The Schrödinger Equation, Reversibility and the Grover Algorithm

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Several aspects of the time-dependent Schrödinger equation are discussed in the context of Quantum Information Theory.

1 Time Dependent Schrödinger Equation and Quantum Computation

In Quantum Information Theory (QIT), the time dependent Schrödinger equation [1] acquires an informational content in addition to its physical content that dictates the time evolution of a quantum system. The functioning of a Quantum Computer (QC) [2] parallels the unitary evolution of a quantum system. Each step of the quantum evolution corresponds to a typical operation on a QC:

i/ A QC starts at some initial state
\[ |\Psi(t_i)\rangle := |\Psi_0\rangle. \tag{1} \]

The preparation of the initial state corresponds to the input data in a computer program. The state \(|\Psi(t_i)\rangle\) belongs to a Hilbert space of many-particle states \(\mathcal{H}^\otimes n\) that is a tensor product of \(n\) single-particle states. When each single Hilbert space \(\mathcal{H}\) is spanned by a two-dimensional basis, the information is quantumly encoded in a qubit. A quantum register is a tensor product of qubit states. Quantum states can be used to encode information. A manageable configuration for the initial state is a factorized tensor product of qubits (unentangled state)
\[ |\Psi(t_i)\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \ldots \otimes |x_n\rangle \in \mathcal{H}^\otimes n, \ x_i = 0, 1 \ \forall i. \tag{2} \]

ii/ A QC evolves in time during an interval \(t\) allowing us to process the information previously encoded
\[ |\Psi(t)\rangle = U(t, t_i)|\Psi(t_i)\rangle. \tag{3} \]
where the unitary evolution operator $U(t, t_i)$ satisfies the time-dependent Schrödinger equation, either in differential form

$$i\hbar \frac{d}{dt} U(t, t_i) = H(t) U(t, t_i),$$

or as an equivalent integral equation

$$U(t, t_i) = I - \frac{i}{\hbar} \int_{t_i}^{t} H(t') U(t', t_i) dt'.$$

The integration of the evolution equation yields

$$U(t, t_i) = T \left[ e^{-\frac{i}{\hbar} \int_{t_i}^{t} H(t') dt'} \right],$$

where $T$ is the temporal ordering operator introduced by Dyson. When the Hamiltonian is time independent as in conservative systems, the integrated form of the evolution operator can be further simplified as

$$U(t, t_i) = e^{-\frac{i}{\hbar} (t-t_i) H}.$$

The evolution operator of Quantum Mechanics corresponds to a quantum logic gate in a QC. Thus, a quantum logic gate is a unitary operator acting on the states of a certain set of qubits (quantum register). It is represented by a $2^n \times 2^n$ matrix in the unitary group $U(2^n)$. Hence, quantum computation is a class of reversible computation. The first experimental proposal for constructing quantum logic gates with ion traps was by Cirac and Zoller [3], [4].

iii/ Quantum programming corresponds to harnessing the reversibility inherent to quantum computation with the purpose of producing a useful task. A task corresponds to the evaluation of a certain Boolean function $f : \{0, 1\}^m \rightarrow \{0, 1\}$. Reversibility requires to split the quantum register storing an initial state $|\Psi_i\rangle$ into two parts: the source register and the target register, namely,

$$|\Psi_0\rangle := |\Psi_s\rangle \otimes |\Psi_t\rangle.$$

To implement a Boolean function $f$ in a QC we need the action of a unitary gate $U_f$ on the registers as follows

$$U_f |x_1 x_2 \ldots x_m\rangle |x_{m+1}\rangle_t = |x_1 x_2 \ldots x_m\rangle |x_{m+1} \oplus f(x_1, x_2, \ldots, x_m)\rangle_t.$$

This action guarantees that whichever the $f$ is, the function evaluation is implemented reversibly [5].

iv/ The final state $|\Psi_f\rangle$ is the outcome of a computation in a QC. It is a superposition of all states in a computational basis $\{ |x_1, \ldots, x_n\rangle \}$

$$|\Psi_f\rangle = U(t_f, t_i) |\Psi(t_i)\rangle = \sum_{x_1, \ldots, x_n=0,1} C_{x_1,\ldots,x_n} |x_1, \ldots, x_n\rangle,$$
and will be an entangled state in contrast to the factorized state that we started with. Entanglement is the result of combining the superposition principle of Quantum Mechanics with the tensor product of single-particle systems. This capability of storing many classical registers \((x_1, \ldots, x_n)\) at the same time is called quantum parallelism. It is the source of the potentially superior efficiency of a QC with respect to a classical computer.

The measurement in Quantum Mechanics is the read out of the QC to retrieve the desired output. Associated to the computational basis there is a set of orthonormal operators \(\Pi_{(x_1, \ldots, x_n)} = |x_1, \ldots, x_n\rangle \langle x_1, \ldots, x_n|\) such that the result of a measurement on the final state is

\[
|\Psi_f\rangle \langle \Psi_f| \rightarrow \frac{\Pi_{(x_1, \ldots, x_n)}|\Psi_f\rangle \langle \Psi_f|\Pi_{(x_1, \ldots, x_n)}}{\text{Tr}\left[\Pi_{(x_1, \ldots, x_n)}|\Psi_f\rangle \langle \Psi_f|\Pi_{(x_1, \ldots, x_n)}\right]} = \Pi_{(x_1, \ldots, x_n)},
\]

with probability

\[
P(x_1, \ldots, x_n) = \text{Tr}\left[\Pi_{(x_1, \ldots, x_n)}|\Psi_f\rangle \langle \Psi_f|\Pi_{(x_1, \ldots, x_n)}\right] = |C_{x_1, \ldots, x_n}|^2.
\]

Thus, the probabilistic nature of Quantum Mechanics implies that a quantum computation is probabilistic: we will find the desired output within a certain probability. The aim of a good quantum programmer is to make this probability as close as possible to 1. This means a pattern of constructive interference of amplitudes towards the desired output amplitude. Examples of good quantum programming are the Shor algorithm, where the task is to factor out a large integer, and the Grover algorithm, where the task is to search for an item in a disordered database.

