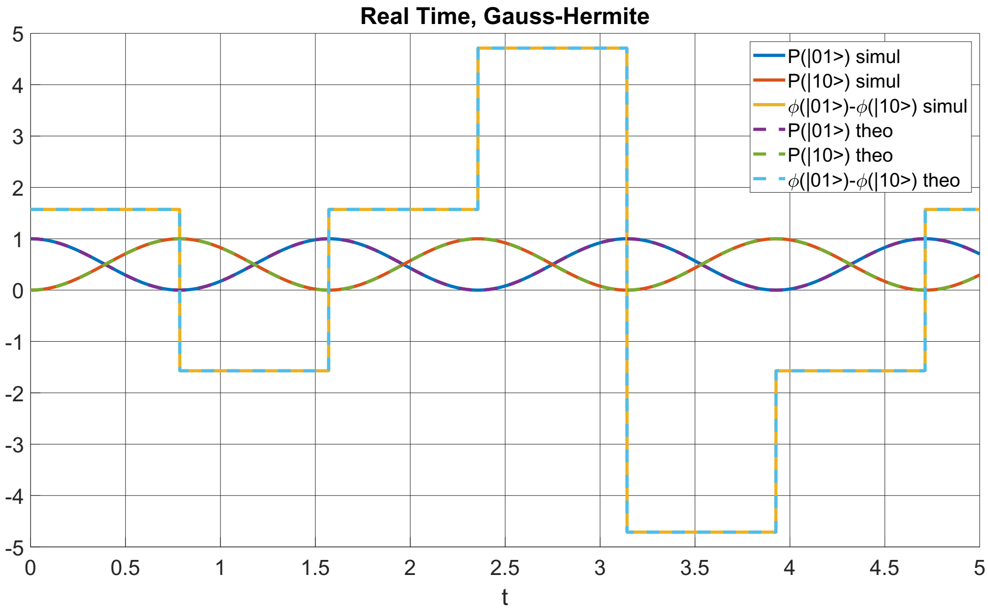


Figure 5.1: Classical evolution in real time of the system in the second example (Chap. 3 Sec. 4) using the Gauss-Hermite procedure with 4 points and $5 \cdot 10^4$ time steps.

again the cost of the simulation was sensibly different: while for each time step the Gauss-Hermite procedure needs only 4 different samples, in order to achieve a similar precision the Monte Carlo technique requires approximately 10^4 times the number of samples, resulting in much longer and possibly error-affected computations.

The dephasing between the 2 components of the state at any given time allows to recover the exact state of the system: such dephasing is easy to get from a simulation, but in a real computation on a quantum machine could be obtained only by performing quantum tomography [23], which would imply repeating several time the same evolution and making at the end a different measurement each time.

1.2 Short time limit

The operators $e^{\frac{1-i}{\sqrt{2}} y \sqrt{t} \hat{\sigma}_j^{(m)}}$ inside the integrals in Eq. (5.2) are not unitary, meaning that some more or less clever methods must be found in order to implement them in a quantum computer (for example I could add an ancilla for each one of the two qubits, as already discussed in Chap. 4 Sec. 3).

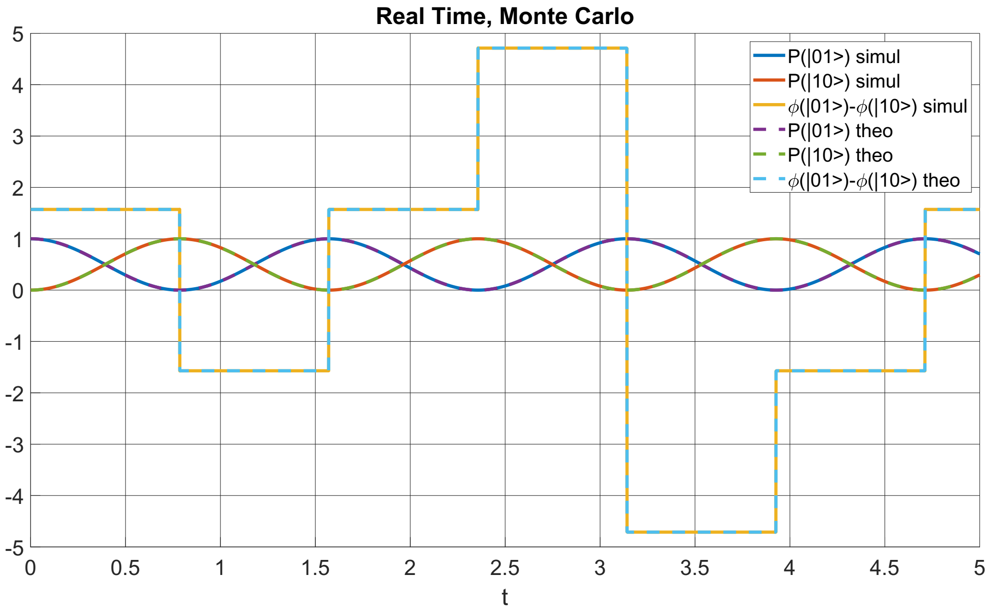


Figure 5.2: Classical evolution in real time of the system in the second example (Chap. 3 Sec. 4) using the Monte Carlo procedure with $5 \cdot 10^3$ time steps and 10^4 samples for each of them.

It may however be interesting to look at the explicit form of these operators:

$$\begin{aligned}
e^{\frac{1-i}{\sqrt{2}}y\sqrt{t}\hat{\sigma}_x^{(m)}} &= \begin{pmatrix} \cos\left(\frac{1+i}{\sqrt{2}}y\sqrt{t}\right) & -i\sin\left(\frac{1+i}{\sqrt{2}}y\sqrt{t}\right) \\ -i\sin\left(\frac{1+i}{\sqrt{2}}y\sqrt{t}\right) & \cos\left(\frac{1+i}{\sqrt{2}}y\sqrt{t}\right) \end{pmatrix} \\
e^{\frac{1-i}{\sqrt{2}}y\sqrt{t}\hat{\sigma}_y^{(m)}} &= \begin{pmatrix} \cos\left(\frac{1+i}{\sqrt{2}}y\sqrt{t}\right) & -\sin\left(\frac{1+i}{\sqrt{2}}y\sqrt{t}\right) \\ \sin\left(\frac{1+i}{\sqrt{2}}y\sqrt{t}\right) & \cos\left(\frac{1+i}{\sqrt{2}}y\sqrt{t}\right) \end{pmatrix} \\
e^{\frac{1-i}{\sqrt{2}}y\sqrt{t}\hat{\sigma}_z^{(m)}} &= \begin{pmatrix} e^{\frac{1-i}{\sqrt{2}}y\sqrt{t}} & 0 \\ 0 & e^{-\frac{1-i}{\sqrt{2}}y\sqrt{t}} \end{pmatrix},
\end{aligned} \tag{5.4}$$

holding $\forall\ m = 1, 2$.

One might in fact wonder whether there are any cases in which these operators become more manageable. As an example, I will now explore how they would be expressed in the short time limit $t \to 0$.

