Single-qubit gates designed by means of the Madelung picture

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Abstract. In this work the Madelung picture is applied to the single qubit systems. The projective aspect of the Madelung quantities and the polar expression of the components of the quantum state allow one to obtain a general dynamical system of equations. Even though this dynamical system of equations is nonlinear, it offers the advantage of designing single quibt gates in a straightforward manner. It only requires the specification of the initial and final points on the Bloch sphere, as well as the gate operation time. This application of the Madelung picture is particularily illustrated for the nuclear magnetic resonance processor case. It turns the problem of specifying the magnetic fields into a simpler problem of substitution.

Keywords: Madelung picture, qubit, Bloch sphere.

1. Introduction

In the current context of the second quantum revolution [1], qubits (two level systems) have acquired a notable importance in both the theoretical and experimental field of quantum computing [2]. Studying the qubit is equivalent to analysing the information storage and information treatment in a quantum way [3]. For this reason, the qubit lies at the core of quantum information. This means that the first step to approach quantum information is first studying the qubit.

Since the introduction of the Madelung picture [4] in 1927, there was a development of the quantum theory in terms of a hydrodynamical framework, notably with the works of Bohm [5, 6] in 1952. From that point in time, there has been progress on this hydrodynamical framework to a great variety of quantum systems particularily in the numerical simulations field [7]. It is also worth noticing the application of the Madelung famework within the quantum engineering as a tool for designing semiconductor devices [8, 9, 10, 11] and even as an alternative way of conceiving quantum engineering systems [12]. Regarding the treatment for qubit systems within the Madelung picture, it is worth mentioning the studies about qubits [13, 14, 15, 16, 17] and the analysis of entangled qubits [18, 19, 20, 21, 22]. An important feature of these treatments of the qubits yields on an exhaustive analysis of the trajectories of the qubit in the configuration space.

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Now, the Madelung picture relies mainly on the trajectory concept, and this concept has been proved to introduce misinterpretations on experiments [23, 24]. For this reason, recently the Madelung picture was revisited and reformulated without introducing additional postulates [25, 26]. It is based on a nonlinear projection of the observables effect over a quantum state. In this way, the Madelung framework is generalized to any basis without having the need to rely on the trajectory concept. The promising advantage of this projective formulation of the Madelung picture is the absence of trajectories as a central element. Instead, the keypoint is the handling of observables through a ratio involving a projection into a given representation. Bearing in mind all the previous information, in this work it is explored how to apply the recent Madelung picture to the single qubit system. In particular, the dynamical equations are obtained regardless of the time-dependency of the magnetic fields. Also, a way to use Madelung picture on the design of single qubit gates is discussed.

The present work is organized as follows: In Section 2 a brief and concise presentation of the Madelung picture is given. Next, in Section 3, the Madelung picture is applied to the two-level system, specifically for the spin 1/2. In particular, in Subsection 3.1, a spin 1/2 under the action of a general magnetic field is considered. Madelung quantities are calculated for the spin components and the Hamiltonian as well. Later, in Subsection 3.2, by combining all the Madelung quantities and regrouping in real and imaginary parts, the dynamical system of equations, for the angles on the Bloch sphere, is obtained. Then, in Subsection 4, a way to use the Madelung picture to implement single qubit gates is discussed. Finally, in Section 5, conclusions are drawn.

2. Madelung picture

The importance of the Madelung picture [3] is apparent when dealing with time-dependent systems such as the linear [27] and quadratic potentials. Its importance also derives from on linking different branches of quantum mechanics, like the Wigner formalism and the trajectory based approach [25].

The Madelung picture consist of treating the observables through the ratio between their effect, projected in a given basis, and the projected quantum state. Particularily, for a system described by the quantum pure state $|\psi(t)\rangle$, the Madelung quantity A of an observable $\widehat{\mathrm{A}}$ in a given representation $\{|q\rangle\}$, is given by,

$$\mathrm{A}(q,t) \doteq \frac{\langle q|\widehat{\mathrm{A}}|\psi(t)\rangle}{\langle q|\psi(t)\rangle}, \tag{1}$$

where the projected state is expressed in the polar form $\langle q|\psi(t)\rangle = \sqrt{\rho(q,t)}\exp\big(\mathrm{i}S(q,t)/\hbar\big)$. Bear in mind that ρ denotes the probability density, while S is related to the phase of the wave function.