This is the time evolution of a quantum system and it encompasses all the principles of Quantum Mechanics, which in turn can also be given an interpretation in QIT.

The basic problems that a QC can address are the same than a classical computer:

- **Computability**: what problems the machines can do and cannot do.
- **Complexity**: scaling of space/time with the size of the problems that can be solved.
- **Universality**: whether one machine can simulate all others, so that we do not need to construct an special-purpose machine for each problem to be solved.

### 2 Reversibility on the Lattice

Reversibility means that we can compute exactly backwards by saving only the final conditions and the number of steps. It is energetically economical compared to current standard computers that work irreversibly.

A QC works reversibly as a consequence of the unitary of the evolution operator. It is also a machine that operates with finite means (Turing
machine): to simulate the evolution of a quantum system we must discretize both time and space. This is done by setting the Schrödinger equation on a space-time lattice. This discretization was implicit in the qubit decomposition of the initial state in (2). From a more fundamental point of view, many theoretical physicists, including Feynman [15], have wondered about what is the underlying structure of the universe beyond the subatomic level and have proposed that it might have a discrete structure. If this were the case, a natural question is how to formulate reversible evolutions in a discretized form.

The finite difference method is a natural scheme to discretize the Schrödinger equation: substitute derivatives of functions by finite differences, which are approximations to a certain degree in a Taylor expansion. There is some freedom in this transition from a differential equation to its finite difference form. It turns out that some of them are not exactly reversible while some of them are. The meaning here of the word exactly is explained below in the context of computer simulations with finite precision.

The key point is whether we use a naive difference formula for the derivative of a given function $F(z)$ as

$$\frac{d}{dz} F(z) = \frac{1}{\epsilon} [F(z_{i+1}) - F(z_i)] + O(\epsilon).$$

This is a non-centered formula. Another possibility is to use centered formulas for derivatives of any degree

$$\frac{d}{dz} F(z) = \frac{1}{2\epsilon} [F(z_{i+1}) - F(z_{i-1})] + O(\epsilon^2),$$

$$\frac{d^2}{dz^2} F(z) = \frac{1}{\epsilon^2} [F(z_{i+1}) - 2F(z_i) + F(z_{i-1})] + O(\epsilon^2).$$

Let us consider the evolution of a single particle in one dimension given by the Schrödinger equation in coordinate representation

$$i\frac{\partial}{\partial t} \psi(x, t) = -\frac{\partial^2}{\partial x^2} \psi(x, t) + V(x, t)\psi(x, t),$$

where $V(x, t)$ is a generic potential and we assume units $\hbar = 2m = 1$. To discretize this equation, let $a$ be the lattice spacing so that the discrete coordinates are $x_m = ma, m \in \mathbb{Z}$ and $\tau$ the time step such that time coordinates are $t_n = n\tau, n \in \mathbb{Z}$. The discretized wave function is $\Psi_{m,n} := \psi(x_m, t_n)$ and similarly for the potential $V_{m,n} := V(x_m, t_n)$.

**Asymmetric Difference Scheme**

This is a (centered space, non-centered time) difference scheme that results from the substitution of (13) for the time derivative and (15) for the spatial derivative.
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\[ \Psi_{m,n+1} = \Psi_{m,n} + i \left[ \frac{\tau}{a^2} (\Psi_{m+1,n} - 2\Psi_{m,n} + \Psi_{m-1,n}) - \tau V_{m,n} \Psi_{m,n} \right]. \]  

(17)

This is a first order difference equation in the time index \( n \) like its continuum version. The initial value problem is determined by giving the values \( \Psi_{m,0} \) along the one-dimensional spatial grid. However, this equation (17) is not an exactly reversible discrete update rule because of roundoff and truncation errors. The matrix form of (17) is, for periodic boundary conditions in a lattice with \( M \) sites,

\[
\Psi_{n+1} = \begin{pmatrix}
1 - iV_{1,n}\tau - 2i\epsilon & i\epsilon & 0 & 0 & \ldots & i\epsilon \\
i\epsilon & 1 - iV_{2,n}\tau - 2i\epsilon & i\epsilon & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
i\epsilon & 0 & 0 & \ldots & 1 - iV_{M,n}\tau - 2i\epsilon \\
\end{pmatrix}
\Psi_n,
\]

(18)

where \( \epsilon := \frac{\tau}{a^2} \) and \( \Psi_n \) is a column vector of dimension \( M \) storing the values of the wave function at time step \( n \). This matrix is unitary only in the limit of infinitesimal \( \epsilon \) and \( \tau \): the norm of each column vector is \( 1 + O(\tau^2) + O(\epsilon^2) \), and the scalar product of two vectors is \( O(\tau^2) + O(\epsilon^2) \). Were it be exactly unitary, its inversion would not need multiplication/division operations since it would be its Hermitian matrix: only simple arithmetic operations would do the job.