It is indeed very common to find such limit while working with any quantum system, since the full time evolution of a system can always be exactly decomposed in a series of briefer evolutions. Furthermore, as already discussed when introducing the Trotterization procedure (see Chap. 3 Sec. 5), sometimes this short time limit of the full evolution must be exploited in order to be able to implement the wanted operator. In these cases the short time limit of operators in (5.4) is even more important, since it is the only meaningful one.

Taking the limit $t \to 0$ for the previous operators yields the following results (neglecting $O(t^{\frac{3}{2}})$ terms):

$$
\begin{aligned}
e^{\frac{1-i}{\sqrt{2}} y\sqrt{t}\hat{\sigma}_x^{(m)}} &\xrightarrow{t\to 0} \begin{pmatrix} e^{-\frac{i}{2}y^2 t} & \frac{1-i}{\sqrt{2}} y\sqrt{t} \\ \frac{1-i}{\sqrt{2}} y\sqrt{t} & e^{-\frac{i}{2}y^2 t} \end{pmatrix} \\
e^{\frac{1-i}{\sqrt{2}} y\sqrt{t}\hat{\sigma}_y^{(m)}} &\xrightarrow{t\to 0} \begin{pmatrix} e^{-\frac{i}{2}y^2 t} & -\frac{1+i}{\sqrt{2}} y\sqrt{t} \\ \frac{1+i}{\sqrt{2}} y\sqrt{t} & e^{-\frac{i}{2}y^2 t} \end{pmatrix} \\
e^{\frac{1-i}{\sqrt{2}} y\sqrt{t}\hat{\sigma}_z^{(m)}} &\xrightarrow{t\to 0} \begin{pmatrix} e^{-\frac{i}{2}y^2 t} + \frac{1-i}{\sqrt{2}} y\sqrt{t} & 0 \\ 0 & e^{-\frac{i}{2}y^2 t} - \frac{1-i}{\sqrt{2}} y\sqrt{t} \end{pmatrix}
\end{aligned}
\tag{5.5}
$$

In order to test the correctness of these expressions I substituted them to their full form (i.e. to operators in (5.4)) in the classical simulation described before (implementing the integral with the Monte Carlo method, dividing the evolution in 10^4 time steps and taking for each of them $5 \cdot 10^4$ samples of the integrand): the obtained result is reported in Fig. 5.3, which is indeed very similar to the one reported in figures 5.1 and 5.2 and coherent with the expectations.

It would now come in very handy if operators in (5.5) were unitary. If that was the case, in fact, by dividing the full time evolution in sufficiently short time steps it would become possible to implement them without the need of adding any ancilla, nor relying on other dissipative procedures.

Unluckily, operators in (5.5) are not unitary, as it can readily be proofed by multiplying each of them for the conjugate transpose of the associated matrix.

Let us still analyze them a bit more in detail. There are only two distinct factors appearing in all the operators: a complex exponential and a second term which is proportional to $\sqrt{t}$. While the complex exponential has modulus 1 for every t, the modulus of the second term decreases with decreasing t.

One might then think that for very short t only the exponential term would need to be

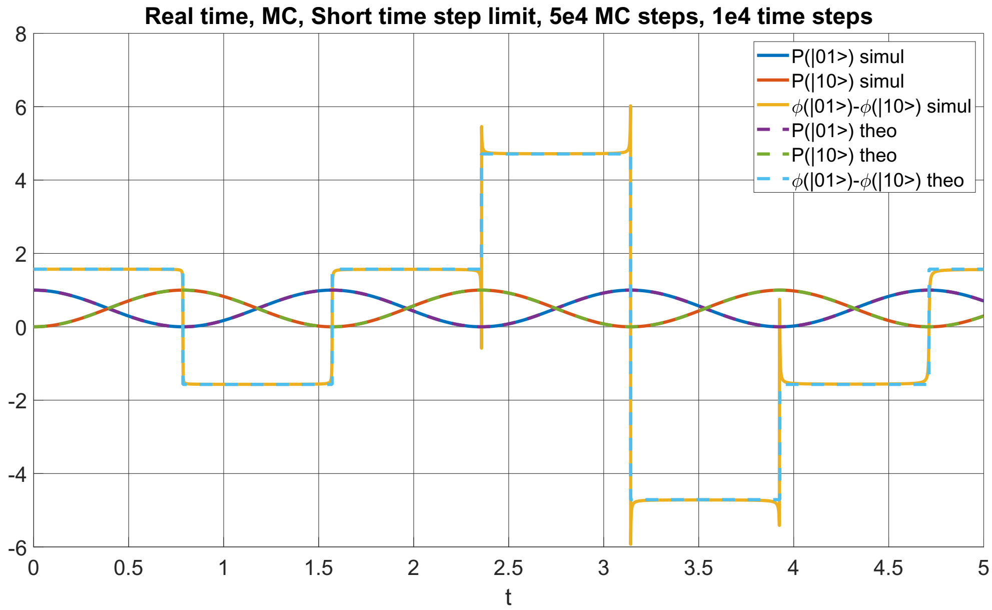


Figure 5.3: Classical evolution in real time of the system in the second example (Chap 3 Sec. 4) using the Monte Carlo procedure with 10^4 time steps, $5 \cdot 10^4$ samples for each of them and the approximated form for short time steps of the operators in the integrand of the Hubbard-Stratonovich form.

considered: in that case all the three matrices would indeed be unitary.

Performing the classical simulation using such approximation (with the same Monte Carlo integration parameters described in the previous section) though, I get the result reported in Fig. 5.4, which differs completely from the expectation.

In order to understand why this happens one needs to explicitly look at how matrices in (5.5) change when neglecting the terms proportional to $\sqrt{t}$:

$$
\begin{aligned}
e^{\frac{1-i}{\sqrt{2}}y\sqrt{t}\hat{\sigma}_x^{(m)}} &\xrightarrow{t\to 0,\ \text{no}\sqrt{t}} \begin{pmatrix} e^{-\frac{i}{2}y^2 t} & 0 \\ 0 & e^{-\frac{i}{2}y^2 t} \end{pmatrix} \\
e^{\frac{1-i}{\sqrt{2}}y\sqrt{t}\hat{\sigma}_y^{(m)}} &\xrightarrow{t\to 0,\ \text{no}\sqrt{t}} \begin{pmatrix} e^{-\frac{i}{2}y^2 t} & 0 \\ 0 & e^{-\frac{i}{2}y^2 t} \end{pmatrix}. \\
e^{\frac{1-i}{\sqrt{2}}y\sqrt{t}\hat{\sigma}_z^{(m)}} &\xrightarrow{t\to 0,\ \text{no}\sqrt{t}} \begin{pmatrix} e^{-\frac{i}{2}y^2 t} & 0 \\ 0 & e^{-\frac{i}{2}y^2 t} \end{pmatrix}
\end{aligned}
$$

In this limit these three operators are indeed unitary, but no longer different. In fact, the Kronecker product of any of these operator with itself is a diagonal operator with

