Estimating the time evolution of NMR systems via quantum speed limit

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The solutions of the equation that governs the dynamics of a given system are pivotal to obtain all information about it. However, by using estimation theory it is possible to obtain under certain limitations some desired informations. The quantum speed limit (QSL) theory was originally used to estimate the shortest time in which a Hamiltonian drives an initial state to a final one for a given fidelity. Using the QSL theory in a slightly different way, we are able to estimate the running time of a given quantum process. For that purpose, we impose the saturation of a Mandelstam-Tamm-like bound in a rotating frame of reference where the state of the system travels slower than in the original frame (lab frame). Through this procedure it is possible to estimate the actual evolution time in the lab frame of reference with good accuracy when compared to previous methods. Our method was tested successfully to predict the time spent in the evolution of nuclear spins 1/2 and 3/2 in Nuclear Magnetic Resonance systems. We found that the estimated time according to our method is better than the approach using the usual QSL theory by until four orders of magnitude.

I. INTRODUCTION

We start by asking the following: Can we know the running time of a given quantum process without solving its dynamical equation? An affirmative answer to this question is particularly useful in the nonrelativistic (relativistic) scenario when is hard to solve the Schrödinger (Dirac) equation. In general, time dependent or many-body Hamiltonians reinforce the difficult to solve such equations. We discuss an explanation to the former question for the particular case in which the initial state of the system is pure and the evolution is unitary. Our approach is based on a variation of the quantum speed limit (QSL) time, i.e., the minimum time required for a system evolves from an initial state to a final one.

In the context of the energy-time uncertainty relations, in 1945 Mandelstam and Tamm (MT) [1] reported a QSL time \( t \geq \hbar \arccos \sqrt{F(t)/\Delta H} \) for a closed quantum system evolving between two distinct pure states \( |\psi(0)\rangle \) and \( |\psi(t)\rangle \), where \( t \) is the actual time of the evolution. Such expression is valid for a time-independent Hamiltonian \( \hat{H} \) with energy uncertainty given by \( \Delta H = \sqrt{\langle \psi(t)|\hat{H}^2|\psi(t)\rangle - \langle \psi(t)|\hat{H}|\psi(t)\rangle^2} \) and the fidelity between the initial and final states defined by

\[
F(t) = |\langle \psi(0)|\psi(t)\rangle|^2.
\]

Later in 1988, Margolus and Levitin [2] resorting to energy as a resource, developed an alternative expression for the QSL time \( t \geq \hbar/\left[4\left(\langle \hat{H} \rangle - E_0\right)\right] \), where the term in parenthesis in the denominator means the average energy above the energy of the reference state. Since these two remarkable works, an intense study on this subject emerged, including generalizations for unitary [3–14] and nonunitary [15–19] evolutions of quantum states.

According to those advances, we call the attention to the two remarkable works of Anandan and Aharonov [5], which proposed a geometrical approach to the QSL problem. Using the Fubini-Study metric in the projective Hilbert space, they found the shortest path between distinct pure states and also determined the speed of the state evolution through the energy uncertainty. The ratio between these two quantities gave origin to the following expression

\[
t \geq t_* = \frac{\hbar \arccos \sqrt{F(t)}}{\Delta H(t)},
\]

where the term \( \arccos \sqrt{F(t)} \) is the geodesic distance between the initial \( |\psi(0)\rangle \) and final \( |\psi(t)\rangle \) states. As the Hamiltonian can be time dependent now, we are able to define the average speed of the state evolution \( \Delta H(t) \equiv \frac{1}{t} \int_0^t \Delta H(\tau) \, d\tau \) [5]. Due to its beautiful geometrical interpretation [5, 7, 15, 19], as shown in Figure 1, the expression for the QSL time (2) will be used henceforth, and \( t_* \) will be called extended Mandelstam-Tamm (EMT) time. The utility of the QSL time has been shown in different scenarios, including quantum communication [20], quantum computation [21], quantum optimal control algorithms [22, 23], quantum thermodynamics [24], and quantum metrology [25]. As highlighted in Ref. [26], the original idea behind the QSL theory is to estimate the shortest time of a given quantum evolution. Conversely, here we apply the QSL theory to estimate the actual time for an initial pure quantum state in the laboratory.

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Let us consider that in the laboratory frame of reference a quantum system is described by the time-dependent Schrödinger equation \( i\hbar \dot{\psi}(t) = \hat{H}(t)\psi(t) \), where \( \hat{H}(t) \) and \( \psi(t) \) are the Hamiltonian and the quantum state of the system at time \( t \), respectively. Given an initial state \( \psi(0) \) and the system Hamiltonian, our main goal is to estimate the actual evolution time of the system to a final state with fidelity \( F(t) \). Notice that we do not know the final state of evolution \( \psi(t) \), just the value of the fidelity, which is given a priori. From Eq. (2) we observe that \( t = t_* \) only when the evolution of the state of the system occurs over the geodesic path. In such case, the quantum state progresses as slower as possible for a fixed time interval, which is equivalent to attain the smallest value for the average energy uncertainty \( \Delta H(t) \). Although the QSL time evaluated in different frames of reference can result different values, the actual evolution time remains the same in all references generated via unitary transformations from the original one. This can be seen through the application of a time-dependent unitary transformation \( R(t) \), such that the quantum state can be expressed as \( \psi(t) = R(t)|\psi_R(t)\rangle \), satisfying the initial condition \( |\psi(0)\rangle = |\psi_R(0)\rangle \). The quantum state \( |\psi_R(t)\rangle \) is represented in the new frame of reference at time \( t \), which evolves according to the time-dependent Schrödinger equation \( i\hbar \dot{\psi}_R(t) = \hat{H}_R(t)|\psi_R(t)\rangle \), where the Hamiltonian in the new frame is defined as \( \hat{H}_R(t) = R^\dagger(t)\hat{H}(t)R(t) - i\hbar R^\dagger(t)\dot{R}(t) \). We denote this new frame as rotating frame for some reasons that will be explained later. Particularly, to estimate the actual time \( t \), we will use the expression for the QSL time \( t_*^R \) in a specific rotating frame