Symmetric Difference Scheme

This is a (centered space, centered time) difference scheme that results from the substitution of (14) for the time derivative and (15) for the spatial derivative

\[ \Psi_{m,n+1} = \Psi_{m,n-1} + i \left[ \frac{\tau}{a^2} (\Psi_{m+1,n} - 2\Psi_{m,n} + \Psi_{m-1,n}) - 2\tau V_{m,n} \Psi_{m,n} \right]. \]  

(19)

This scheme was discovered by Fredkin and Barton in 1975 \[16\] in their quest for exact reversibility of discretized Schrödinger equation following discussions with Feynman \[16, 17, 18\]. This discretized update rule have very interesting properties:

i/ It is a second order difference equation: the initial value problem is defined by providing the values of the wave function at two earlier time steps. This is in sharp contrast with the original continuous differential equation.

ii/ It is exactly reversible after \( n \) steps of computation.

iii/ It is exactly reversible even if the RHS cannot be computed exactly.

iv/ It is exactly reversible even if \( \Psi_{m,n} \) has finite precision values.

v/ It is a complex equation. However, the real part of \( \Psi_{n+1} \) depends only on the real part of \( \Psi_{n-1} \) and the imaginary part of \( \Psi_n \). Likewise, the imaginary part of \( \Psi_{n+1} \) depends only on the imaginary part of \( \Psi_{n-1} \) and the real part of \( \Psi_n \).
The exact reversibility expressed in properties ii/, iii/ and iv/ is related to property i/ and follows from the backwards recurrence relation:

$$\Psi_{m,n-1} = \Psi_{m,n+1} - i \left[ \frac{\tau}{a^2} (\Psi_{m+1,n} - 2\Psi_{m,n} + \Psi_{m-1,n}) - 2\tau V_{m,n}\Psi_{m,n} \right].$$  (20)

Property v/ is also useful to see the exact reversibility more explicitly: we can select the real parts of the wave function at all even time steps $n = 2l$ and the imaginary parts at all odd time steps $n = 2l + 1$. Thus, v/ guarantees that the evolution under (19) respects this structure and the rest of components of $\Psi_{2l}, \Psi_{2l+1}$ can be ignored self-consistently.

As a warmup, let us consider a typical update rule for a set of variables $\{X_{2l}, Y_{2l+1}\}_{l=0}^{\infty}$, ordered according to the time evolution of the real and imaginary parts described above: $X_0, Y_1, X_2, Y_3, X_4, Y_5, X_6, \ldots$. The initial data is $X_0, Y_1$. Let us assume that the update rule has the following form:

$$\begin{align*}
X_{2l+2} &:= X_{2l} + F(Y_{2l+1}), \\
Y_{2l+3} &:= Y_{2l+1} + F(X_{2l}),
\end{align*}$$  (21)

where $F$ is an arbitrary function. This is an example of an exactly reversible recurrence relation: the backwards update rule follows immediately,

$$\begin{align*}
Y_{2l+1} = Y_{2l+3} - F(X_{2l}), \\
X_{2l} = X_{2l+2} - F(Y_{2l+1}).
\end{align*}$$  (22)

Notice that in doing this reverse operation there is no need for multiplication/division operations, instead the simple arithmetic of addition/substraction can do the job. This fact is important when implementing the exact reversibility on a computer.

Let us now turn to the evolution difference equations for the real and imaginary parts of the wave function:

$$\Psi_{m,n} := R_{m,n} + iI_{m,n}.$$  (23)

From (19), they are given by

$$\begin{align*}
R_{m,n+1} &= R_{m,n-1} - [2\epsilon (I_{m+1,n} - 2I_{m,n} + I_{m-1,n}) - 2\tau V_{m,n}I_{m,n}], \\
I_{m,n+1} &= I_{m,n-1} + [2\epsilon (R_{m+1,n} - 2R_{m,n} + R_{m-1,n}) - 2\tau V_{m,n}R_{m,n}].
\end{align*}$$  (24)

For simplicity we have assumed that the potential is time-independent $V_{m,n} := V_m, \forall n$. Thus, setting $n = 2l + 1$ and $n = 2l + 2$ in the first and second equations of (24) respectively, we can discard the real parts at all odd time steps and the imaginary parts at all even time steps, yielding

$$\begin{align*}
R_{m,2l+2} &= R_{m,2l} - [2\epsilon (I_{m+1,2l+1} - 2I_{m,2l+1} + I_{m-1,2l+1}) - 2\tau V_{m}I_{m,2l+1}], \\
I_{m,2l+3} &= I_{m,2l+1} + [2\epsilon (R_{m+1,2l+2} - 2R_{m,2l+2} + R_{m-1,2l+2}) - 2\tau V_{m}R_{m,2l+2}].
\end{align*}$$  (25)

They have precisely the same form as (21).
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\[
\begin{align*}
R_{m,2l+2} &= R_{m,2l} - F_m(I_{m,2l+1}), \\
I_{m,2l+3} &= I_{m,2l+1} + F_m(R_{m,2l}),
\end{align*}
\]  
(26)

with \(F_m\) given by

\[
F_m(C_{m,n}) := 2\epsilon(C_{m+1,n} - 2C_{m,n} + C_{m-1,n}) - 2\tau V_mC_{m,n}.
\]  
(27)

Therefore, we have an exactly reversible update rule for the real and imaginary parts of the wave function \(\Psi_n\) at successive time steps. This does not produce the values of \(\Psi_n\) at arbitrary times, but assuming that the change in \(\Psi_n\) is smooth when \(\tau\) is small enough, then we can define the complex value of the wave function at any time as

\[
\Psi_{m,l} := R_{m,2l} + iI_{m,2l+1}.
\]  
(28)

A more compact form of the update recursion relations are obtained if we arrange the spatial components of the wave function in a vector array:

\[
\begin{align*}
R_{2l} &= (R_{m,2l}), \\
I_{2l+1} &= (I_{m,2l+1}).
\end{align*}
\]  
(29)

Moreover, we may want to implement the evolution equations directly in a computer with only integer arithmetics and resorting to only summation/substraction operations. The update rules (26) are precisely well suited for this type of implementations using for instance the C/C++ language operations ++ and -=. With these provisos, the computer-like form of the evolution difference equations is

\[
\begin{align*}
R - &= F(I), \\
I + &= F(R).
\end{align*}
\]  
(30)

The total probability \(P(t) := ||\Psi(x,t)||^2\) for finding the particle is a conserved quantity in the evolution of the quantum system (16). This quantity admits a discretized implementation like

\[
P_l := R_{2l}^2 + I_{2l+1}^2.
\]  
(31)

However, it is not exactly reversible for the discretized time evolution (26). Feynman found \([16]\) the following invariant

\[
P_l^{(t)} := R_{2l}^2 - I_{2l+1} \cdot I_{2l-1},
\]  
(32)

that is exactly reversible under the evolution (26).