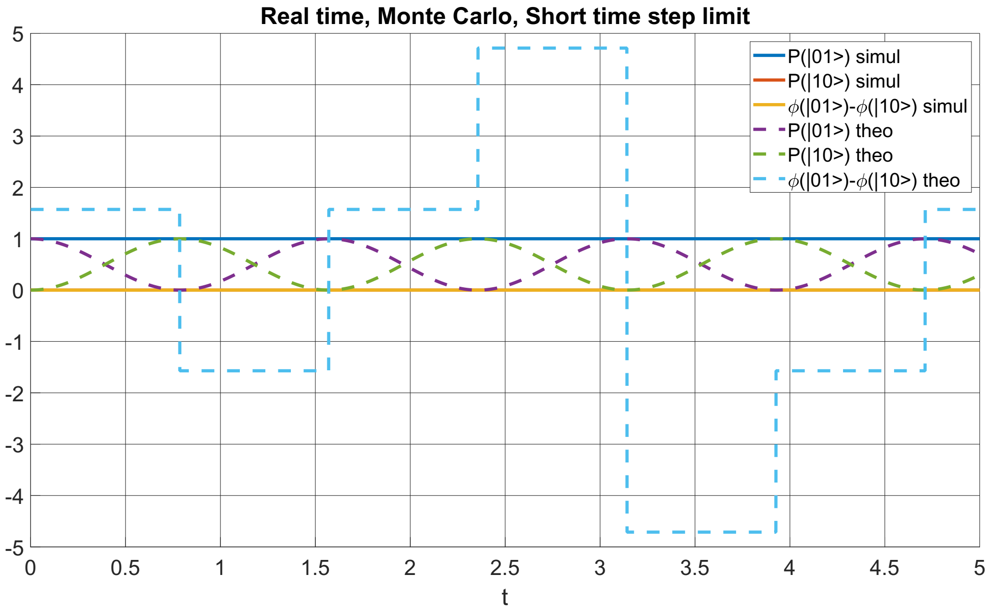


Figure 5.4: Classical evolution in real time of the system in the second example (Chap 3 Sec. 4) using the Monte Carlo procedure with $5 \cdot 10^3$ time steps, 10^4 samples for each of them and the approximated form for short time steps of the operators in the integrand of the Hubbard-Stratonovich form neglecting terms proportional to $\sqrt{t}$. Red and orange lines are one on the top of the other.

all diagonal elements being identical one with the other:

$$e^{\frac{1-i}{\sqrt{2}} y\sqrt{t}\hat{\sigma}_j^{(1)}} \otimes e^{\frac{1-i}{\sqrt{2}} y\sqrt{t}\hat{\sigma}_j^{(2)}} \xrightarrow{t\to 0,\ \text{no}\sqrt{t}} \begin{pmatrix} e^{-iy^2 t} & 0 & 0 & 0 \\ 0 & e^{-iy^2 t} & 0 & 0 \\ 0 & 0 & e^{-iy^2 t} & 0 \\ 0 & 0 & 0 & e^{-iy^2 t} \end{pmatrix} \quad \forall\, j \in \{x, y, z\}.$$

This means that considering this limit in Eq. (5.2) will produce an operator proportional to the identity, as shown in Fig. 5.4.

Actually, one could have already predicted the failure of such approach by remembering the expansion for short t at order t of $e^{-\frac{i}{2}y^2 t}$, which is $1 - \frac{1}{2} i y^2 t$. This means that one should not have neglected in (5.5) the terms proportional to $\sqrt{t}$ while also keeping the exponential factor, since this would mean keeping terms at higher order in t then those discarded.

This result, which is however specific of the considered case, may suggest the existence of a fundamental problem in the Hubbard-Stratonovich decomposition of a multi-qubit gate in only one-qubit gates. While the procedure is well defined, and the results consistent, such procedure is indeed possible, these result can only be obtained provided if dissipation (i.e. non-unitary operators) is introduced in the system.

Nonetheless the fundamental result still holds, that by taking a system (2 qubits + 2 ancillas) divided into two not entangled parties (1 qubit + 1 ancilla each) and by only acting separately on each of these, I was able to reproduce the results of an evolution of such system which entangles the two parties.

Whether or not the original system actually gets entangled after the application of the Hubbard-Stratonovich procedure or if the obtained results can instead only be "statistically interpreted" is still not fully clear and a further investigation is needed in order to give a satisfying answer.

1.3 Quantum simulation

In order to check the correctness of the previously mentioned method for the implementation of a non-unitary operator acting on a system by means of a unitary operator acting on an extended system comprehensive also of some ancillas (see Chap. 4 Sec. 3), I repeated the previous simulation on a quantum computer simulator following the said procedure.

In particular, rather than applying the operators $\hat{\hat{O}}_{y,j}^{(m)}(\hat{H}) = e^{\frac{1-i}{\sqrt{2}} y\sqrt{t}\hat{\sigma}_j^{(m)}}$ in Eq. (5.2) to the single qubits, I added two ancillas in total (one for each qubit present in the system) and applied to each qubit + ancilla couple the operators $\hat{O}_M \hat{\hat{O}}_{y,j}^{(m)(\mathrm{tot})}(\hat{H})$ as defined in Eqs. (4.4) and (4.5).

In order to double check the simulation and to be able to perform a comparison, I employed once again two different integration methods: firstly I implemented the integral for each time step with the vanilla Riemann integration technique, choosing 2000 different values for y equally spaced in the interval $[-8, 8]$; then I repeated the simulation with the Monte Carlo procedure, sampling 10^4 points from a Gaussian (actually I only sampled half the number of points, taking for every sample also the opposite value in order to reduce the error in the evaluation of the integral).

In both the simulations I divided the evolution from $t = 0$ to $t = 5$ in $5 \cdot 10^4$ equally-long shorter time steps, obtaining the results reported in Figs. 5.5, 5.6. Once again,

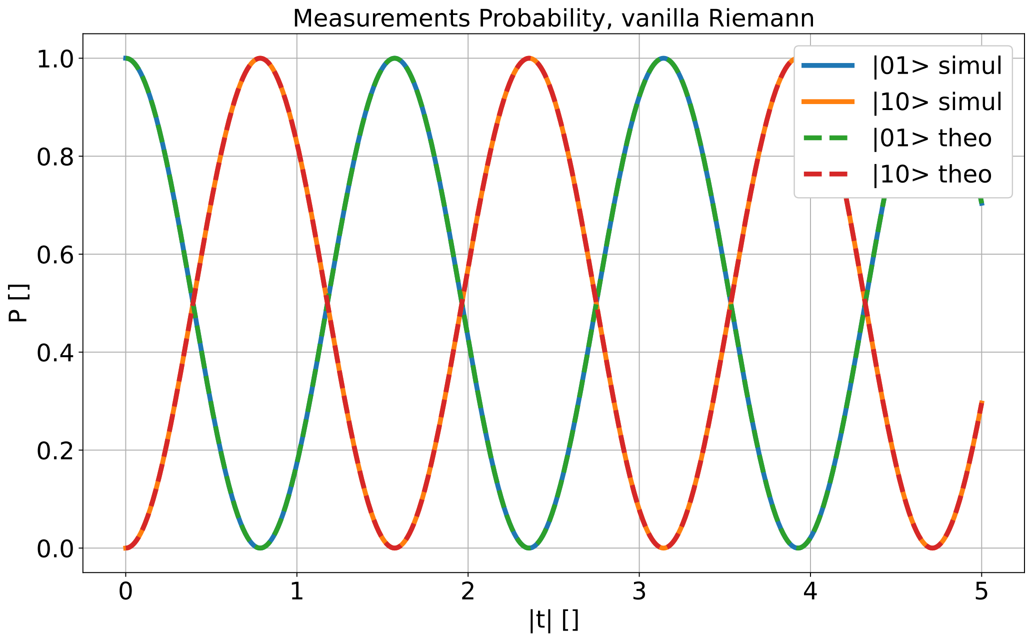


Figure 5.5: Quantum simulation of the evolution in real time of the system in the second example (Chap 3 Sec. 4) using the vanilla Riemann integration procedure with 2000 equally spaced points in the interval $[-8, 8]$ for each of the $5 \cdot 10^4$ time steps.