\[
t \geq t_*^R = \frac{\hbar \arccos \sqrt{F_R(t)}}{\Delta H_R},
\]

where the average energy uncertainty \( \Delta H_R \) is chosen to be smaller than its counterpart in the lab frame \( \Delta H(t) \). Hence, we hope to find \( t_*^R \) closer to the actual time \( t \) when compared to the same prediction made in the lab frame, see Eq. (2). Choosing an appropriate unitary transformation \( R(t) \), the rotating Hamiltonian \( \hat{H}_R \) becomes time independent and consequently its average variance, \( \Delta H_R(t) = \Delta H_R \). The later imposition was made for the sake of simplicity and also because the average energy uncertainty becomes time independent, i.e., it does not depend on the actual time of the evolution. Naturally, the expression for the fidelity in the rotating frame also changes, \( F_R(t) = \langle \psi_R(0)|\psi_R(t)\rangle^2 = \langle \psi(0)|R^\dagger(t)|\psi(t)\rangle^2 \).

To summarize the idea behind our method, we rewrite Eq. (2) as

\[
t_* = \frac{\ell_{\text{geodes}}}{\pi},
\]
where $\ell_{\text{geodes}}$ is geodesic path length and $\overline{v}$ is the average speed of the quantum state evolution. On the other hand, the average speed can be written as

$$\overline{v} = \frac{\ell_{\text{real}}}{t},$$

with $\ell_{\text{real}}$ being the real path length and $t$ the actual evolution time. Therefore, the QSL time is expressed as

$$t_* = \frac{\ell_{\text{geodes}}}{\ell_{\text{real}}} t.$$

Once the actual time is the same in all frames of reference, we only have to maximize the ratio $\ell_{\text{geodes}}/\ell_{\text{real}}$ in order to obtain a good estimate of the actual evolution time. When we move to a frame of reference where the energy uncertainty is smaller than in the lab frame, the real path length is getting closer to the geodesic length. Indeed, this can be observed in the video in the Supplemental Material [27].

To implement our method, first we notice that even for time-independent Hamiltonians in the rotating frame, the utility of Eq. (3) remains limited, provided that it is necessary to know the quantum state to obtain the fidelity $F_R(t)$. In order to overcome this problem, we replace $F_R(t)$ by $\overline{F}_R(t^*_R)$ in Eq. (3), resulting in the following transcendental equation

$$\arccos \sqrt{\overline{F}_R(t^*_R)} = \frac{\Delta H_R t^*_R}{\hbar}. \quad (4)$$

The expression for the new fidelity is

$$\overline{F}_R(t^*_R) = |\langle \psi(0)| R^d(t^*_R)|\overline{\psi}(t^*_R)\rangle|^2, \quad (5)$$

with the quantum state at time $t^*_R$ being written as

$$|\overline{\psi}(t^*_R)\rangle = \sqrt{F}|\psi(0)\rangle + \sum_{j=1}^{n-1} a_j e^{i\varphi_j} |\psi^j_\perp\rangle. \quad (6)$$

The quantum states $|\psi^j_\perp\rangle$ are orthogonal to $|\psi(0)\rangle$, the time dependent coefficients $a_j, \varphi_j \in \mathbb{R}$ satisfy $\sum_{j=1}^{n-1} |a_j|^2 = 1 - F$, and $n$ is the dimension of the Hilbert space. The reason why we have written the evolved quantum state $|\psi(t)\rangle$ as in Eq. (6) is that it recovers the expression (1), i.e., $F = |\langle \psi(0)| \overline{\psi}(t^*_R)\rangle|^2$. Therefore, we can express $\overline{F}_R(t^*_R)$ as

$$\overline{F}_R(t^*_R) = \left| \sqrt{F} \langle \psi(0)| R^d(t^*_R)|\psi(0)\rangle + \sum_{j=1}^{n-1} a_j e^{i\varphi_j} \langle \psi(0)| R^d(t^*_R)|\psi^j_\perp\rangle \right|^2. \quad (7)$$

We can obtain the set of $n-1$ orthogonal states by using the Gram-Schmidt orthogonalization procedure over the initial state. Hence, given the initial quantum state, the fidelity $F$ and the Hamiltonian in the lab frame, and after we have chosen the time-dependent unitary transformation $R(t)$, we find numerically the root of Eq. (4) for the shortest time $t^*_R$. We observe that the transcendental equation depends on several variables $\{\varphi_1, \ldots, \varphi_{n-1}, a_1, \ldots, a_{n-1}\}$, beyond $t^*_R$. Our strategy to solve such equation is to sweep over the whole set of parameters to minimize $t^*_R$ as the first chronological root of the transcendental equation. We are looking for the first chronological root because different final states can have the same value of fidelity. This may occur mainly in periodical systems. It is also possible to obtain numerically the best unitary transformation that leads to the best time estimation, although this is not our goal here. This can be reached by numerically sweeping over all the parameters of the unitary transformation.

Nonetheless, to analyze how effective is the method proposed here, in the next section we show its application to estimate the necessary time for an initial state to evolve to a final state in systems constituted of spins $1/2$ and $3/2$ in NMR scenario. Our predictions are compared to experimental data for both evolutions.

### III. APPLICATIONS

**Spin 1/2 systems** — In order to put in practice our method, we implemented experimentally the dynamics of a spin $I=1/2$ NMR system composed by molecules of $o$-Phosphoric Acid, see Appendix C. Phosphorous nuclei ($^{31}$P) interacts with an external magnetic field according to the Hamiltonian,

$$\hat{H}(t) = \hbar \{ \omega_0 \hat{I}_z + \omega_1 \left[ \cos(\omega_p t) \hat{I}_x + \sin(\omega_p t) \hat{I}_y \right] \}, \quad (8)$$

where $\omega_0$ is the Larmor frequency and $\omega_1$ is proportional to the intensity of the magnetic field applied in the $x-y$ plane which rotates around the $z$ axis with frequency $\omega_p$, while $\hat{I}_z = \hat{\sigma}_z/2, i = x, y, z$, and $\hat{\sigma}_i$ are the Pauli spin matrices. We observe that the Hamiltonian (8) does not commute with itself for different times, which introduces some degree of difficulty to solve the Schrödinger equation, despite its simple form.