The stability of the exactly reversible Schrödinger equation is analysed in appendix A.

So far we have considered the reversible vs. non-reversible implementation of the time-dependent Schrödinger equation in a classical computer. We can also implement it in a QC. Feynman proposed \([19]\) that one of the most important tasks that a QC could carry out is simulating quantum physics in an efficient way, contrary to the inefficiency showed by classical computers. The Abrahams-Lloyd scheme can serve for implementing differential equations in a QC \([20]\).
3 The Schrödinger Equation and the Grover Algorithm

The initial steps pursued by Schrödinger to formulate his evolution equation for the wave function of a quantum mechanical system bears little similarity with the final outcome he arrived at. In fact, he first came up with a scalar relativistic wave equation, later known as the Klein-Gordon equation. The process of creation of a new theory usually is not a straight line but rather a long a winding road, whose final results are not as polished and neat as they look at the end. Likewise, the final formulation of Grover algorithm does not show the initial steps that his author followed. In fact, Grover wandered around the discretized time-dependent Schrödinger equation \[21\] until he arrived to his beutiful algorithm in its final form \[7\], \[21\], \[22\].

The Grover algorithm is a quantum searching algorithm that outperforms any classical searching algorithm. The problem of searching an item in a disordered list or database with \(M\) items is known to be one of the most fundamental tasks that any computer is oftenly doing. Classically, no algorithm can do better than a brute force algorithm \[2\]. The number of queries is order \(O(M)\). Remarkly enough, the quantum search algorithm can do better with the help of the quantum parallelism and constructive interference of amplitudes in the evolution of a QC described in Sect. \[4\]. In the quantum case, the number of queries is reduced to order \(O(\sqrt{M})\), which is a major improvement.

The basic steps that led Grover to the quantum search algorithm starting from the discretized time-dependent Schrödinger equation are the following:

1/ Discretize the time-dependent Schrödinger equation on a space-time lattice with lattice spacing \(a\) and time steps of \(\tau\) duration as described in Sect. \[2\] using an asymmetric difference scheme \[17\], \[18\]. This evolution is approximately unitary up to order \(O(\epsilon^2) + O(\tau^2)\).

It is interesting to notice that Grover does not resort to an exactly reversible implementation of the evolution equation as in a symmetric difference scheme \[13\]. He employs a different pathway to achieve an exact unitary transformation since he needs to stick to a first order difference equation in the time variable.

2/ Introduce Diffusion \(D\) and Rotation \(R\) operators. This is a decomposition of the matrix evolution equation \[18\] as follows

\[
\Psi_{n+1} := DR\Psi_n, \quad \text{(33)}
\]

\[
D := \begin{pmatrix}
1 - 2i \epsilon & i \epsilon & 0 & 0 & \ldots & i \epsilon \\
i \epsilon & 1 - 2i \epsilon & i \epsilon & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
i \epsilon & 0 & 0 & \ldots & 1 - 2i \epsilon
\end{pmatrix}, \quad \text{(34)}
\]
We have assumed that the potential is time independent. This decomposition is correct within the approximation of order $O(\epsilon^2) + O(\tau^2)$. Notice also that while $R$ is exactly unitary, $D$ is only within the approximation $O(\epsilon^2)$.

The motivation for doing this decomposition is the key idea behind the construction of the searching algorithm: the matrix $D$ may be interpreted as a diffusion transformation (Markov process) with imaginary transition probabilities $\epsilon$, and the matrix $R$ is a phase rotation at every site of the lattice $m = 1, 2, \ldots, M$ induced by the application of the external potential $V_m$.

In the searching process, at time step $n = 0$ the system is initially in an equally probable superposition of states from the database to be searched for

$$\Psi_{m,0} := \frac{1}{\sqrt{M}}, \quad m = 1, 2, \ldots, M. \quad (36)$$

The goal is to find a marked state or item that is represented by a marked component of the wave function $\Psi_{m,N}$, after a number $N$ of iterations that represent the queries of the disordered database. This can be achieved taming these transformations $D, R$ in order to drive the system towards a final wave function that has the marked component highly amplified with respect to the rest of components.

The diffusion process represented by $D$ affects only to nearest-neighbour components of the wave function. This can also be viewed as the hopping of a single particle along the lattice in the presence of a potential. A classical analogy is useful: we may think that this particle will roll down towards the sites of lower potential like in a potential well. This is the amplification effect needed in the quantum search.

3/ Global diffusion and localized rotation: it is advantageous to extend the local diffusion of eq. (14) globally, as follows

$$D_L := \begin{pmatrix} 1 - (M - 1)\epsilon & \epsilon & \epsilon & \ldots & \epsilon \\ \epsilon & 1 - (M - 1)\epsilon & \epsilon & \ldots & \epsilon \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \epsilon & \epsilon & \epsilon & \ldots & 1 - (M - 1)\epsilon \end{pmatrix} \quad (37)$$

Now, the particle may hop to any site of the lattice. This is an example of long-range hopping. The sum of every column in $D_L$ is $1$.