both results are perfectly compatible with the predictions. The theoretical predictions (dotted lines) lay on top of the data obtained from simulations (continuous lines). From this fact it is possible to conclude that the described method employed for the implementation of the non-unitary one-qubit gates $\hat{\hat{O}}_{y,j}^{(m)}(\hat{H}) = e^{\frac{1-i}{\sqrt{2}} y \sqrt{t} \hat{\sigma}_j^{(m)}}$ has proven to work fine, at least in the simulation of the considered case.

2 Imaginary time evolution

I consider now the evolution in imaginary time of the system described in Chap. 3 Sec. 4, which means choosing $t = t_i \in \mathbb{R}$ in Eq. (5.1)[1].

The Hubbard-Stratonovich formulation of such operator allows me to write it in the

[1]As previously done, t_i will still be shortened into t throughout this section, assuming the last to be real

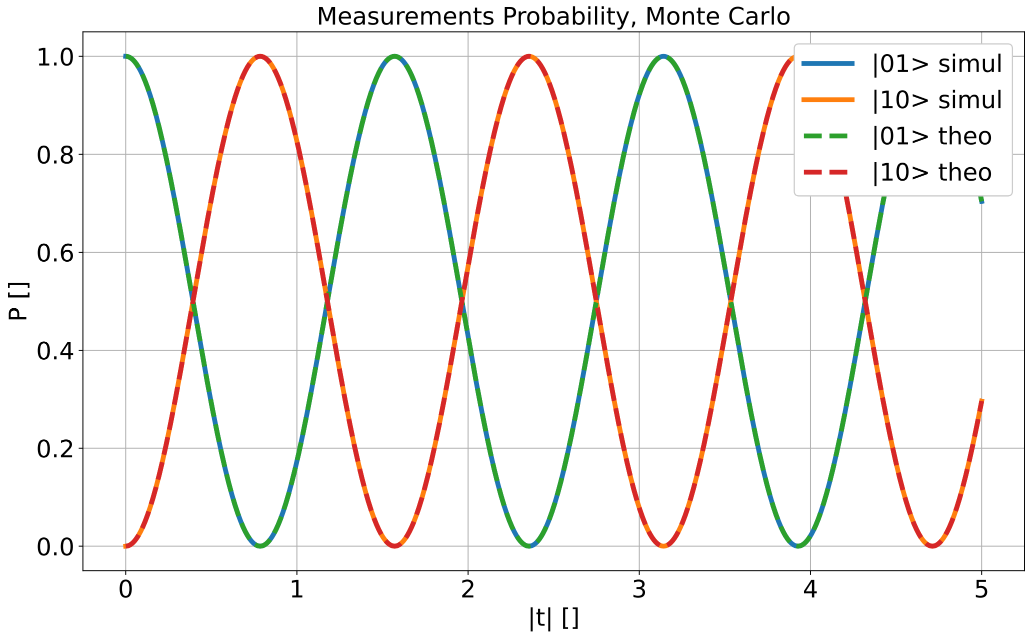


Figure 5.6: Quantum simulation of the evolution in real time of the system in the second example (Chap 3 Sec. 4) using the Monte Carlo procedure with $5 \cdot 10^4$ time steps and 10^4 samples for each of them.

following way:

$$\begin{aligned} \hat{O}(\hat{H}) &= e^{-\hat{H}t} = e^{3t} \prod_{j=x,y,z} e^{-\frac{\left(\hat{\sigma}_j^{(1)}+\hat{\sigma}_j^{(2)}\right)^2}{2}t} \\ &= e^{3t} \prod_{j=x,y,z} \int dy \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} e^{-iy\sqrt{t}\hat{\sigma}_j^{(1)}} \otimes e^{-iy\sqrt{t}\hat{\sigma}_j^{(2)}} \end{aligned} \tag{5.6}$$

where I recall that I'm applying this operator on a two qubit system in the state $|01\rangle \equiv |0\rangle \otimes |1\rangle$.

There is a very interesting thing to notice in this last equation: since y is a real variable, t is a real positive time and all the Pauli matrices $\hat{\sigma}_j$ are Hermitian, it follows that all the one-qubit operators $e^{-iy\sqrt{t}\hat{\sigma}_j^{(m)}}$ are now unitary.

This means that I could apply them on the system in an actual quantum computer in the usual way, without the need of introducing ancillas and to use the procedure described in Chap. 4 Sec. 3 (or other dissipative methods).

Let us now move on to considering the action of $\hat{O}(\hat{H})$ on the initial state $|01\rangle$. We have already seen in Chap. 3 Sec. 4.1 that such action is expressed by Eq. (3.12), which leads to the following relation when specifying to the case of imaginary time (I recall that we are considering $t = t_i \in \mathbb{R}$):

$$\hat{O}(\hat{H})\,|01\rangle = \frac{1}{2}\left(e^{-t} + e^{3t}\right)|01\rangle + \frac{1}{2}\left(e^{-t} - e^{3t}\right)|10\rangle\,. \tag{5.7}$$

It is then worth looking at the long time limit behaviour of such evolution:

$$\hat{O}(\hat{H})\,|01\rangle \xrightarrow{t\to\infty} \frac{e^{3t}}{2}\left(|01\rangle - |10\rangle\right) = \frac{e^{3t}}{\sqrt{2}}\,|-\rangle\,.$$

This last expression makes it evident that, if the system is appropriately renormalized, the pure maximally entangled state (i.e. Bell state) $|-\rangle$ would be produced by evolving for a sufficient time the initial state $|01\rangle$.

This consequence is even more striking than the analogous result for the real time evolution of the same system. Indeed, by separately acting on the two qubits (which is what the Hubbard-Stratonovich procedure allows to do, as discussed before) it is possible to filter out a stable maximally entangled state from the initial separable state.

Besides that, it is also worth noting that Eq. (5.7) implies that now the difference in phase during the evolution between the amplitudes associated to the states $|01\rangle$ and $|10\rangle$ is always constant and equal to π. This constant phase is not going to be shown in the following plots.