The unitary transformation that removes the time dependence from the Hamiltonian (8) is $R(t) = e^{-i \hat{\sigma}_z \omega_p t}$, which is a rotation around the $z$-axis, explaining why we called the new frame as rotating frame. The resulting Hamiltonian is $\hat{H}_R = \hbar \left( \hat{\Delta} \hat{I}_z + \omega_1 \hat{I}_x \right)$, with $\Delta = \omega_0 - \omega_p$. We considered as the initial state of the system a general pure state on the Bloch sphere $|\psi(0)\rangle = |\psi(\theta, \phi)\rangle = \cos(\theta/2)|0\rangle + e^{i\phi} \sin(\theta/2)|1\rangle$. It can be written as function of the polar $\theta$ and azimuthal $\phi$ angles and the eigenstates $\{|0\rangle, |1\rangle\}$ of the Pauli matrix $\hat{\sigma}_z$. In this case, the fidelity (7) depends only on the parameter $\varphi_1$ and the QSL time, as shown below.
The perpendicular state is easily obtained by \(|\psi^\perp_1\rangle = |\psi(\theta - \pi, \phi)\rangle\). According to the experimental setup (see Appendix C), the axial Larmor frequency is \(\omega_0 = \omega_p = 2\pi(161.975\text{MHz})\) and the Radio frequency in the perpendicular direction is \(\omega_1 = 2\pi(21.930\text{kHz})\), while the initial state is defined by the angles \(\theta = 24.48^\circ\) and \(\phi = 4.02^\circ\). Under these circumstances, in Fig. 2 we show at some discrete times the experimental fidelity of the system state in the lab frame (green asterisks). To obtain these values we performed quantum state tomography at each 0.5\(\mu\text{s}\) in the time interval \([0, 22\mu\text{s}]\) and used the Eq. (1) to obtain the fidelity at each time.

The system dynamics is well described by the unitary evolution governed by Hamiltonian (8) provided that the relaxation times \(T_1 = 1.96\mu\text{s}\) and \(T_2 = 170\mu\text{s}\) are much longer. In order to establish a comparison with the theoretical predictions, first we solve the Schrödinger equation (Appendix A). This solution is used to calculate the fidelity (1) in the lab frame \(F(t)\) (solid black line). Due to its very fast oscillating behavior, it looks like a black belt. It is possible to see in the inset of the picture the oscillating behavior of the fidelity as the system state evolves in time with the help of a time scale one thousand shorter. Such oscillations are proportional to the ratio between the values of \(\omega_0\) and \(\omega_1\) and depend on the chosen system initial state. Indeed, the experimental values do not present oscillating behavior, once the measurements are performed in a time interval that is two orders of magnitude greater than one period of oscillation of the fidelity.

In analogy to Ref. [17], we use the QSL time to estimate the actual time evolution of the quantum system. There, the authors make use of different norms of the generator of the evolution to get tighter bounds for QSL time. They found that the operator norm furnishes the best estimate for the actual evolution time. In Appendix B, we compare the QSL time for different norms, as proposed in Ref. [17], with that one obtained via EMT bound (2) and through our method (4) for spin 1/2 case. We observed that predictions made by the EMT and operator norm approaches are similar, although the former provides a tighter bound. That is why we have used the EMT bound as the usual approach to compare with our method (blue circles). In Fig. 2, predictions made by the EMT bound (2) in the lab frame are represented by red dashed line. This last result is a consequence of the high average speed in which the system state evolves in the lab frame, or equivalently, it is due to its higher uncertainty energy \(\Delta H(t)\), as presented in Fig. 3. We emphasize that predictions of our method (first roots of transcendental equation) are closer to the actual evolution time, providing in some cases times estimates until four orders of magnitude better than the EMT bound. If we compute the ratio \(\frac{\Delta H(t)}{\Delta H_R} \sim 10^4\), then it corroborates the predictions made above.

Despite that result, some attention must be taken at this point. As emphasized earlier, the original idea about the meaning of the QSL time was not to use it to estimate the actual evolution time, but the minimum time for a quantum state to become distinguishable from the previous one. That is why the original EMT bound does not give satisfactory results when applied within the present purpose, only for very short time scales. Our method, which consists in to find the first chronological roots of the transcendental equation (4), produces good estimations of the actual time of the evolution, providing results (blue points) that are at least in the same order of magnitude of the actual value. Similar observations cannot be pointed out by applying the original EMT bound, which one can predict in the worst case times that are four orders of magnitude lesser than the actual time. For short times, see inset of Fig. 2, we observe that our method works very well, although few roots were predicted a little bit later compared to the actual evolution time obtained theoretically. This fact is attributed to numerical errors due to the high value of the Larmor frequency \(\omega_1\) in relation to the radio frequency \(\omega_1\).

**Spin 3/2 system** — We are interested in to apply the method exposed in this work in a slightly more complex quantum system, aiming to understand how hard the application of the method becomes with the increasing of
spins are 2.6. The Hamiltonian for this is the Casimir operator of the 
the Hilbert space dimension. The physical system is constituted by spins 3/2 of Na nuclear present in sodium dodecyl sulfate of a lyotropic liquid crystal evolving under the action of an external magnetic field and an internal electric field gradient. The Hamiltonian for this system is

\[ H(t) = \hbar \left\{ \omega_0 \mathbf{I}_z + \omega_1 \left[ \cos(\omega_\rho t) \mathbf{I}_x + \sin(\omega_\rho t) \mathbf{I}_y \right] + \frac{\omega_Q}{6} \left( 3\mathbf{I}_z^2 - \mathbf{I}^2 \right) \right\}, \tag{10} \]

where \( \mathbf{I}_j \) \( (j = x, y, z) \) are the components of the nuclear spin operator and \( \mathbf{I}^2 \) is the Casimir operator of the \( su(2) \) algebra. The first term is due to Zeeman interaction with frequency \( \omega_0 \), the second term describes the coupling with the radio frequency field, as in the previous example, while the third one is due to the interaction of the quadrupole moments of the nuclei with the internal electric field gradient, whose coupling strength is \( \omega_Q \). The strength of the Larmor frequency \( \omega_0 \), the radio frequency pulse \( \omega_1 \), and quadrupolar coupling \( \omega_Q \) are \( 2\pi(16.85\text{MHz}), 2\pi(62.50\text{kHz}), \) and \( 2\pi(2.39\text{kHz}) \), respectively, which enable us to neglect the quadrupolar term in the Hamiltonian (Appendix C). Additionally, we chose the precession frequency \( \omega_\rho = \omega_0 \). Therefore, in this approximation the Hamiltonian (10) becomes quite similar to (8), except by the fact that the spin is no longer 1/2. As the \( T_2 \) and \( T_1 \) relaxation times of the \( ^{23}\text{Na} \) nuclear spins are 2.6±0.3 ms and 12.2±0.2 ms, respectively, the time evolution of the system is very well approximated by a unitary dynamics.