Note that the Madelung quantity $\mathrm{A}(q,t)$ is, in general, a complex function of two variables: the time t due to the time-dependence of the quantum state $|\psi(t)\rangle$, while the variable q arises from the chosen representation, in this case $\{|q\rangle\}$. For further details on the computation of the Madelung quantities in different representations, please refer to [25].

Now, let us consider a non relativistic system of mass m with an associated Hamiltonian $\widehat{\mathrm{H}}$,

$$\widehat{\mathrm{H}} = \frac{1}{2m}\widehat{\mathrm{P}}^2 + U(\widehat{\mathrm{X}}), \tag{2}$$

where $\widehat{\mathrm{X}}$, $\widehat{\mathrm{P}}$ are the position and momentum operators respectively. Besides, U denotes de potential energy function.

Regardless of the considered representation, the effect of the Hamiltonian is determined by the Schrödinger equation $\widehat{\mathrm{H}}|\psi(t)\rangle = \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle$. Bearing in mind Eq. (1), the Madelung quantity for the Hamiltonian (2) takes the following form,

$$\mathrm{H}(q,t) = f(\mathrm{X},\mathrm{P};q,t), \tag{3}$$

with f a function involving the individual Madelung quantities X, P. It is worth noticing that the form of function f depends on the structure of the potential energy. As it is extensively shown in [25], the real and imaginary parts of Eq. (3) are respectively the dynamical equations of the function $S(q,t)$ and the probability density $\rho(q,t)$. The former corresponds to a modified Hamilton–Jacobi equation and the latter, to a continuity equation.
It is important to point out that the equations resulting from the Madelung picture has facilitated the obtention of dynamical invariants among other applications, see [27].
So far, the madelung picture has been applied to continuous representations, for example position and momentum. The application of the Madelung picture to discrete representations needs to be addressed, in particular, the simplest case, the qubit (two-level system).

3. Madelung treatment for the qubit

3.1. Madelung quantities for the qubit

The application of the Madelung picture, on one hand, needs the knowledge of the effect of the observables and, on the other hand, it requires to express the quantum state in a polar form.
Let us consider a spin 1/2 system whose states are given by $\{|0\rangle, |1\rangle\}$. In this case, the system is finite dimensional and the requirement of expressing the quantum state in polar form means that for every energy level a polar form must be introduced. This is straightforward if we bear in mind that, in this case, the quantum state $|\psi(t)\rangle$ is expressed by means of the two parameters $\theta \in \{0,\pi\}$ and $\phi \in \{0,2\pi\}$ in the following way,

$$|\psi(t)\rangle = \cos\frac{\theta}{2}|0\rangle + e^{\mathrm{i}\phi}\sin\frac{\theta}{2}|1\rangle. \tag{4}$$

This already fulfills the requirement of rewritting the state in polar form. Now, let us remember the effect of the observables, in particular the spin components $\widehat{\mathrm{S}}_x$, $\widehat{\mathrm{S}}_y$, $\widehat{\mathrm{S}}_z$:

$$\widehat{\mathrm{S}}_x|0\rangle = \frac{\hbar}{2}|1\rangle, \quad \widehat{\mathrm{S}}_y|0\rangle = \mathrm{i}\frac{\hbar}{2}|1\rangle, \quad \widehat{\mathrm{S}}_z|0\rangle = \frac{\hbar}{2}|0\rangle, \tag{5}$$

$$\widehat{\mathrm{S}}_x|1\rangle = \frac{\hbar}{2}|0\rangle, \quad \widehat{\mathrm{S}}_y|1\rangle = -\mathrm{i}\frac{\hbar}{2}|0\rangle, \quad \widehat{\mathrm{S}}_z|1\rangle = -\frac{\hbar}{2}|1\rangle. \tag{6}$$