2.1 Classical simulation

In analogy to the case of the real time evolution, I implemented the RHS of Eq. (5.6) on a classical computer, simulating the evolution of the system by representing the initial state $|01\rangle$ as the Kronecker product of two 2-dimensional vectors and the operators

$e^{-iy\sqrt{t}\hat{\sigma}_j^{(m)}}$ with the following 2x2 unitary matrices:

$$e^{-iy\sqrt{t}\hat{\sigma}_x^{(m)}} = \begin{pmatrix} \cos\left(y\sqrt{t}\right) & -i\sin\left(y\sqrt{t}\right) \\ -i\sin\left(y\sqrt{t}\right) & \cos\left(y\sqrt{t}\right) \end{pmatrix}$$
$$e^{-iy\sqrt{t}\hat{\sigma}_y^{(m)}} = \begin{pmatrix} \cos\left(y\sqrt{t}\right) & -\sin\left(y\sqrt{t}\right) \\ \sin\left(y\sqrt{t}\right) & \cos\left(y\sqrt{t}\right) \end{pmatrix}$$
$$e^{-iy\sqrt{t}\hat{\sigma}_z^{(m)}} = \begin{pmatrix} e^{-iy\sqrt{t}} & 0 \\ 0 & e^{iy\sqrt{t}} \end{pmatrix}$$

Once again, two distinct simulations were performed, implementing in one case the integrals with the Gauss-Hermite technique while in the other with the Monte Carlo procedure (parameters of the integrations were the same as those described in Chap. 5 Sec. 1.1). The results of these simulations are presented in Figs. 5.7 and 5.8.

Figure 5.7: Classical evolution in imaginary time of the system in the second example (Chap 3 Sec. 4) using the Gauss-Hermite procedure with 4 points and $5 \cdot 10^4$ time steps.

Figs. 5.7 and 5.8 show exactly the results predicted by the analysis presented in the previous section. Starting with the system in the state $|01\rangle$, the probability of finding again such state at time t decreases monotonically, in agreement with the prediction, until it settles at 0.5, while the probability of finding the other separable state $|10\rangle$ also

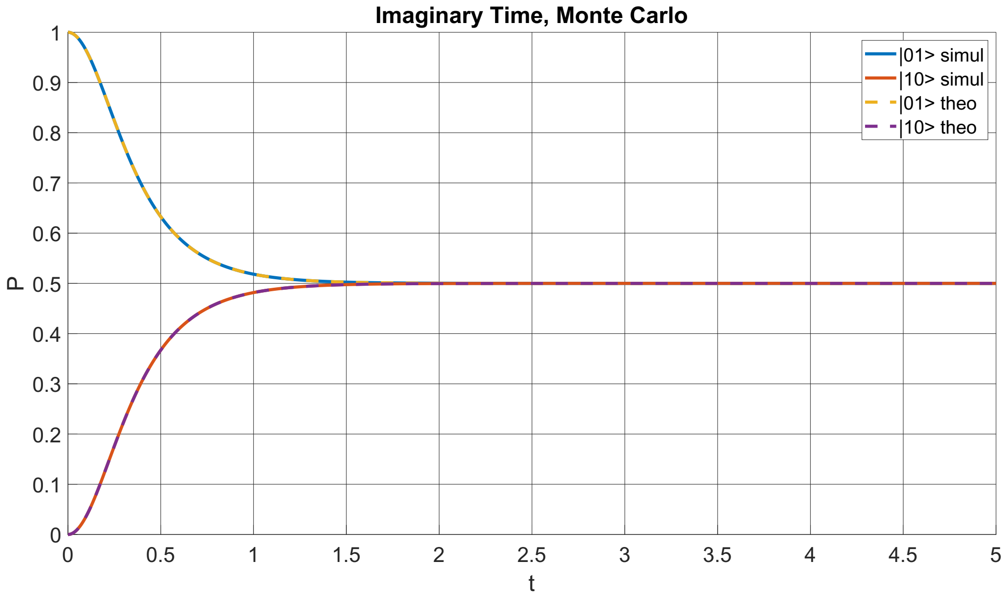


Figure 5.8: Classical evolution in imaginary time of the system in the second example (Chap 3 Sec. 4) using the Monte Carlo procedure with $5 \cdot 10^3$ time steps and 10^4 samples for each of them.

reaches 0.5 for high t, but increasing monotonously from 0 at $t = 0$.

The phase difference between the amplitudes relative to the two separable states is not reported because, as already anticipated, it is always equal to π. This fact, together with the previous point, means that the asymptotic state reached by the system at $t \to \infty$ is indeed the $|-\rangle$ state (neglecting normalization).

This behaviour is nothing more than the system "decaying" in its ground state. We indeed saw in Chap. 3 Sec. 4.1 that the only eigenstates of the Hamiltonian $\hat{\vec{\sigma}}^{(1)} \cdot \hat{\vec{\sigma}}^{(2)}$ involved in the evolution are $|+\rangle$ and $|-\rangle$, which respectively have eigenvalues 1 and -3. The imaginary time evolution then projects the system in the eigenstate with the lower energy, namely $|-\rangle$.

As already discussed when studying the real time evolution of the system, also in this case the implementation by means of the Gauss-Hermite integration is way more efficient than the Monte Carlo one, since it allows to obtain a result having the same precision but by taking much less samples of the integrand for each evolution time step.

2.2 Quantum simulation

Considering what has been anticipated in Chap. 5 Sec. 2, there would not be any need of performing a quantum simulation in the case of the imaginary time evolution, since the one-qubit operators involved are already unitary and can then always be implemented in a quantum computer by means of consecutive single qubit rotations.
Nonetheless, the operator defined in Eq. (4.4) is still unitary even if $\hat{\hat{O}}_{x,k}(\hat{H})$ is by itself a unitary operator. For completeness I chose then to perform a quantum simulation implementing with the method described in Chap. 4 Sec. 3 the one-qubit unitary operators $e^{-iy\sqrt{t}\hat{\sigma}_j^{(m)}}$.
As I did in the case of the quantum simulation for the real time evolution of the system, I performed two distinct simulations. In the first one I implemented the integrals with the vanilla Riemann technique, choosing 2000 different values for y equally spaced in the interval $[-8, 8]$. In the second I instead implemented them with the Monte Carlo procedure, sampling each time 10^4 points.
In both simulations I divided the evolution from $t = 0$ to $t = 5$ in $5 \cdot 10^4$ equally-long shorter time steps, obtaining the results reported in Figs. 5.9 and 5.10.