The initial state is a pseudo-nuclear spin coherent state defined by the angles \( \theta = 0 \) and \( \phi = 0 \), i.e., an eigenvector of \( \mathbf{I}_z \) which points out to the north pole of the Bloch sphere, \( |j = 3/2, m = +3/2\rangle \). For more details about the state preparation, tomography of the system dynamics, see Ref. [28].

Given the similarities between the spin 1/2 Hamiltonian (8) and the spin \( I = 3/2 \) Hamiltonian, we directly conclude that the unitary transformation that removes the time dependence of the Hamiltonian in the rotating frame is \( R(t) = e^{-i\mathbf{I}_z \omega_\rho t} \) and the corresponding Hamiltonian is \( \hat{H}_R = \hbar \omega_\rho \mathbf{I}_z \). Then, the fidelity of the system state in the rotating frame as function of the lab fidelity and the estimated actual time can be expressed as

\[
F(t_R) = \left[ \sqrt{F(\psi(0)) R^\dag(t_R^\ast)\psi(0)} + a_1 e^{i\varphi_1} \langle \psi(0)|R^\dag(t_R^\ast)|\psi_1^\perp \rangle \right. \\
+ a_2 e^{i\varphi_2} \langle \psi(0)|R^\dag(t_R^\ast)|\psi_2^\perp \rangle + a_3 e^{i\varphi_3} \langle \psi(0)|R^\dag(t_R^\ast)|\psi_3^\perp \rangle \left] \right|^2, 
\tag{11}\]

where \( \varphi_1, \varphi_2, \varphi_3 \in \mathbb{R} \) are relative phases to the initial state. According to the normalization condition, we have that \( a_1^2 + a_2^2 + a_3^2 = 1 - F \), which is a sphere equation of radius \( \sqrt{1-F} \). In virtue of this, we can parametrize \( a_1, a_2, a_3 \in \mathbb{R} \) by \( u, v \in [0, \pi/2] \) through the relations: \( a_1 = \sqrt{1-F} \sin u \cos v \), \( a_2 = \sqrt{1-F} \sin u \sin v \), and \( a_3 = \sqrt{1-F} \cos u \). Observe that we are restricted to one octant of the sphere only, once the others ones can be recovered by choosing the correct sign of the relative phases \( \varphi_1, \varphi_2, \varphi_3 \). In that way, solving the transcendental equation (4) numerically for each combination of parameters in the set \( \{ \varphi_1, \varphi_2, \varphi_3, u, v \} \) and looking for its firsts chronological roots for a given fidelity \( F \), we present ours results in Fig. 4.

By performing quantum state tomography on the nuclear spin 3/2 evolving under the action of the Hamiltonian (10) at each discrete time \( t_n = n \frac{\text{ms}}{48} \) \( (n = 0, 1, \ldots, 18) \) it was possible to obtain the experimental fidelity (green asteriks) with the help of Eq. (1). The theoretical description (solid black line) was achieved through the exact solution of the Schrödinger equation for the same Hamiltonian [28], resulting in the time-dependent fidelity in the lab frame (see Appendix A)

\[
F(t) = \cos^6 \left( \frac{\omega_1 t}{2} \right). \tag{12}\]

We observe that after 8 µs the spin is totally inverted achieving the final state \( |j = 3/2, m = -3/2\rangle \). Differently from the spin 1/2 case, we do not observe fast oscillations in the fidelity behavior. This happens because the initial state of the system acquires only a global phase under the action of the rotation that connects the lab and rotating frames. Furthermore, we used Eq. (12) and the exact expression for the average energy uncertainty \( \Delta H(t) \) applied to the EMT bound in lab frame to estimate the actual evolution time (red solid line) (see also Appendix
A). Similarly to the spin 1/2 case, the higher values of the average energy uncertainty (speed) in the lab frame produces poor predictions of the actual evolution time. While using the predictions made by the first chronological roots of the transcendental equation (blue points), we obtain very close results to the actual evolution time. This occurs because this time estimation is performed in a rotating frame where the energy uncertainty is smaller than in the lab frame.

We call the attention to the fact that the dynamics of the 3/2 spin is quite similar to the NOT gate, since the initial state $|j = 3/2, m = +3/2\rangle$ subjected to the Hamiltonian Eq. (10) returns after 8 µs the state $|j = 3/2, m = -3/2\rangle$. Therefore, we are also estimating the running time of a quantum gate.

IV. DISCUSSIONS AND PERSPECTIVES

In this work we proposed a method to estimate the actual evolution time of a quantum system based on the notion of quantum speed limit time evaluated in a reference frame where the system state evolves as close as possible to the geodesic path over the underlying Hilbert space. Such method enabled us to obtain good time estimation for given 1/2 and 3/2 nuclear spin dynamics, obtaining values until four orders of magnitude better than the EMT bound. There are two important issues related to the implementation of our method: the first one is the chosen of a reference frame where the speed of the state evolution (average energy uncertainty) is smaller than in the lab frame. The second one is the computational cost to implement it. Related to the first issue, our strategy was to find a reference frame where the Hamiltonian becomes time independent. This is interesting because it is possible to evaluate exactly the energy uncertainty using only the initial state and the new Hamiltonian, so that none approximation at this part of the calculation is necessary.