At the same time, we tune the form of the potential well to be localized at the marked state as follows
\[ R_L(v) := \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ 0 & e^{-iv\tau} & 0 & \ldots & 0 \\ 0 & 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & 1 \end{pmatrix}, \quad (38) \]

where \( v \) is the value of the potential at that site. When it is negative it means attraction. The marked state is unknown, but we can selectively rotate its phase by an amount given by \( v \).

With a global diffusion operation \((37)\) there is no net hopping between unmarked sites since they have the same amplitude and the hopping in both directions cancels out. The hopping occurs towards the marked site from the rest of all states. This is the mechanism of amplitude amplification in the search algorithm. This amplification is maximum for a value of the rotation parameter \( v = \frac{\pi}{2} \). After this rotation and at time step \( n \), let the amplitudes of the marked and unmarked states be given by

\[ \tilde{\Psi}_{m_0,n} = \frac{iC_n}{\sqrt{M}}, \quad \tilde{\Psi}_{m \neq m_0,n} = \frac{c_n}{\sqrt{M}}. \quad (39) \]

Initially, \( C_0 := 1 =: c_0 \) \((36)\). After the diffusion transformation, they become

\[ \psi_{m_0,n} = \frac{1}{\sqrt{M}}[iC_n + (ic_n + C_n)(M - 1)c], \]
\[ \psi_{m \neq m_0,n} = \frac{1}{\sqrt{M}}[c_n - (ic_n + C_n)c]. \quad (40) \]

This means that the marked state changes its magnitude an amount of the order \( O(\sqrt{M}c) \), since by normalization \((39)\) \( \frac{1}{2} < c_n < 1 \), assuming \( C_n < \sqrt{\frac{M}{2}} \).

We wish to make \( \epsilon \) as large as possible in order to get the highest magnitude change in the marked state. However, we recall that the diffusion operation \((37)\) is unitary assuming that \( \epsilon \ll \frac{1}{M} \).

As the change of the marked state is order \( O(\sqrt{M}c) \), if we take \( \epsilon = O(\frac{1}{M}) \), then this change becomes \( O(M^{-\frac{3}{2}}) \). Thus, after the application of the diffusion transformation \((37)\) a number of time steps \( N = O(\sqrt{M}) \), the amplification of the marked state will become of the order of \( 1 \).

4/ Exactly unitary diffusion operation. Let us get rid off the infinitesimal character of the diffusion \((37)\) introducing a finite \( D_F \) transformation

\[ D_F(x, y) := \begin{pmatrix} x & y & y & \ldots & y \\ y & x & y & \ldots & y \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y & y & y & \ldots & x \end{pmatrix}, \quad (41) \]

where \( x, y \) are complex amplitudes satisfying the unitary constraints.
\[
|x|^2 + (M - 1)|y|^2 := 1, \quad (xy^* + x^*y) + (M - 2)|y|^2 := 0.
\] (42)

The infinitesimal transformation (37) corresponds to the particular case \(x = 1 - (M - 1)i\epsilon, \ y = i\epsilon\). Solving (42) we find that the highest value of \(y\) can be obtained on real solutions as
\[
x = -1 + \frac{2}{M} := x_M, \ y = \frac{2}{M} := y_M.
\] (43)

Then, the best diffusion operation is \(D_F(x_M, y_M)\) which corresponds to a hopping amplitude as high as \(\frac{2}{M}\).

This is the pathway followed by Grover in order to implement an exactly reversible evolution while retaining the first order character of the iteration process.

5/ The quantum searching algorithm: iterate a number \(N\) of time steps the basic operations (41) and (38), starting from the uniformly distributed state (36). When the diffusion operation is exactly unitary (41), the maximum hopping into the marked site occurs for a rotation of \(v = \pi\) (38), instead of \(v = \frac{\pi}{2}\) that is the case when the diffusion is infinitesimal (37). Thus,
\[
\Psi_N = [D_F(x_M, y_M)R_L(\pi)]^N \Psi_0.
\] (44)

This is an example of Trotter-Suzuki transformation [23, 24]. The counting of the number of iterations –queries of the database– is the same as in iv/ but with the application of (41), (42) to the state
\[
\tilde{\Psi}_{m_0,n} = \frac{c_n}{\sqrt{M}}, \quad \tilde{\Psi}_{m\neq m_0,n} = \frac{c_n}{\sqrt{M}}.
\] (45)

The result is,
\[
\Psi_{m_0,n} = \frac{1}{\sqrt{M}}[C_n + \frac{2}{M}(M - 1)c_n + C_n],
\Psi_{m\neq m_0,n} = \frac{1}{\sqrt{M}}[-c_n + \frac{2}{M}(Mc_n - C_n)].
\] (46)

In the limit \(M \to \infty\), the increase in the amplitude of the marked state is of order \(O(c_n/\sqrt{M})\), and the amplitude of the unmarked states remains approximately the same. As \(c_n\) remains order \(O(1)\) during the evolution, the net amplification is order \(O(M^{-\frac{1}{2}})\). Therefore, we need a number of iterations (44) of the order \(N = O(\sqrt{M})\) to make the probability of success for finding the searched item close to 1.

The origin of the higher efficiency of the quantum search algorithm over the classical algorithms is thus a neat combination of quantum parallelism and constructive interference of amplitudes. In addition, the Grover algorithm (44) is an example of the evolution of a quantum system like in Sect. 4 with \(\Psi_N \to \Psi_f\) and \(\Psi_0 \to \Psi_i\), in order to implement a useful task in Quantum Information Theory.
4 Conclusions

It has been two decades now since the BB84 quantum cryptography protocol was presented [25] and one decade ago that Shor algorithm was introduced [6]. I has been specially during this last decade that Quantum Information Theory has emerged an matured as a solid and complete discipline. QIT has part of its roots in the fundamentals of Quantum Mechanics, and thus it has become a part of Theoretical Physics by now. It has ramifications in other disciplines like Information Theory, Computer Science etc. which guarantees that findings in QIT may have applications to other fields beyond. Specially rewarding is the fact that QIT is a discipline in which there are experiments testing its theoretical findings. All these aspects have made QIT a very exciting field so far and we expect that it will continue to be so in the future.