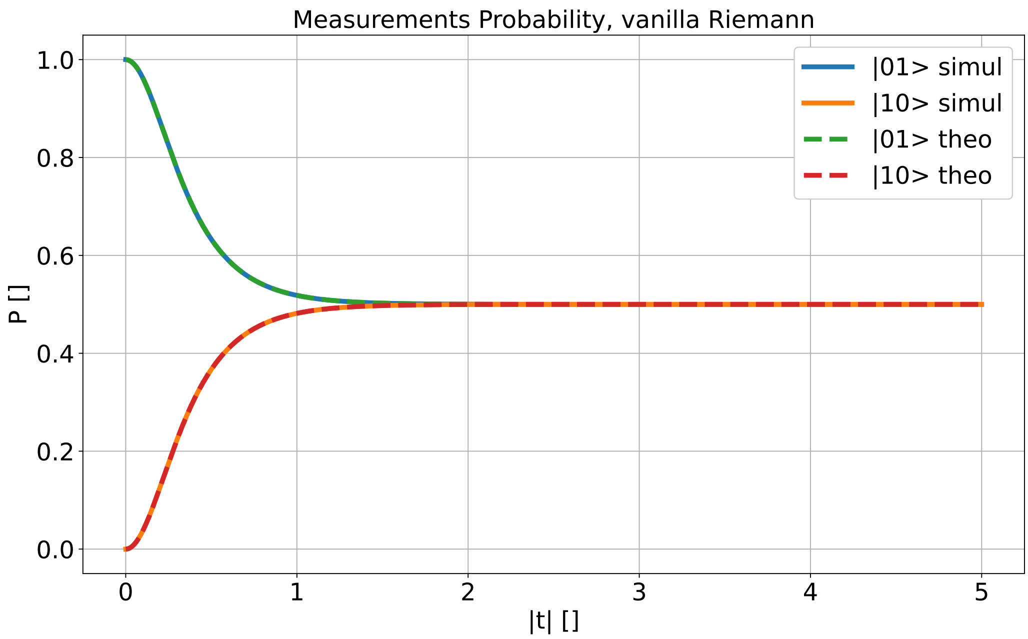


Figure 5.9: Quantum simulation of the evolution in imaginary time of the system in the second example (Chap 3 Sec. 4) using the vanilla Riemann integration procedure with 2000 equally spaced points in the interval $[-8, 8]$ for each of the $5 \cdot 10^4$ time steps.

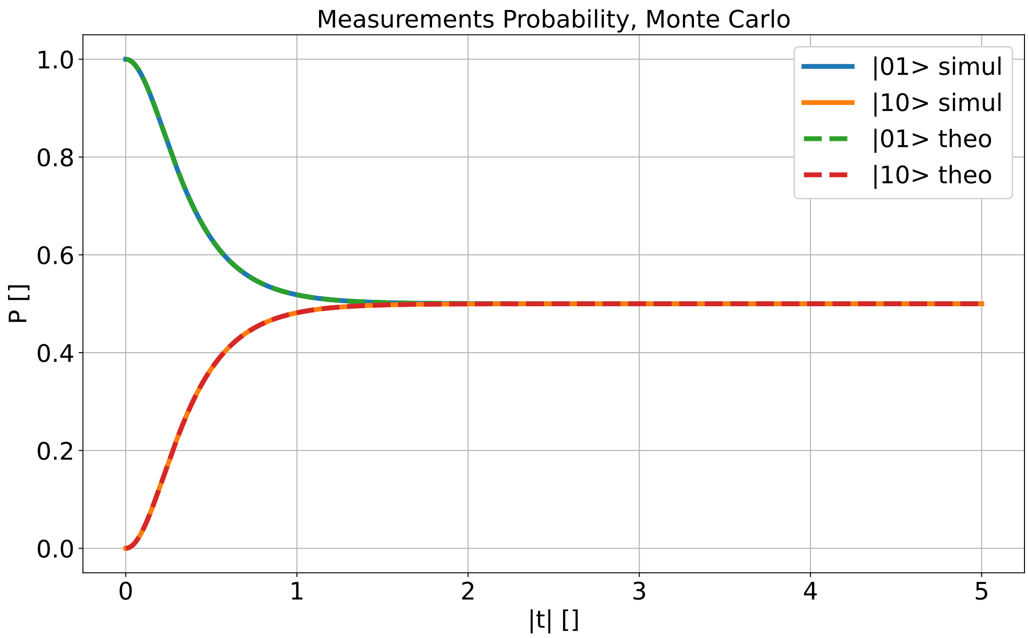


Figure 5.10: Quantum simulation of the evolution in imaginary time of the system in the second example (Chap 3 Sec. 4) using the Monte Carlo procedure with $5 \cdot 10^4$ time steps and 10^4 samples for each of them.

As expected, the results of these simulations matches once again the expectations: adding the ancillas is in this case an unnecessary complication, however it still produces the correct states during the evolution.

In case that the unitarity of the exponential operators appearing inside the integral of Eq. (3.6) is not certain then, it is always possible to accurately implement them as described in Chap. 4 Sec. 3.

Chapter 6

Fundamental Implications

In this last chapter some further remarks about the Hubbard-Stratonovich formulation of quantum gates will be made, focusing on its similarity with the predictions of local hidden-variable theories.

1 Local hidden-variable theories

Hidden-variable theories [24] are all those physical theories which try to explain the intrinsic probabilistic character of nature arising from quantum mechanics by postulating the existence of some inaccessible well defined quantities of classical nature (the hidden variables). From this perspective, the values of such quantities define the result of the measurement of any observable on the considered system. The fact that the hidden variables values cannot be known allows for these theories to reproduce the same probabilistic results found with quantum mechanics, whose results would in this case only be an approximation of a more fundamental, "inaccessible", theory.

The interest in these theories arose primarily as a consequence of a paper published in 1935 by Einstein, Podolsky and Rosen [25], where they claimed to have found the way of showing that quantum mechanics was not a complete theory, in the sense that it was not compatible with the assumptions of locality and realism as defined by them.

In particular, they spoke about reality by imagining the existence of the so called *elements of reality*, i.e. quantities in a system, the value of which can be obtained with absolute precision without perturbing the system by the slightest amount. A complete theory, according to the authors of the paper, must be able to provide a well definite value for any element of reality. On the other hand, the assumption of locality comes directly from the theory of relativity and consists in postulating that no instantaneous action can take place in the considered system, i.e. that any influence must travel at a finite speed which must be at most equal to that of light.

The argument starts by considering an entangled two-particle system such that the sum of the two particles momenta is 0 and also the difference of their positions is known, this last being big enough to allow local measurements on either of the two particles without involving the other.

Given these premises, it must always be possible to measure the position or the momentum of one of the two particles alone: from the results of such measurements one could then deduce the value of the same quantities but for the remaining particle, without acting in any way on the latter.

According to what was just stated earlier, the presented arguments imply that both the position and the momentum of the untouched particle must be elements of reality. Therefore, a complete theory should be able to predict a value for each of them. It is well known however that in quantum mechanics it is not possible to measure exactly the position and the momentum of a given particle at the same time, which means that such theory must be incomplete under the assumptions made earlier.

An important point to make at this point is that before the first particle is measured, in quantum mechanics the values of position and momentum of the two particles are not defined. When taking the measurement, however, both such quantities become well defined for each of the two particles, simultaneously. Action is performed only on one particle though, which may be interpreted as if a certain influence is instantaneously transferred from the measured particle to the other, regardless of the distance separating them.

This fact allows for the introduction of the local hidden-variable theories: Quantum mechanics is interpreted as an approximation of a more fundamental local theory characterized by some unknown variables, thanks to which it is possible to predict the correct values for every observable of any system. Calling x the set of all the hidden variables, a system in a certain quantum state $|\psi\rangle$ will correspond to a statistical mixture of states with a well defined x, mixture defined by the the probability distribution $\rho_\psi(x)$ of having a particular value for the hidden variables. States with a precise value of x will have a precise value $\hat{O}(x)$ for any possible observable $\hat{O}$, so that the value of such observable computed on the quantum state $|\psi\rangle$ will be given by the average of the various $\hat{O}(x)$ weighted by the probability density $\rho_\psi(x)$:

$$\langle \hat{O} \rangle_\psi = \int dx \rho_\psi(x) \hat{O}(x).$$

2 Bell inequalities

A question that may arise is whether or not all the results of quantum mechanics could be reproduced by a local hidden-variable theory. In order to address this problem let's consider a slightly different version of the arguments discussed in the paper by Einstein, Podolsky and Rosen.