This clearly implies that the effect of those observables over the quantum state, in the polar form (4), is given by,

$$\widehat{\mathrm{S}}_x|\psi(t)\rangle = \frac{\hbar}{2}\Big(\sin\frac{\theta}{2}e^{\mathrm{i}\phi}|0\rangle + \cos\frac{\theta}{2}|1\rangle\Big) \tag{7}$$

$$\widehat{\mathrm{S}}_y|\psi(t)\rangle = \frac{\hbar}{2}\Big(-\mathrm{i}\sin\frac{\theta}{2}e^{\mathrm{i}\phi}|0\rangle + \mathrm{i}\cos\frac{\theta}{2}|1\rangle\Big) \tag{8}$$

$$\widehat{\mathrm{S}}_z|\psi(t)\rangle = \frac{\hbar}{2}\Big(\cos\frac{\theta}{2}|0\rangle - \sin\frac{\theta}{2}e^{\mathrm{i}\phi}|1\rangle\Big). \tag{9}$$

Bear in mind that the Madelung quantity associated to the operator $\widehat{\mathrm{A}}$ is given by $\mathrm{A} = \langle x|\widehat{\mathrm{A}}|\psi\rangle/\langle x|\psi\rangle$. For the case of spin, since there are only two levels, that means that we have two different effects for every spin component. Explicitly,

$$\mathrm{S}_x(s,t) = \frac{\langle s|\widehat{\mathrm{S}}_x|\psi(t)\rangle}{\langle s|\psi(t)\rangle}, \quad \mathrm{S}_y(s,t) = \frac{\langle s|\widehat{\mathrm{S}}_y|\psi(t)\rangle}{\langle s|\psi(t)\rangle}, \quad \mathrm{S}_z(s,t) = \frac{\langle s|\widehat{\mathrm{S}}_z|\psi(t)\rangle}{\langle s|\psi(t)\rangle}, \tag{10}$$

where $s \in \{0, 1\}$. The Madelung quantities associated to those observables are therefore,

$$\mathrm{S}_x(0,t) = \frac{\hbar}{2}\tan\frac{\theta}{2}e^{\mathrm{i}\phi}, \quad \mathrm{S}_y(0,t) = -\mathrm{i}\frac{\hbar}{2}\tan\frac{\theta}{2}e^{\mathrm{i}\phi}, \quad \mathrm{S}_z(0,t) = +\frac{\hbar}{2}, \tag{11}$$

$$\mathrm{S}_x(1,t) = \frac{\hbar}{2}\cot\frac{\theta}{2}e^{-\mathrm{i}\phi}, \quad \mathrm{S}_y(1,t) = \mathrm{i}\frac{\hbar}{2}\cot\frac{\theta}{2}e^{-\mathrm{i}\phi}, \quad \mathrm{S}_z(1,t) = -\frac{\hbar}{2}. \tag{12}$$

Next, we need to write down the effect of the Hamiltonian $\widehat{\mathrm{H}}$, taking into account the Schrödinger equation,

$$\widehat{\mathrm{H}}|\psi(t)\rangle = \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle. \tag{13}$$

If we take into account the polar form of the quantum state (4), then it yields,

$$\widehat{\mathrm{H}}|\psi(t)\rangle = -\mathrm{i}\frac{\hbar}{2}\frac{\mathrm{d}\theta}{\mathrm{d}t}\sin\frac{\theta}{2}|0\rangle + \Big(-\hbar\frac{\mathrm{d}\phi}{\mathrm{d}t}\sin\frac{\theta}{2} + \mathrm{i}\frac{\hbar}{2}\frac{\mathrm{d}\theta}{\mathrm{d}t}\cos\frac{\theta}{2}\Big)e^{\mathrm{i}\phi}|1\rangle. \tag{14}$$