Furthermore, insofar as in NMR systems it always possible to go to a rotating frame defined by the time-dependent radio frequency field [29], the remaining Hamiltonian becomes time independent or varies slowly in time. Related to the computational cost to solve the transcendental equation (4) for the shortest time, there are efficient methods to solve this kind of equation [30], although we did not approach this problem by solving a multi parameter transcendental equation. Instead, if we solve the equation for each possible configuration of any set of parameters in a $d$-dimensional Hilbert space, then it will be need to solve $(2d-1) \times n$ transcendental equations, where $n$ is the number of steps to sweep over each coefficient. After that we take the first chronological root (time) among all solutions. Therefore, although this method can provide good results, it can become expensive for higher dimensional systems. Another possibility to improve the method, it would be to find the unitary transformation that forces the quantum state to evolve over a geodesic length in the new reference frame.

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Appendix A: Exact solution of the Schrödinger equation

Our goal here is to solve the Schrödinger equation

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H}(t)|\psi(t)\rangle,$$

(A1)

for the 1/2 and 3/2 spins dynamics and to obtain the time-dependent fidelity $F(t)$ in order to compare with the predictions of our method and experimental data. Spin 1/2 system — The spin 1/2 Hamiltonian is

$$\hat{H}(t) = \hbar \left\{ \omega_0 \hat{I}_z + \omega_1 \left[ \cos(\omega_p t) \hat{I}_x + \sin(\omega_p t) \hat{I}_y \right] \right\}.$$  

(A2)
First we apply the unitary transformation \( R(t) = e^{-i\hat{H} \omega_p t} \) on Eq. (A1), obtaining the transformed Hamiltonian
\[
\hat{H}_R = R^\dagger(t) \hat{H}(t) R(t) - i \hbar R^\dagger(t) \dot{\hat{R}}(t),
\]
where we set \( \omega_p = \omega_0 \). Then, the evolved state in this new frame is
\[
|\psi_R(t)\rangle = e^{-i\hat{R} \omega_1 t} |\psi_R(0)\rangle, \quad (|\psi_R(0)\rangle = |\psi(0)\rangle). \tag{A4}
\]
Coming back to the original picture, we obtain the exact solution of the Schrödinger equation as
\[
|\psi(t)\rangle = e^{-i\hat{H} \omega_1 t} e^{-i\hat{R} \omega_1 t} |\psi(0)\rangle. \tag{A5}
\]
A general pure state on the Bloch sphere can be written as \(|\psi(0)\rangle = \cos(\theta/2) |0\rangle + e^{i\phi} \sin(\theta/2) |1\rangle\), with \( \theta \) and \( \phi \) defining the polar and azimuthal angles, respectively. Therefore, the evolved state at time \( t \) is represented in matrix form as
\[
|\psi(t)\rangle = \begin{pmatrix}
  e^{-\omega_0 t/2} [ e^{-i \Omega t/2} c_+ \cos(\chi/2) + e^{i \Omega t/2} c_- \sin(\chi/2) ] \\
  e^{i \omega_0 t/2} [ e^{-i \Omega t/2} c_+ \sin(\chi/2) - e^{i \Omega t/2} c_- \cos(\chi/2) ]
\end{pmatrix}, \tag{A6}
\]
with \( \Omega = \sqrt{\omega_0^2 + (\omega_1 - \omega_0)^2} \), \( \cos \chi = (\omega_1 - \omega_0)/\Omega \), \( \sin \chi = \omega_0/\Omega \) and,
\[
c_+ = (\cos(\chi/2) \cos(\theta/2) + e^{i\phi} \sin(\chi/2) \sin(\theta/2)), \quad c_- = (\sin(\chi/2) \cos(\theta/2) - e^{i\phi} \cos(\chi/2) \sin(\theta/2)). \tag{A7}
\]
Evaluating the fidelity we get
\[
F(t) = \left[ \cos\left(\frac{\omega_0 t}{2}\right) \cos\left(\frac{\Omega t}{2}\right) \cos \chi \sin \left(\frac{\omega_0 t}{2}\right) \sin \left(\frac{\Omega t}{2}\right) \right]^2
+ \left[ \cos \theta \cos \chi + \cos \phi \sin \theta \sin \chi \right] \left[ \cos\left(\frac{\omega_0 t}{2}\right) \sin \left(\frac{\Omega t}{2}\right) \cos \chi \sin \left(\frac{\omega_0 t}{2}\right) \cos \left(\frac{\Omega t}{2}\right) \right]
+ \sin \left(\frac{\omega_0 t}{2}\right) \sin \chi \left[ \cos\left(\frac{\omega_0 t}{2}\right) \cos \theta \sin \chi - \cos \phi \sin \theta \cos \chi \right] \sin \left(\frac{\omega_0 t}{2}\right) \sin \phi \sin \varphi \right]^2. \tag{A8}
\]
Now we are able to evaluate the energy uncertainty in both frames of reference. Using the Hamiltonian (A3) and the quantum state (A4), we find that
\[
\Delta H_R = \frac{\hbar \Omega}{2} \sqrt{1 - (\cos \chi \cos \theta + \cos \phi \sin \chi \sin \theta)^2}, \tag{A9}
\]
while the energy uncertainty in the lab frame is obtained through Eqs. (A2) and (A6), i.e.,
\[
\Delta H(t) = \sqrt{\frac{\hbar^2}{4} (\omega_0^2 + \omega_1^2) - (\langle \psi(t) | \hat{H}(t) | \psi(t) \rangle)^2}, \tag{A10}
\]
where
\[
\langle \psi(t) | \hat{H}(t) | \psi(t) \rangle = \frac{\hbar}{2} \left( |c_+|^2 - |c_-|^2 \right) (\Omega + \omega_0 \cos \chi)
+ \hbar \omega_0 \sin \chi \left[ \cos (\Omega t) \mathbf{Re}(c_+^* c_-) - \sin (\Omega t) \mathbf{Im}(c_+^* c_-) \right], \tag{A11}
\]
with
\[
|c_+|^2 - |c_-|^2 = \cos \theta \cos \chi + \cos \phi \sin \theta \sin \chi, \tag{A12}
\]
and
\[
\mathbf{Re}(c_+^* c_-) = \frac{1}{2} (\cos \theta \sin \chi - \cos \phi \sin \theta \cos \chi), \quad \mathbf{Im}(c_+^* c_-) = -\frac{1}{2} \sin \theta \sin \phi. \tag{A13}
\]
The EMT bound in the lab frame depends only on the fidelity (A8) and the time average of the energy uncertainty (A10). Such bound is evaluated numerically and is plotted in Fig. 2 as the red dashed line.