In 1951 David Bohm showed that by considering a two-particle quantum system in the singlet spin state $|-\rangle$ (see Chap. 3 Sec. 4.1) with the two particles being sufficiently spatially separated (enough for the measurement of single particles to be possible), any component of the spin of one of the two particles could indeed be considered as an element of reality [26].

Different components of the spin of a particle cannot be simultaneously measured according to quantum mechanics, though. This is then the same problem presented in the last section, formulated now in more precise and mathematical terms. This is also known as the *EPR paradox*, by the names of the authors of the original paper.

Relying on this example it is fairly simple to show the result published by Bell in a paper in 1965 [27], where he demonstrated that quantum mechanics can make predictions which are not reproducible by a real local hidden-variable theory.

Let us think about measuring the spin of each particle (I called them A and B) along certain directions with two separated measurements, choosing independently the direction for each of them and representing such choice with a for the first particle and b for the other: the results of the measurements may be respectively indicated by $\hat{\sigma}^{(A)}(a, b, x)$ and $\hat{\sigma}^{(B)}(a, b, x)$, since in principle each of them could depend on both the chosen directions a and b, but once these are chosen each measurement will be uniquely determined by the hidden variables x (when computed on the system in a state with a well defined x).

The system however is in the singlet state $|-\rangle$, which is a quantum entangled state and as such doesn't correspond to a precise choice of the hidden variables, rather it will be defined by a certain probability distribution $\rho_-(x)$. The result of the measurements as predicted by quantum mechanics will then be a weighted average of the possible results with a fixed x.

Let us consider the observable $\langle\hat{\sigma}_a^{(A)} \otimes \hat{\sigma}_b^{(B)}\rangle_- \equiv \langle -|\hat{\sigma}_a^{(A)} \otimes \hat{\sigma}_b^{(B)}|-\rangle$. According to a general hidden-variable theory, such observable should have the following form, as stated at the end of the previous section:

$$\langle\hat{\sigma}_a^{(A)} \otimes \hat{\sigma}_b^{(B)}\rangle_- = \int dx \rho_-(x)(\widehat{\sigma\sigma})(a,b,x), \tag{6.1}$$

where I defined $(\widehat{\sigma\sigma})(a,b,x) \doteq \hat{\sigma}^{(A)}(a,b,x) \otimes \hat{\sigma}^{(B)}(a,b,x)$.

Specifying to a local hidden-variable theory means assuming that $\hat{\sigma}^{(A)}(a,b,x)$ and $\hat{\sigma}^{(B)}(a,b,x)$ do not depend respectively on b and a, i.e. that the measurement performed on a particle does not depend on the measurement performed on the other particle (at least when the 2 measurements are space-like separated, in the relativistic sense). According to a local hidden-variable theory, then, Eq. (6.1) becomes the following:

$$\langle\hat{\sigma}_a^{(A)} \otimes \hat{\sigma}_b^{(B)}\rangle_- = \int dx \rho_-(x)\hat{\sigma}^{(A)}(a,x) \otimes \hat{\sigma}^{(B)}(b,x). \tag{6.2}$$

This is exactly the important point: It is possible to show explicitly that if Eq. (6.2) holds, then there are many different inequalities (collectively called *Bell inequalities*) among quantity $\langle\hat{\sigma}_a^{(A)} \otimes \hat{\sigma}_b^{(B)}\rangle_-$ chosen with different values of a and b that must be satisfied.

Two examples of such inequalities are reported below [27] [28]:

$$\left|\langle\hat{\sigma}_a^{(A)} \otimes \hat{\sigma}_b^{(B)}\rangle_- - \langle\hat{\sigma}_a^{(A)} \otimes \hat{\sigma}_c^{(B)}\rangle_-\right| \leq 1 + \langle\hat{\sigma}_b^{(A)} \otimes \hat{\sigma}_c^{(B)}\rangle_-$$

$$\left|\langle\hat{\sigma}_a^{(A)} \otimes \hat{\sigma}_b^{(B)}\rangle_- - \langle\hat{\sigma}_a^{(A)} \otimes \hat{\sigma}_c^{(B)}\rangle_-\right| + \langle\hat{\sigma}_d^{(A)} \otimes \hat{\sigma}_b^{(B)}\rangle_- + \langle\hat{\sigma}_d^{(A)} \otimes \hat{\sigma}_c^{(B)}\rangle_- \leq 2.$$

However, quantum mechanics provides values $\langle \hat{\sigma}_a^{(A)} \otimes \hat{\sigma}_b^{(B)} \rangle_-$, which *do not satisfy such inequalities*. Since these are measurable quantities it must be possible to set up various experiments which could test whether or not nature is found to comply with the aforementioned inequalities.

Many such experiments were actually carried out, leading to the result that it is actually quantum mechanics, rather than the local hidden-variable theories, that correctly reproduces the observed correlations. This fact implies then that quantum mechanics cannot be interpreted as an approximation of an underlying local hidden-variable theory, but at the very least only of a non-local one.

3 Relation with Hubbard-Stratonovich

In the light of what has just been discussed in the last sections, let us consider again Eq. (3.10), choosing $N = 2$ and renaming $\hat{O}_i$ the one-qubit operators that was called $\hat{\tilde{O}}_i$ before, for ease of notation. This is the complex time evolution operator of a two qubit system under an Hamiltonian $\hat{H}$ being the squared sum of two operators acting each on a single qubit:

$$e^{-\hat{H}t} = e^{-\frac{1}{2}\left(\hat{O}_1+\hat{O}_2\right)^2 t} = \int dy \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} e^{-iy\sqrt{t}\hat{O}_1} \otimes e^{-iy\sqrt{t}\hat{O}_2}. \tag{6.3}$$

It is immediately evident that this equation looks formally equivalent to Eq. (6.2). In particular, it might be easy to consider the classical field y in Eq. (6.3) as an hidden variable and $\frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}}$ as a probability distribution in y (it is always greater or equal to 0 for every y and its integral over the full domain is 1). At the same time, $e^{-iy\sqrt{t}\hat{O}_1}$ and $e^{-iy\sqrt{t}\hat{O}_2}$ are already one-qubit operators depending on y only, like $\hat{\sigma}^{(A)}(a, x)$ and $\hat{\sigma}^{(B)}(b, x)$ in Eq. (6.2).