This means that the Madelung quantity associated to the Hamiltonian is

$$\mathrm{H}(0,t) = -\mathrm{i}\frac{\hbar}{2}\frac{\mathrm{d}\theta}{\mathrm{d}t}\tan\frac{\theta}{2}, \quad \mathrm{H}(1,t) = -\hbar\frac{\mathrm{d}\phi}{\mathrm{d}t} + \mathrm{i}\frac{\hbar}{2}\frac{\mathrm{d}\theta}{\mathrm{d}t}\cot\frac{\theta}{2}. \tag{15}$$

3.2. Dynamical equations

Let us consider a spin 1/2 system under the action of a general magnetic field $\vec{\mathrm{B}} = (\mathrm{B}_x, \mathrm{B}_y, \mathrm{B}_z)$. The corresponding Hamiltonian is

$$\widehat{\mathrm{H}} = \gamma\mathrm{B}_x\widehat{\mathrm{S}}_x + \gamma\mathrm{B}_y\widehat{\mathrm{S}}_y + \gamma\mathrm{B}_z\widehat{\mathrm{S}}_z, \tag{16}$$

where γ denotes the gyromagnetic ratio of the system. The associated Madelung quantities satisfy the following system of equations,

$$\mathrm{H}(0,t) = \gamma\mathrm{B}_x\mathrm{S}_x(0,t) + \gamma\mathrm{B}_y\mathrm{S}_y(0,t) + \gamma\mathrm{B}_z\mathrm{S}_z(0,t) \tag{17}$$

$$\mathrm{H}(1,t) = \gamma\mathrm{B}_x\mathrm{S}_x(1,t) + \gamma\mathrm{B}_y\mathrm{S}_y(1,t) + \gamma\mathrm{B}_z\mathrm{S}_z(1,t). \tag{18}$$

Once we define $\omega_x \doteq \gamma\mathrm{B}_x$, $\omega_y \doteq \gamma\mathrm{B}_y$, $\omega_z \doteq \gamma\mathrm{B}_z$, the system of equations can be rewritten as follows,

$$\mathrm{H}(0,t) = \omega_x\mathrm{S}_x(0,t) + \omega_y\mathrm{S}_y(0,t) + \omega_z\mathrm{S}_z(0,t) \tag{19}$$

$$\mathrm{H}(1,t) = \omega_x\mathrm{S}_x(1,t) + \omega_y\mathrm{S}_y(1,t) + \omega_z\mathrm{S}_z(1,t), \tag{20}$$

after substitution of the corresponding quantities (11)-(12) and factorizing $\hbar/2$,

$$-\mathrm{i}\frac{\mathrm{d}\theta}{\mathrm{d}t}\tan\frac{\theta}{2} = \omega_x\tan\frac{\theta}{2}e^{\mathrm{i}\phi} - \omega_y\mathrm{i}\tan\frac{\theta}{2}e^{\mathrm{i}\phi} + \omega_z \tag{21}$$

$$-2\frac{\mathrm{d}\phi}{\mathrm{d}t} + \mathrm{i}\frac{\mathrm{d}\theta}{\mathrm{d}t}\cot\frac{\theta}{2} = \omega_x\cot\frac{\theta}{2}e^{-\mathrm{i}\phi} + \omega_y\mathrm{i}\cot\frac{\theta}{2}e^{-\mathrm{i}\phi} - \omega_z. \tag{22}$$

Let us express this system of equations in real and imaginary part,

$$-\mathrm{i}\frac{\mathrm{d}\theta}{\mathrm{d}t}\tan\frac{\theta}{2} = \Big(\omega_x \tan\frac{\theta}{2}\cos\phi + \omega_y\tan\frac{\theta}{2}\sin\phi + \omega_z\Big) + \mathrm{i}\Big(\omega_x\tan\frac{\theta}{2}\sin\phi - \omega_y\tan\frac{\theta}{2}\cos\phi\Big) \tag{23}$$

$$-2\frac{\mathrm{d}\phi}{\mathrm{d}t} + \mathrm{i}\frac{\mathrm{d}\theta}{\mathrm{d}t}\cot\frac{\theta}{2} = \Big(\omega_x\cot\frac{\theta}{2}\cos\phi + \omega_y\cot\frac{\theta}{2}\sin\phi - \omega_z\Big) + \mathrm{i}\Big(- \omega_x\cot\frac{\theta}{2}\sin\phi + \omega_y\cot\frac{\theta}{2}\cos\phi\Big). \tag{24}$$