Spin 3/2 system — This system was already studied in Ref.[28]. A particular case in which \( \omega_0, \omega_1 \gg \omega_Q \) and \( \omega_p = \omega_0 \), the Hamiltonian in the Schrödinger picture (10) simplifies to
\[
\hat{H}(t) = \hbar \left\{ \omega_0 \hat{I}_z + \omega_1 \left[ \cos(\omega_0 t) \hat{I}_z + \sin(\omega_0 t) \hat{I}_y \right] \right\}.
\]
Going to the rotating frame through the unitary transformation \( R(t) = e^{-iA \omega_p t} \), the new Hamiltonian is
\[
\hat{H}_R = \hbar \omega_1 \hat{I}_x, \tag{A14}
\]
and the evolved state in the rotating frame is
\[
|\psi_R(t)\rangle = e^{-i\omega_1 A \hat{I}_x} |\psi(0)\rangle. \tag{A15}
\]
Immediately we obtain the general expression for the evolved state in the lab frame as

\[ |\psi(t)\rangle = e^{-i\omega_0 t} |\psi(0)\rangle. \]  

(A16)

By choosing the initial state as a pseudo-nuclear spin coherent state characterized by the angles \( \theta=0, \phi=0 \) [28], or simply \( j=3/2, m=+3/2 \), the system state at time \( t \) in the lab frame is

\[
\begin{pmatrix}
\sin^3 (\omega_1 t/2) \\
-\sqrt{3}\sin(\omega_1 t/2) \cos(\omega_1 t/2) \\
-\sqrt{3}\sin(\omega_1 t/2) \cos^2(\omega_1 t/2) \\
e^{i3\omega_0 t/2} \cos^3(\omega_1 t/2)
\end{pmatrix}.
\]

(A17)

Consequently, the fidelity becomes

\[ F(t) = \cos^6 \left( \frac{\omega_1 t}{2} \right). \]  

(A18)

Its behavior is represented by the solid black line in Fig. 4. To do the time estimation it is necessary the energy uncertainty in the rotating frame, which reads as

\[ \Delta H_R = \frac{\sqrt{3}}{2} \hbar \omega_0, \]  

(A19)

while in the lab frame it is obtained through the substitution of (A14) and (A17) in the expression \( \Delta H(t) = \sqrt{\langle \psi(t)|\hat{H}^2(t)|\psi(t)\rangle - \langle \psi(t)|\hat{H}(t)|\psi(t)\rangle^2} \). Due to its long length, the expressions for \( \Delta H(t) \) and \( \Delta \hat{H}(t) \) were evaluated numerically. Therefore, by combining \( \Delta \hat{H}(t) \) and (A18) according to Eq. (2), we obtain the EMT bound for the 3/2 spin system, which is reported in Fig. 4 by the dashed red line.

**Appendix B: Comparing quantum speed limit bounds**

It was deduced in Ref. [17] the following expressions for the QSL time for unitary dynamics,

\[ \tau_{tr,op} = \frac{\hbar \sin^2 (L)}{2 \Lambda_{tr,op}}, \quad \tau_{HS} = \frac{\hbar \sin^2 (L)}{\Lambda_{HS}}, \]  

(B1)

where \( L = \arcsin \left( \frac{1}{F(t)} \right) \) is the geodesic length between the initial and final states and

\[ \Lambda^i = \frac{1}{t} \int_0^t \left\| \hat{H}(t)|\psi(t')\rangle\langle \psi(t')| \right\| dt'. \]

The index \( \ell \) refers to the type of norm being used. For operator norm

\[ \left\| \hat{H}(t)|\psi(t')\rangle\langle \psi(t')| \right\|_{op} = \sigma^i, \]  

(B2)

\( \sigma^i \) are singular values of \( \hat{H}(t)|\psi(t')\rangle\langle \psi(t')| \) and are written in descending order as \( \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \). In Fig. 5 we compare the expressions given by Eq. (B1) with that ones from the EMT bound (2) and transcendental equation (4) for the example of the spin 1/2 system. Despite the hierarchic relation \( \Lambda_{op} \leq \Lambda_{HS} \leq \Lambda_{tr} \) [17], in Fig. 5 we noticed that \( \tau_{HS} \) is bigger than the other two expressions obtained in [17], but smaller than the EMT bound because of the inequality \( L \geq \sin^2 L \). Altogether \( \tau_{tr} \) (green thin solid line), \( \tau_{op} \) (orange dotted line), \( \tau_{HS} \) (blue thin dashed line), and the EMT bound (2) (red thick dashed line) furnish similar results for the time estimates. Nevertheless, the best result is given by
the solution of the transcendental equation (4) (blue circles). Therefore, for the sake of simplicity, hereafter we will compare the predictions for the actual time made by EMT bound (2), first roots of transcendental equation (4), and experimental data.

Appendix C: Experimental data of the spin system

The NMR implementation is carried out using an Ascend Bruker of 400 MHz spectrometer (Larmor frequency of \(^1\)H nuclei) at State University of Ponta Grossa (UEPG). A double channel probe-head for liquid samples is used to apply a transverse magnetic field of a few gauss. The channel configuration obeys the label (H/F)X, it means that the first channel is dedicated into detect \(^1\)H and \(^{13}\)C nuclei signals; the second channel detects signals of any number species between 162 MHz and 40 MHz, such as \(^{31}\)P, \(^{13}\)C, \(^{23}\)Na, \(^{15}\)N.