Eq. (6.3), though, is an exact representation of the complex time evolution operator, while Eq. (6.2) expresses the average value of the Kronecker product between two one-qubit operators, evaluated on a state defined by the distribution $\rho_-(x)$. This means that one cannot blindly compare these two equations. Rather, one should use Eq. (6.3) to compute the same quantity involved in Eq. (6.2) and then compare these last two. Let us then proceed with such computation, evaluating the expectation of $\hat{O}_1' \otimes \hat{O}_2'$ on the state $|\psi(t)\rangle$ evolved from the separable state $|\psi(0)\rangle \equiv |\phi_1\phi_2\rangle \doteq |\phi_1\rangle \otimes |\phi_2\rangle$ with the Hubbard-Stratonovich formulation (where $\hat{O}_1'$ and $\hat{O}_2'$ are one-qubit operators acting respectively on particle 1 and 2):

$$\langle \hat{O}_1' \otimes \hat{O}_2' \rangle_{\psi(t)} \doteq \langle\psi(t)|\, \hat{O}_1' \otimes \hat{O}_2'\, |\psi(t)\rangle = \left\langle e^{-\hat{H}t}\psi(0) \right| \hat{O}_1' \otimes \hat{O}_2' \left| e^{-\hat{H}t}\psi(0) \right\rangle =$$
$$= \left\langle \left(\int \tfrac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} e^{-ix\sqrt{t}\hat{O}_1} \otimes e^{-ix\sqrt{t}\hat{O}_2} dx \right) \psi(0) \right| \hat{O}_1' \otimes \hat{O}_2' \left| \left(\int \tfrac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} e^{-iy\sqrt{t}\hat{O}_1} \otimes e^{-iy\sqrt{t}\hat{O}_2} dy \right) \psi(0) \right\rangle =$$
$$= \langle\psi(0)| \left(\int \tfrac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} e^{ix\sqrt{t}\hat{O}_1} \otimes e^{ix\sqrt{t}\hat{O}_2} dx \right) \left(\hat{O}_1' \otimes \hat{O}_2' \right) \left(\int \tfrac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} e^{-iy\sqrt{t}\hat{O}_1} \otimes e^{-iy\sqrt{t}\hat{O}_2} dy \right) |\psi(0)\rangle =$$
$$= \langle\phi_1\phi_2| \iint \tfrac{1}{2\pi} e^{-\frac{x^2+y^2}{2}} \left(e^{ix\sqrt{t}\hat{O}_1} \otimes e^{ix\sqrt{t}\hat{O}_2} \right) \left(\hat{O}_1' \otimes \hat{O}_2' \right) \left(e^{-iy\sqrt{t}\hat{O}_1} \otimes e^{-iy\sqrt{t}\hat{O}_2} \right) dxdy |\phi_1\phi_2\rangle =$$
$$= \langle\phi_1\phi_2| \iint \frac{1}{2\pi} e^{-\frac{x^2+y^2}{2}} \left(e^{ix\sqrt{t}\hat{O}_1} \hat{O}_1' e^{-iy\sqrt{t}\hat{O}_1} \right) \otimes \left(e^{ix\sqrt{t}\hat{O}_2} \hat{O}_2' e^{-iy\sqrt{t}\hat{O}_2} \right) dxdy\, |\phi_1\phi_2\rangle =$$
$$= \iint \frac{1}{2\pi} e^{-\frac{x^2+y^2}{2}} \langle\phi_1|\, e^{ix\sqrt{t}\hat{O}_1} \hat{O}_1' e^{-iy\sqrt{t}\hat{O}_1}\, |\phi_1\rangle \langle\phi_2|\, e^{ix\sqrt{t}\hat{O}_2} \hat{O}_2' e^{-iy\sqrt{t}\hat{O}_2}\, |\phi_2\rangle\, dxdy. \tag{6.4}$$

Since $\int \frac{1}{2\pi} e^{-\frac{x^2+y^2}{2}} dxdy = 1$ and $\frac{1}{2\pi} e^{-\frac{x^2+y^2}{2}} \geq 1\ \forall x, y \in [-\infty, \infty]$, the quantity $\frac{1}{2\pi} e^{-\frac{x^2+y^2}{2}}$ can be interpreted as a probability distribution over the variables x and y, while once again both $\langle\phi_1|\, e^{ix\sqrt{t}\hat{O}_1} \hat{O}_1' e^{-iy\sqrt{t}\hat{O}_1}\, |\phi_1\rangle$ and $\langle\phi_1|\, e^{ix\sqrt{t}\hat{O}_2} \hat{O}_2' e^{-iy\sqrt{t}\hat{O}_2}\, |\phi_1\rangle$ are one-qubit operators depending on the two variables x and y.

This seems to imply that the form of Eq. (6.4) is the same of that in Eq. (6.2), which in turn would mean that the Hubbard-Stratonovich formulation is in a sense introducing some local hidden variables in the system and using these to rephrase the evolution.

There is something sounding very bad about this conclusion, however. The Hubbard-Stratonovich transformation is in principle an exact transformation, and as such one would expect that when used to formulate a quantum operator it would produce the same identical effect as if that operator was applied in the standard way. On the other hand, if the Hubbard-Stratonovich transformation of a quantum operator reformulates the latter in terms of local hidden variables, than the two procedures cannot be the same, since from what has been presented in the previous sections it should be clear that a local hidden-variable theory cannot reproduce all the results expected by a quantum theory.

This subject is of fundamental importance for understanding whether a quantum gate implementation method relying on the Hubbard-Stratonovich transformation could actually be achieved and needs a thorough investigation which is left for future work. As a last remark, I would like to point out that the results of the simulations reported in the earlier parts of this work seem to show that the Hubbard-Stratonovich formulation of evolution operators is indeed able to generate entanglement and to produce Bell states (i.e. completely entangled pure states), where it can be shown (see for example [29]) that such states always violate at least some Bell inequalities.

Chapter 7

Conclusions

Inspired by the problem of optimizing gate implementation in quantum computers, a method based on the Hubbard-Stratonovich transformation is presented.
This exact mathematical transformation has been shown to correctly allow the rephrasing of numerous multi-qubit gates in terms of a combination of one-qubit gates, which are generally characterized by a better fidelity. This is achieved by combining both a "quantum step" (the actual implementation on the quantum computer of each needed one-qubit gate) and a "classical step" (the realization of the integral of the aforementioned gates). This strategy might be therefore classified as a quantum-classical hybrid method.
The application of the HS transformation has been proved to be able to evolve the state of a system in both imaginary and real time (according to a two-body trial Hamiltonian), providing the correct amplitudes (on the computational basis of the Hilbert space in which the system lives) even when such state is expected to be entangled. Whether or not the state that is reached in a physical machine is a truly entangled state is still a debatable matter and will be further investigated.
By means of several simulations, different algorithms for the classical implementation of the integral were compared, all of which produced the correct results at the same level of accuracy, although requiring a different amount of computational resources. Furthermore, under many circumstances, the HST has been shown to require the application on the system of non-unitary gates. A procedure for the implementation of such gates by expanding the Hilbert space of the system through the addition of ancil-

lary qubits has been exploited and successfully tested with quantum simulations.
In the last part of the thesis, similarities between the HST and local hidden-variable theories are highlighted, which raises some questions about the actual range of application and reliability of this approach.
Future perspectives of this work include:

- further testing of the described procedure changing the various aspects from those investigated in this work (different systems, Hamiltonians, algorithms for the implementation of the integral and the non unitary gates...);
- as already mentioned, analyzing precisely the relations between the HST and local hidden-variable theories, consolidating the foundations of the first and hopefully gaining a deeper understanding of its operating principles;
- realizing the implementation of an actual multi-qubit gate on a real quantum computer by means of the HST, benchmarking it with the standard procedures;
- verifying the actual nature of the entanglement that the HST seems to be able to generate in a system, testing which correlations among parts of a system can actually be realized;
- Improving the described procedure upgrading it to a fully quantum form.

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