This is then equivalent to the following system of four equations

$$\begin{aligned}
0 &= \omega_x\tan\frac{\theta}{2}\cos\phi + \omega_y\tan\frac{\theta}{2}\sin\phi + \omega_z && (25)\\
0 &= \Big(\omega_x\sin\phi - \omega_y\cos\phi + \frac{\mathrm{d}\theta}{\mathrm{d}t}\Big)\tan\frac{\theta}{2} && (26)\\
0 &= \omega_x\cot\frac{\theta}{2}\cos\phi + \omega_y\cot\frac{\theta}{2}\sin\phi - \omega_z + 2\frac{\mathrm{d}\phi}{\mathrm{d}t} && (27)\\
0 &= \Big(- \omega_x\sin\phi + \omega_y\cos\phi - \frac{\mathrm{d}\theta}{\mathrm{d}t}\Big)\cot\frac{\theta}{2}. && (28)
\end{aligned}$$

Since Eqs. (26) and (28) hold for all $\theta \in [0\,,\,\pi]$, then necessarily it yields,

$$\begin{aligned}
0 &= \tan\frac{\theta}{2}\Big(\omega_x\cos\phi + \omega_y\sin\phi\Big) + \omega_z && (29)\\
-\frac{\mathrm{d}\theta}{\mathrm{d}t} &= \omega_x\sin\phi - \omega_y\cos\phi && (30)\\
-2\frac{\mathrm{d}\phi}{\mathrm{d}t} &= \cot\frac{\theta}{2}\Big(\omega_x\cos\phi + \omega_y\sin\phi\Big) - \omega_z && (31)\\
\frac{\mathrm{d}\theta}{\mathrm{d}t} &= -\omega_x\sin\phi + \omega_y\cos\phi. && (32)
\end{aligned}$$

Since Eqs. (30) and (32) are the same, we only need to write down the following system of differential equations,

$$\begin{aligned}
\omega_x\cos\phi + \omega_y\sin\phi &= -\omega_z\cot\frac{\theta}{2} && (33)\\
-2\frac{\mathrm{d}\phi}{\mathrm{d}t} &= \cot\frac{\theta}{2}\Big(\omega_x\cos\phi + \omega_y\sin\phi\Big) - \omega_z && (34)\\
-\frac{\mathrm{d}\theta}{\mathrm{d}t} &= \omega_x\sin\phi - \omega_y\cos\phi. && (35)
\end{aligned}$$

After combining Eqs. (33) and (34), it yields,

$$\begin{aligned}
2\frac{\mathrm{d}\phi}{\mathrm{d}t} &= \frac{\omega_z(t)}{\sin^2\frac{\theta(t)}{2}} && (36)\\
-\frac{\mathrm{d}\theta}{\mathrm{d}t} &= \omega_x(t)\sin\phi(t) - \omega_y(t)\cos\phi(t). && (37)
\end{aligned}$$

We have now a system of nonlinear differential equations with *a priori* time-dependent coefficients. It would seem that we loose already the linear treatment provided by the conventional treatment of Schrödinger picture; and therefore we do not gain any new insight on the dynamics of the single qubit, using the Madelung picture. Nevertheless, if we use these equations of motion as a way of designing specific single qubit gates, then we gain a lot of advantages with those equations, as it will be shown in the next Section.

4. Design of single qubit gates

Let us consider the following problem: we have an nuclear magnetic resonance (NMR) quantum processor [28, 29] and we need to design a single qubit gate $\widehat{\mathrm{U}}$ that performs the transformation on the Bloch sphere, as shown in Figure 1.