Solution-NMR experiment is performed using molecules of α-phosphoric acid (H\(_3\)PO\(_4\)) dissolved in deuterated water (D\(_2\)O), at room temperature (\(\sim 25^\circ\)C). The stoichiometry of our sample obeys 12.5% of H\(_2\)O and 87.5% of D\(_2\)O, a solution of 650 ml was placed in a glass of 5 mm NMR tube. In Fig. 6(a) is sketched a picture of H\(_3\)PO\(_4\) molecular structure. The choice of H\(_3\)PO\(_4\) molecule to achieve an isolated 1 qubit system using \(^{31}\)P nuclei obeys some chemical characteristics. First, the \(^{31}\)P isotope is naturally abundant at one hundred percent. Second, oxygen nuclei has zero nuclear spin, so there is not any coupling strength between oxygen nuclei and \(^{31}\)P. Third, the electrons of the four oxygen nuclei are arranged in such away that they shell the interaction between \(^1\)H nuclei and \(^{31}\)P nuclei. Fourth, to verify the efficiency of this shielding process, in Fig. 7c we present the spectrum of \(^{31}\)P. The peak width at half height is \(\sim 2.1\) Hz, meaning that if there exist any kind of coupling between any neighborhood nuclei of \(^{31}\)P, then the strength of the interaction is less than \(2.1\) Hz, which is considered weak. The calibration parameters on the X-channel of the probe-head in to apply and to detect \(^{31}\)P nuclei signals are: tuning of the radio-frequency is \(\omega_p = 2\pi (161.975\) MHz), \(\pi/2\)-pulse time calibrated at 11 \(\mu\)s which corresponds to a strength radio-frequency of \(\omega_1 = 2\pi (21.93\) kHz), recycle delay \(d_1 = 20\)s, acquisition time \(\tau_{Acq.} = 2.5\) s.

At room temperature, the theoretical formalism to describe the quantum state of any nuclear spin system is the maximum mixture state [31]

\[
\hat{\rho} \approx \frac{1}{2} \mathbf{I} + \frac{\beta \hbar \omega_0}{2} \mathbf{I}_z,
\]  

(C1)

where \(\beta = 1/k_B T, \ Z = \text{Tr} \left[ e^{-\beta \hbar \omega_0 \mathbf{I}_z} \right] \) is partition function, \(T \) is temperature, \(k_B \) is Boltzmann’s constant, \(\hbar \) is reduced Planck’s constant and \(\omega_0 = 2\pi (161.975\) MHz) is Larmor frequency for \(^{31}\)P nuclei at 9.39 Tesla. So, the polarization factor is \(\epsilon = \frac{\beta \hbar \omega_0}{2} = 0.652 \times 10^{-5} \), which is a slight deviation from the normalized identity matrix \(\mathbf{I}/\mathbf{Z} \). In this sense, the thermal state of Eq. (C1) can be rewritten

\[
\hat{\rho} \approx \left( \frac{1}{2} - \epsilon \right) \mathbf{I} + \epsilon \hat{\rho}_0,
\]  

(C2)

where \(\hat{\rho}_0 \) represents the pure part of density matrix with unitary trace.

1. The quantum state tomography procedure

The pure part of the density matrix was tomographed and reconstructed using global rotations [32]. In this sense, the NMR technique detects magnetization along the x-axis and y-axis which correspond to first order coherences of any density matrix, and this characteristic has been explored into detect other orders of coherences. So, we present a brief explanation for spin \(I = 1/2\), and analogous procedure is extended for spin \(3/2\), see details in [28, 32].

In order to apply the tomography procedure on a spin system \(I = 1/2\), we identify zero and first order coherences on its density matrix. Thus, we must use appropriate rotations to transfer intensities from zero order of coherences into first order. The density operator for one qubit is represented by \(2 \times 2\) operator. Therefore, as an example, lets us reconstruct the density matrix of the nuclear spin in its ground state, \(|\uparrow\rangle\). So, we represent the elements of any density matrix as

\[
\hat{\rho}_0 = \begin{bmatrix}
\rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\
\rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow}
\end{bmatrix} = \begin{bmatrix}
x_1 & x_2 + ix_3 \\
x_2 - ix_3 & x_4
\end{bmatrix},
\]  

(C3)

and to compute numerical values for their elements, we proceed with a protocol that can be summarized into three stages:

*The first stage:* NMR observables are spin angular momentum operators \(\hat{I}_x\) and \(\hat{I}_y\), such that their average values correspond to magnetization along the \(x\)- and \(y\)-axis, respectively. By simple calculation for any density matrix \(\hat{\rho}_0\), see Eq. (C3), it is possible to show that

\[
M_x (\hat{\rho}_0) = \text{Tr} \left\{ \hat{I}_x \hat{\rho}_0 \right\} = x_2,
\]  

(C4a)

\[
M_y (\hat{\rho}_0) = \text{Tr} \left\{ \hat{I}_y \hat{\rho}_0 \right\} = -x_3,
\]  

(C4b)

bring information on the real and imaginary parts of the element \(\rho_{\uparrow\downarrow}/\rho_{\downarrow\uparrow}\) and also its complex conjugate \(\rho_{\downarrow\uparrow}/\rho_{\uparrow\downarrow}\).

*The second stage:* We transform \(\hat{\rho}_0\) applying the operator \(R_y (\pi/2)\) and each element of the transformed density matrix can be represented by

\[
\hat{\rho}' = \frac{1}{2} \begin{bmatrix}
x_1 + x_4 - 2x_2 & x_1 - x_4 + 2ix_3 \\
x_1 - x_4 - 2ix_3 & x_1 + x_4 + 2x_2
\end{bmatrix}.
\]  

(C5)

Again, if the NMR signal is detected, so the magnetiza-
Figure 6. (Color online) We sketch a cartoon of the molecules used in the present study. (a) O-phosphoric acid molecule (H$_3$PO$_4$). (b) Sodium dodecil sulfate (Na-C$_{12}$H$_{25}$SO$_4$).