Dedicated to Prof. Alberto Galindo Tixaire on occasion of his 70th birthday.

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A Numerical Stability of the Exactly Reversible Schrödinger Equation

In the analysis of the finite difference equations obtained from the time-dependent Schrödinger equation (16), we have focused on the exact reversibility on the lattice as the main issue.

Another very important issue is whether the difference equations are well-posed: a solution of the difference equation must be a reasonable approximation to the solution of the differential equation. This is the notion of convergence: in the limit of both the lattice spacing \( a \to 0 \) and the time step \( \tau \to 0 \), the solution of the difference equation must converge to the solution of the differential equation. The convergence is measured with a \( L^2 \)-norm:

\[
\| \Psi_n \|_a^2 := \sum_m |\Psi_{m,n}|^2 a.
\]

A related issue is the consistency of the difference equation. It means that the difference equation itself must converge to the differential equation pointwise at each grid point as \( a, \tau \to 0 \). Consistency implies that a smooth solution of the differential equation is an approximate solution of the difference equation. While a direct proof of convergence is a rather difficult problem, the proof of consistency is simpler. For the exactly reversible Schrödinger difference equation (19), consistency is a direct consequence of the Taylor expansions (14), (15) and it is checked directly.

Consistency is a necessary condition for convergence, but it is not sufficient. Additional properties must be required for a consistent difference equation to be convergent. This is where the notion of numerical stability enters [18], [26].
The essence of stability is that the solutions of the difference equation must be bounded in some sense, in order to prevent the finite solution to explode in the continuum limit. More precisely, a difference equation is stable when the solution at a time step \(n\) is bounded by

\[
||\Psi_n||_a^2 \leq C_T \sum_{n'=0}^{N_0} ||\Psi_{n'}||_a^2,
\]

with \(C_T\) some constant, and \(N_0\) some integer that depends on the order of the difference equation. The meaning of this bound is that as time goes by, the growth of the solution is limited. This concept of stability is closely related to the concept of well-posedness of initial value problems for partial differential equations:

\[
\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx \leq C_T \int_{-\infty}^{+\infty} |\Psi(0, t)|^2 dx, \quad t \in [0, T].
\]

The fundamental theorem in the theory of finite difference equations is the Lax-Richtmyer equivalence theorem: a consistent finite difference equation for a partial differential equation, for which the initial value problem is well-posed, is convergent if and only if it is stable.

This theorem is a very powerful characterization of convergence since the determination of consistency and stability is much easier. Let us apply the Lax-Richtmyer theorem to the exactly reversible Schrödinger difference equation (19) with vanishing external potential. We already know that the equation is consistent from the Taylor expansions (14), (15). Let us focus on stability. In this particular case, we have translational invariance and we also assume an infinite spatial lattice. This allows us to Fourier transform to momentum space the solution \(\Psi_{m,n}\) in coordinate space,

\[
\hat{\Psi}_{m,n}(k) := \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{+\infty} e^{-ima} \Psi_{m,n} a, \quad k \in [-\pi/a, \pi/a].
\]

Using the inversion formula

\[
\Psi_{m,n} = \frac{1}{\sqrt{2\pi}} \int_{-\pi/a}^{+\pi/a} e^{ima} \hat{\Psi}_{m,n}(k) dk,
\]

we obtain the recursion relation satisfied by the Fourier components

\[
\hat{\Psi}_{n+1}(k) = \hat{\Psi}_{n-1}(k) - 2if_\epsilon(ka)\hat{\Psi}_n(k),
\]

\[
f_\epsilon(ka) := 4\epsilon \sin^2 \frac{ka}{2a}.
\]

This is a simpler recursion relation since it is only on the time-step label \(n\). The Parseval relation
\[\|\hat{\Psi}_n\|_a^2 = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} |\hat{\Psi}_n(k)|^2 dk = \sum_{m,n=0}^{+\infty} |\hat{\Psi}_{m,n}|^2 a = \|\Phi_n\|_a^2, \quad (53)\]