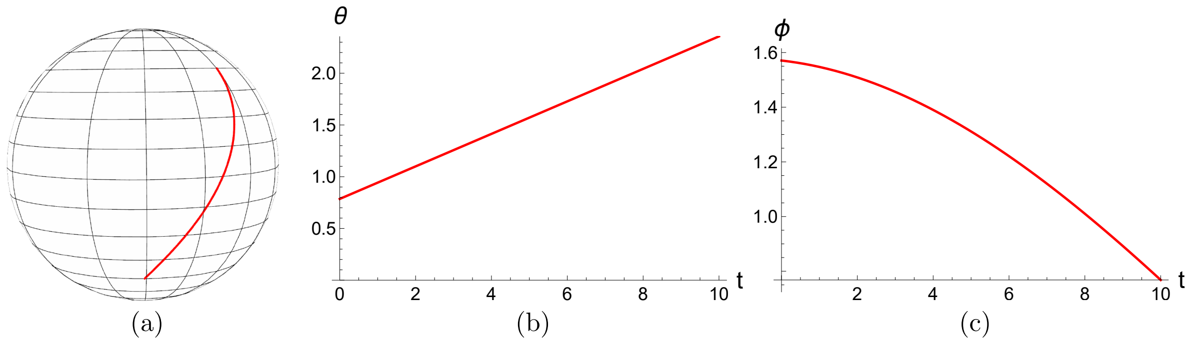

Figure 1. (a) Trajectory of the qubit under the action of the gate $\widehat{\mathrm{U}}$ (b) Behavior of the angle θ over time (c) Behavior of the angle ϕ over time.

Namely,

$$(\theta_0 = \pi/4, \phi_0 = \pi/2) \longmapsto (\theta_f = 3\pi/4, \phi_f = 0)$$

within a time interval $T = 10$ $[a.u.]$.

For that, we need to specify the time-dependency of the magnetic fields. Usually, an NMR processor has two coils producing magnetic fields in orthogonal directions. For this reason, we will set $\omega_y = 0$. Therefore, the dynamics of the qubit are ruled by,

$$2\frac{\mathrm{d}\phi}{\mathrm{d}t} = \frac{\omega_z}{\sin^2\frac{\theta}{2}} \quad \text{and} \quad -\frac{\mathrm{d}\theta}{\mathrm{d}t} = \omega_x \sin\phi \tag{38}$$

In order to perform the above-mentioned single qubit gate, the angles on the Bloch sphere must be

$$\theta(t) = \frac{\pi}{20}t + \frac{\pi}{4} \quad \text{and} \quad \phi(t) = \frac{\pi}{2}\cos(0.1t)\exp(-0.01t).$$

With this information, the task is to find the time-dependency of the coils in order to assure such behavior. In the Madelung picture this is straightforward. Indeed, the desired behavior is substituted in Eq. (38) and the required coils must satisfy,

$$\mathrm{B_z}(t) = 2\left(\sin\left(\frac{\pi}{40}t + \frac{\pi}{8}\right)\right)^2\left(-0.1\frac{\pi}{2}\sin(0.1t)\exp(-0.01t) - 0.01\frac{\pi}{2}\cos(0.1t)\exp(-0.01t)\right) \tag{39}$$

$$\mathrm{B_x}(t) = -\frac{\pi/20}{\sin\left(\frac{\pi}{2}\cos(0.1t)\exp(-0.01t)\right)} \tag{40}$$

where $\omega_x = \gamma \mathrm{B_x}$, $\omega_y = \gamma \mathrm{B_y}$ and γ was set to the unity for illustrative purposes. The time dependency of the magnetic field are depicted in Figure 2 during the gate operation time $T = 10$.

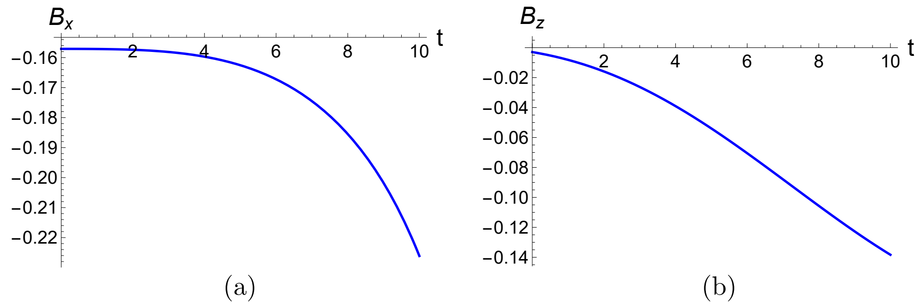

Figure 2. (a) Time dependency of the magnetic field for the gate $\widehat{\mathrm{U}}$ in x direction (b) Time dependency of the magnetic field in z direction.