The third stage: In order to reconstruct the density matrix, we need to identify each equation of the previous stages with those four spectra on Fig. 7. In this sense, the spectra in Fig. 7a and 7b represent magnetizations $M_x (\hat{\rho}_0)$ and $M_y (\hat{\rho}_0)$ which are quantified by Eq. (C4a) and (C4b). Similarly, the spectra in Fig. 7c and 7d represent magnetizations, after a $\pi/2$-rotation, generating from Eqs. (C6a) and Eq. (C6b) information on the state $\rho'$. In this procedure, we use and apply a normalization factor 2, because the amplitude of magnetization goes from -1 to 1, see Fig. 7, such that the magnetization $M_x (\hat{\rho}')=0.5$ (those values are rounded with one decimal place in this example). Summarizing, the equations are

$$x_2 = 0,$$
$$x_3 = 0,$$
$$x_1 - x_4 = 1,$$
$$x_1 + x_4 = 1.$$

Solving this system of coupled equations, we find the cor-

Figure 7. (Color online) NMR spectra of $^{31}$P nuclei in order to detect the initial quantum state $|\uparrow\rangle$ represented by the density matrix $\hat{\rho}_0$. A spectral window of 120 Hz is established to show the magnetization: (a) along $x$-axis with $M_x (\hat{\rho}_0)$, (b) along $y$-axis, with $M_y (\hat{\rho}_0)$, (c) along $x$-axis, with $M_x (\hat{\rho}')$ such that $\hat{\rho}' = R_y (\frac{\pi}{2}) \hat{\rho}_0 R_y (\frac{\pi}{2})$, (d) along $y$-axis, with $M_y (\hat{\rho}')$.

Figure 8. (Color online) Tomographed quantum state. The quantum state $\hat{\rho} = |\uparrow\rangle \langle \uparrow|$ is showed at its matrix representation using bar charts. Left (Right) bar chart corresponds to real (imaginary) elements.
The initialization of the quantum state. Third, the rotation delay $d$ allows to achieve the thermal equilibrium state of all nuclei in the sample. Second, the procedure to initialize the quantum state is depicted by the first box (dashed line) of the pulse sequence with $\tau_1$ the required time to perform the initialization of the quantum state. Third, the rotation $R_{-x}(\tau_r)$ allow us to control the dynamics of the nuclear spin system. Fourth, the quantum state tomography procedure performing any rotation of the protocol [32] is represented by the black dashed line box. Finally, the read out of the free induction decay (FID) is performed under $\tau_{Acq}$ the acquisition time.

The development of the protocol can be summarized as an initialization of the quantum state and the register of the dynamics protocol. First, recycle delay $d_1$ allows to achieve the thermal equilibrium state of all nuclei in the sample. Second, the procedure to initialize the quantum state is depicted by the first box (dashed line) of the pulse sequence with $\tau_1$ the required time to perform the initialization of the quantum state. Third, the rotation $R_{-x}(\tau_r)$ allow us to control the dynamics of the nuclear spin system. Fourth, the quantum state tomography procedure performing any rotation of the protocol [32] is represented by the black dashed line box. Finally, the read out of the free induction decay (FID) is performed under $\tau_{Acq}$ the acquisition time.

The NMR experiments are performed on a VARIAN INOVA 400 MHz spectrometer at the Institute of Physics in São Carlos (IFSC-USP). In this second setup we use Sodium dodecyl sulfate sample (see Fig. 6(b)) in order to excite and to detect $^{23}$Na nuclei signals. The stoichiometry of this sample obeys 21.3 wt % of sodium dodecyl sulfate, 3.7 wt % of decanol, and 75 wt % of deuterated water in a regime of a lyotropic liquid crystal. At strength static magnetic field of 9.34 Teslas, the Larmor frequency and quadrupolar couplings are $2\pi(16.85)$MHz and $2\pi(2.39)$kHz, respectively. Also, $\pi$-pulse lengths of 8 $\mu$s and recycle delays of 500 ms are calibrated. The $T_2$ and $T_1$ relaxation times of $^{23}$Na nuclei are 2.6 ± 0.3 ms and 12.2 ± 0.2 ms, respectively.

Appendix D: Spin system $I = 3/2$

The NMR experiments are performed on a VARIAN INOVA 400 MHz spectrometer at the Institute of Physics in São Carlos (IFSC-USP). In this second setup we use Sodium dodecyl sulfate sample (see Fig. 6(b)) in order to excite and to detect $^{23}$Na nuclei signals. The stoichiometry of this sample obeys 21.3 wt % of sodium dodecyl sulfate, 3.7 wt % of decanol, and 75 wt % of deuterated water in a regime of a lyotropic liquid crystal. At strength static magnetic field of 9.34 Teslas, the Larmor frequency and quadrupolar couplings are $2\pi(16.85)$MHz and $2\pi(2.39)$kHz, respectively. Also, $\pi$-pulse lengths of 8 $\mu$s and recycle delays of 500 ms are calibrated. The $T_2$ and $T_1$ relaxation times of $^{23}$Na nuclei are 2.6 ± 0.3 ms and 12.2 ± 0.2 ms, respectively.

At thermal equilibrium, most NMR systems are represented by their almost maximum mixture states, such as Eq.(C1). Using suitable pulse sequences – spin rotations and free evolutions – any pseudo pure state is prepared [33–35] as depicted in Fig. 9. In this sense, the first dashed square of Fig. 9 represents the initialization procedure performed by strongly modulated pulses[35], such that in this study we prepare the pseudo-nuclear spin coherent state [28] $|\psi(0)\rangle = |3/2, +3/2\rangle \equiv |\zeta(0,0)\rangle$; the second square represents a hard pulse with variable length $\tau_r$ to control the spin rotation; the third dashed square represents the tomography pulse [32]. In particular, the initial quantum state means, from the NMR point of view, the precession of the magnetic moment around an axis defined by the orientation of the strong static magnetic field $B_0$. For more details on the experimental setup, the initialization of the pseudo-nuclear spin coherent state, and the register of the dynamics to flip the spin 3/2, see Ref. [28].
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[27] In this video we make a qualitative comparison among the real path length of the Bloch vector evolution for a spin 1/2 system described in three different reference frames: lab frame (left), rotating frame in resonance condition (middle), and rotating frame out of resonance (right). These frames are related by a rotation around the z-axis. The geodesic length at instant of time is the path length over the Bloch sphere between the North Pole and the Bloch vector position along a given meridian. Particularly in this example, the geodesic length is the same in all three reference frames for each instant of time. See https://youtu.be/TOWNTnSzCS4.
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