guarantees that the stability property is preserved under the Fourier transform. There are several ways for solving (52). Let us introduce a generating function
\[\hat{G}_k(u) := \sum_{n=0}^{\infty} \hat{\Psi}_n(k)u^n, \quad (54)\]
defined on the complex plane \(u \in \mathbb{C}\). Knowing \(\hat{G}_k(u)\), we can recover the Fourier components through the Cauchy theorem,
\[\hat{\Psi}_n(k) = \frac{1}{2\pi i} \oint_{\Gamma_0} \hat{G}_k(u)u^{-n-1} du, \quad (55)\]
where \(\Gamma_0\) is a contour encircling the origin counterclockwise. Using the recursion relation we can find the generating function. It is given by
\[\hat{G}_k(u) = \left[1 + 2if_x(ka)u\right] \hat{\Psi}_0(k) + u\hat{\Psi}_1(k), \quad (56)\]
where \(\hat{\Psi}_0(k), \hat{\Psi}_1(k)\) are the Fourier transform of the initial data (50). To find the solution via (55) it is convenient to change variables \(v := \frac{1}{u}\),
\[\hat{\Psi}_n(k) = \frac{1}{2\pi i} \oint_{\Gamma_{\infty}} \hat{G}_k\left(\frac{1}{v}\right)v^{n+1} \frac{dv}{v^2}, \quad (57)\]
where \(\Gamma_{\infty}\) is a contour encircling the point of infinity and enclosing all the poles of the generating function. Using Cauchy’s residue’s theorem, we can obtain the general solution as
\[\hat{\Psi}_n(k) = \frac{1}{2\pi i} \oint_{\Gamma_{\infty}} \hat{G}_k(v)v^{n} dv = \sum_{\text{poles}} \text{Res}[\hat{H}_k(v)v^n], \quad (58)\]
\[\hat{H}_k(v) := \frac{\left[1 + 2if_x(ka)\right] \hat{\Psi}_0(k) + \hat{\Psi}_1(k)}{v^2 + 2f_x(ka)v - 1}. \]
This solution depends on the roots of the equation
\[v^2 + 2if_x(ka)v - 1 = 0, \quad v_{\pm} = -if_x(ka) \pm \sqrt{1 - f_x^2(ka)}. \]
When the roots are distinct \(v_+ \neq v_-\), we have simple poles in (58) and the solution has the following form
\[\hat{\Psi}_n(k) = \frac{1}{2\sqrt{1 - f_x^2(ka)}} \sum_{s = \pm} s \left[(v_s + 2if_x(ka))\hat{\Psi}_0(k) + \hat{\Psi}_1(k)\right] v_n^{s}. \quad (60)\]
The roots are equal \(v_+ := v_- := v_0\), when \(f_x(ka) = \pm 1\) and then \(v_0 = \mp i\). Thus, we have a double pole in \(58\) and the solution takes the form
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\[ \hat{\Psi}_n(k) = \left[ (n-1)\hat{\Psi}_0(k) \mp in\hat{\Psi}_1(k) \right] e^{\mp i(n-2)\pi} \tag{61} \]

The stability analysis can be done with the help of the explicit solutions. To simplify, let us assume that the limit \( a, \tau \to 0 \) is taken with \( \epsilon \) kept fixed [26]. When there are two different roots, the solution (60) is bounded when

\[ |v_\pm(ka)| \leq 1, \tag{62} \]

and this determines the stability. If \( 4|\epsilon| > 1 \), then there exists values of \( ka \) for which \( |v_\pm(ka)| > 1 \) and becomes unstable. It is when \( 4|\epsilon| \leq 1 \) that we can guarantee condition (62) \( \forall ka \), since then \( |v_+(ka)| = |v_-(ka)| = 1 \).

When there is a single root, the solution (61) is not bounded due to the linear growth with \( n \). This instability occurs at \( 4|\epsilon| \sin^2 \frac{ka}{2} = 1 \). Since from the previous case we already know that \( 4|\epsilon| \) can be at most 1, removing this possibility we avoid the case of solution (61). Therefore, the condition for numerical stability is \( 4|\epsilon| < 1 \). In this case, the solution (60) can be further simplified as

\[ \hat{\Psi}_n(k) = \frac{1}{2\cos \theta_\epsilon(ka)} \sum_{s=\pm} \left[ e^{is\theta_\epsilon(ka)} \hat{\Psi}_0(k) + s\hat{\Psi}_1(k) \right] s^n e^{i(1-s)n\theta_\epsilon(ka)}, \tag{63} \]

where we have introduced the following parametrization

\[ f_\epsilon(ka) := \sin \theta_\epsilon(ka), ~ 4|\epsilon| < 1. \tag{64} \]

Let us point out that the stability analysis carried out here can be repeated for the exactly reversible Schrödinger equation in terms of real and imaginary parts [26], [27]. In this case we would need to introduce a couple of generating functions, one for each component.

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5. At first sight this splitting of registers looks awkward but otherwise, we run into problems since the direct function evaluation is doom to failure. Imagine we implement the function evaluation as

\[ U_f |x_1, x_2, \ldots, x_m \rangle = |f(x_1, x_2, \ldots, x_m)\rangle, \tag{65} \]

and \( f \) is not a one-to-one application: there exists \( (x_1, \ldots, x_m) \neq (y_1, \ldots, y_m) \) such that \( f(x_1, \ldots, x_m) = f(y_1, \ldots, y_m) \). Choose the states as orthonormal
\[(x_1, \ldots, x_m)\langle (y_1, \ldots, y_m) = 0.\] Then, the implementation (65) implies that the transformed states are not orthogonal:
\[\langle f(x_1, \ldots, x_m)\rangle\langle f(y_1, \ldots, y_m) = 1.\] This violates unitarity. In fact, we know that an orthonormal basis of states is transformed onto another orthonormal basis of states under a unitary transformation. Whence the necessity for splitting registers (8), (9).

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8. The Principles of Quantum Mechanics admit an interpretation in the light of Quantum Information Theory as follows:

- **PI States:** To each physical system there corresponds a complex and separable Hilbert space \( \mathcal{H} \) of states. A pure state at instant \( t \) is represented by a unitary ray \( |\Psi(t)\rangle_R \in \mathcal{H} \). A mixed state is represented by a density matrix \( \rho \): \( \rho^\dagger = \rho, \text{Tr} \rho = 1, \rho \geq 0 \).

  In QIT this corresponds to encoding information in a quantum way in those states. The superposition principle encoded in the Hilbert space structure implies the quantum parallelism for the information stored. When the Hilbert space \( \mathcal{H} \) is constructed by tensor product of single-particle states, there appears entanglement that allows for non-classical capabilities of information processing and communication.