This methodology can be followed to design any single qubit gate once the initial and final points, as well as the gate operation time, are specified. For instance, a Hadamard gate described by the trajectory depicted in Figure 3, can be implemented by the magnetic fields from Figure 4 by means of equation (38).

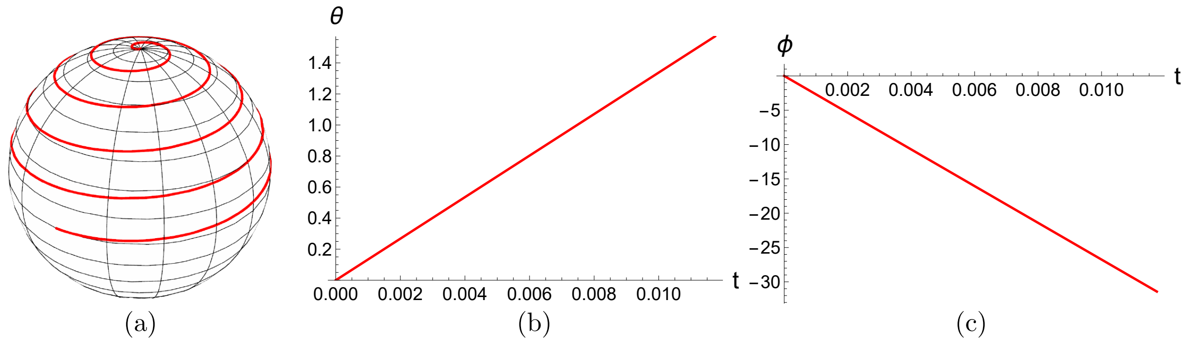

Figure 3. (a) Trajectory of the qubit under the action of the Hadamard gate (b) Behavior of the angle θ over time (c) Behavior of the angle ϕ over time.

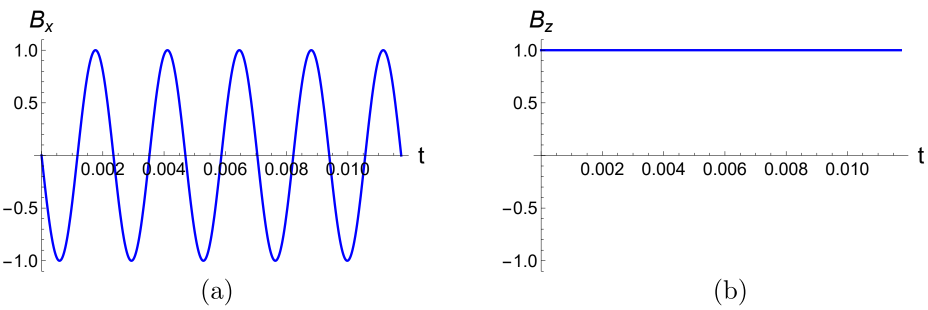

Figure 4. (a) Time dependency of the magnetic field for the Hadamard gate in x direction (b) Time dependency of the magnetic field in z direction.

It is worth noticing that the resulting magnetic fields correspond to the usual fields employed in this quantum gate. Namely, a constant field in z-direction and a cosine pulse in x-direction with a phase shift of $\pi/2$ [28], compare with [30]. In the same way, for the quantum gate X described by the trajectories in Figure 5, the magnetic fields are obtained by applying (38); these fields are shown in Figure 6.

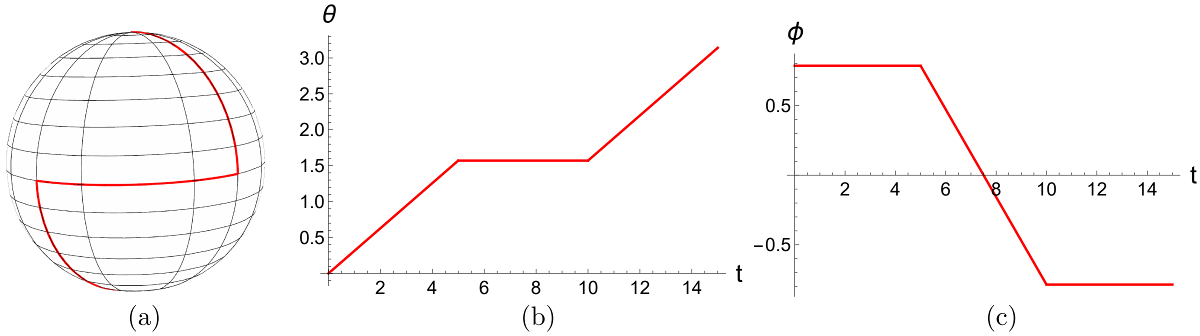

Figure 5. (a) Trajectory of the qubit under the action of the X gate (b) Behavior of the angle θ over time (c) Behavior of the angle ϕ over time.

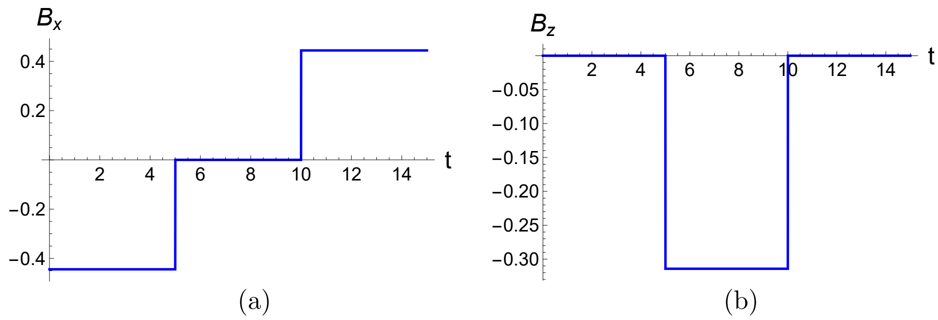

Figure 6. (a) Time dependency of the magnetic field for the X gate in x direction (b) Time dependency of the magnetic field in z direction.

5. Conclusion

In the second quantum revolution, quantum computing and quantum communications play an important role. Therefore, the treatment of the information carried by a qubit is crucial. This is manipulated by applying a succesive series of quantum gates. This means that the design of specific quantum gates is relevant. In this paper, it was shown how this task becomes straightforward when using the Madelung picture.

For this purpose, in Section 2, a brief and concise reminder of the Madelung picture was given, especially the projective definition of the Madelung quantities (1). In Section 3 the single qubit was addressed within the Madelung picture. Specifically, in Subsection 3.1, the Madelung quantities associated to the spin components were determined. For a quantum pure state in polar form (4), the spin components have the Madelung quantities given by Eqs. (11)-(12), as well as the Hamiltonian (15). Iin Subsection 3.2, by decoupling the real and imaginary parts of the Madelung quantity of the Hamiltonian, we obtained the dynamical system of equations associated to the single qubit system, see Eqs. (36) and (37). Finally, with these equations, in

Subsection 4, we found the required magnetic field functions providing a specific single qubit gate, *i.e.*, a specific trajectory on the Bloch sphere.

The advantage of our methodology is twofold: On one hand, it provides a simple way of substituting the desired trajectory on the Bloch sphere in order to determine the time-dependency of the magnetic field, and hence, to implement the corresponding single qubit gate. On the other hand, when dealing with a specific NMR processor the decoherence time of the qubit sets an upper limit for the duration of the quantum gate, this means that when specifying the trajectory on the Bloch sphere, the duration of the trajectory can be specified so that it will not take more time than the decoherence time. This is particularily important in the design of hardware for quantum computing and communications. As future work, the application of the Madelung picture for the design of multiple qubit gates can be studied.

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