- **PII Observables:** Each observable of a physical system is represented by a linear self-adjoint operator \( A \) acting on the Hilbert space of states \( \mathcal{H} \):

  \[\langle \varphi|A|\psi\rangle = \langle A^\dagger \varphi|\psi\rangle, \quad \forall \varphi \in D(A), \forall \varphi \in D(A^\dagger).\] (66)

  In QIT this corresponds to the particular physical realization of a computational basis associated to the spectral decomposition of the operator \( A \). For instance, it may be the third component of the spin of a spin-\( \frac{1}{2} \) particle.

- **PIII Measurements:** If a physical system is in a pure state \( |\psi\rangle \in \mathcal{H} \), normalized, then the probability of obtaining a value \( a \) when measuring a certain observable \( A \) is

  \[P_\psi(a) = \left| \langle \psi|E_a|\psi\rangle \right|^2,\] (67)

  where \( \{E_a\} \) is an orthonormal set of projectors \( E_a^\dagger = E_a : E_a E_b = \delta_{ab} E_a, \sum_a E_a = I \), associated to the spectral decomposition of \( A : A(a) = a|a\rangle \), \( E_a = |a\rangle\langle a| \). Generalized measurements are described with POVMs.

  In QIT this corresponds to the probabilistic nature for the result of a quantum calculation. It implies that good quantum programming amounts to maximizing that probability above a finite threshold. This is summarized as the need for constructive interference of final amplitudes towards the desired output amplitude.

- **PIV Collapse:** If a given physical system is in a state \( \rho \), the result state of an ideal measurement of an observable \( A \), with respect to a set of values in a set \( \Delta \), is described by the following density matrix

  \[\rho \rightarrow \rho_{A,\Delta} = \frac{1}{\text{Tr}[\rho E_A(\Delta)]} \sum_{a \in \Delta} E_a \rho E_a\] (68)
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In QIT this corresponds to the final state of the QC after the computation has finished.

- **PV Schrödinger Equation**: Between two consecutive measurements, the pure states of a physical system remain pure, and there exists in each unit ray \(|\Psi(t)\rangle\) some representative state vector \(|\Psi(t)\rangle\) such that the time evolution is given by the Schrödinger Equation

\[
i\hbar \frac{d}{dt} |\Psi(t)\rangle = H(t)|\Psi(t)\rangle.
\] (69)

In QIT this corresponds to quantum logic gates represented as unitary evolution operators and the reversibility of quantum computation. The conditional logic needed to process information is achieved by acting on Hilbert spaces with at least two-particle states. This conditional logic is realized in the Hamiltonian \(H(t)\) of the system, as the physical interaction between two parts or particles in the Hilbert space of states.

- **PVI Quantization Rules**: In a physical system with cartesian coordinates of position \(q_1, q_2, ..., q_N\) and conjugate momenta \(p_1, p_2, ..., p_N\), then the corresponding operators \(X_r, P_r\) that represent those observables must fulfill the commutation rules in the Weyl form

\[
U_\alpha V_\beta = e^{-i\frac{\alpha \cdot \beta}{\hbar}} V_\beta U_\alpha \quad \forall \alpha, \beta \in R
\] (70)

\[
U_\alpha := e^{-i\frac{\alpha \cdot X}{\hbar}} \quad V_\beta := e^{-i\frac{\beta \cdot P}{\hbar}}
\]

If the system has an observable whose classical expression is \(A(q_r, p_r, t)\), then the corresponding operator is obtained from this expression, written in a convenient form, upon substitution of the variables \(q_r, p_s\) by \(X_r, P_s\).

In QIT this corresponds to the transition from a classical computation to a quantum computation. A physical system can be used to compute classically or quantumly depending on its physical description. This is the meaning of information is physical.

9. Irreversibility implies heat dissipation according to the second law of thermodynamics: information cannot be lost and every erased or lost bit of information is shed as a tiny puff of heat. This shedding of information is happening permanently at each step of the fast and long chains of computations. Intermediate results in these calculations are discarded since they are apparently useless and the computer needs to reset the memory registers. This erasure produces heat that must be removed from the machine to prevent from malfunctioning. The nature of this heating is fundamental, intrinsic to information erasure.

There are other sources of heating in a computer like the dragging of electrons in the currents inside the wires due to resistance. In actual computers this heat dissipation due to resistance is larger by far than the heating due to information erasure. There is still a lot of room for reducing resistance heating, for instance, introducing superconducting electron currents. When this would be achieved, then we face the heating due to dumping information. Landauer first quantified \[10\] in energy this loss per bit as

\[
\Delta E = k_B T \ln 2.
\] (71)

This is an irreducible amount of heat that must unavoidably be shed when a computer clears its registers by erasing a bit of information. The less information systems erase, the less power they use. Bennett found \[11\] a way to
overcome this heating introducing the concept of a reversible computer that is universal as a Turing machine. Lecerf had introduced \[12\] this idea of a reversible Turing machine earlier in the sixties. In the Bennett machine, information is never throw out, thus causing no heat. The problem then becomes one of a machine with an infinitely large memory. To continue working, the computer needs somehow to be reset and here is where reversibility comes in: rewind the machine till the initial state without erasing any single bit. These computers operate with reversible algorithms that do not require data to be erased. Bennett designed a memory-saving method in which a computer would carry out a few steps of the calculation, copy the result and rewind. This is at the expense of processing time.

There has been recent interest in reversible classical computers for reducing a system’s heat level while allowing chip performance to scale. The first reversible computer is a chip called Flattop \[13\] developed at the MIT’s Reversible Computing research group. It is based on the reversible and adiabatic transfer of charge in digital circuits implemented in standard silicon. Flattop implements the Billiard Ball Cellular Automaton \[14\], a universal and reversible model of computation introduced by Fredkin. It is not a practical architecture for performing arbitrary computations, but it is regarded as a proof-of-concept reversible machine showing that universal reversible computers may be accessible in the near future.

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