Quantum transitions and semiquantum chaos in an SU(2) nonlinear dynamics

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Abstract. A semi-quantum nonlinear Hamiltonian, associated with the SU(2) Lie algebra, is used to model the confinement of a particle of spin $\frac{1}{2}$ in a double well potential generated by a classical particle of mass $m$ (CPm). We discuss the manner in which the nonlinear coupling between the quantum and classical subsystems induces transitions between the (spin) two levels system’s states. Also, we elaborate on how the associated transition probabilities’ behave as the coupling constant varies. The role played by the uncertainty principle during these transitions is also described.

Keywords. Nonlinear semiquantum dynamics; quantum transitions; two-level systems.

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1. Introduction

Semiquantum Hamiltonians are often found in the literature [1–24], and, according to Ref. [1], they are defined as those composed by a full quantum part, a full classical part, and an interaction term which takes into account the interaction between the quantum system and the classical one. In the interaction term one finds both classical and quantum variables, coupled in nonlinear fashion. Thus, generally speaking, we are allowed to represent the ensuing Hamiltonian in the form used by Ref. [3]:

\[ \hat{H} = \hat{H}_q + \hat{H}_{cl} + \hat{H}_{int}, \]

where $\hat{H}_q$ and $\hat{H}_{cl}$ stand for the pure quantum and pure classical parts of the system, respectively, and $\hat{H}_{int}$ is the interaction term. There are many phenomena which can be modeled by semiquantum Hamiltonians and described within the framework of semiquantum dynamics, like molecular transistors, carbon nanotubes, quantum dots and SQUIDs (interested readers can consult Ref. [14]). It is well known that the nonlinear coupling of a quantum system with a classical one can lead to chaotic dynamics not only for certain values of the system’s parameters, but also for adequate initial conditions. Signatures of chaos are observed not only in the behavior of classical quantities but also in quantum ones (see Refs [1, 2, 6, 10–12, 19–21, 25].

Among the kinds of Hamiltonian described by eq. (1), there exists a particular case in which the quantum degrees of freedom (quantum operators) appearing in the $\hat{H}_q$ and $\hat{H}_{int}$ terms may be expressed as a linear superposition of the generators of a certain Lie algebra. When this is the case, it is possible to find some invariants of the motion for the system, given that the quantum variables close a partial semi Lie algebra under commutation with the Hamiltonian (see Refs [12, 26–28] for more details).

In this contribution we are going to consider a semi-quantum nonlinear Hamiltonian associated with the SU(2) Lie algebra and are able to model the confinement of a spin $\frac{1}{2}$ in a double well potential generated by a classical particle of mass $m$ (CPm). Quantum degrees of freedom appear in the Hamiltonian as a linear superposition of the generators of the SU(2) Lie algebra $\{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$ (i.e. the components of spin $\frac{1}{2}$). Because the Hamiltonian closes a partial Lie algebra under commutation, the associated dynamical invariant that the system exhibits is the uncertainty principle (UP) itself (see Refs [12, 26, 27] for more details).

In Ref. [7], we took advantage of this invariant and made a complete study of this systems’ fixed points and of their instabilities and bifurcation curves. We showed
how their emergence/disappearance is related to a certain parameter, associated with the UP-invariant. Here, our goal is (1) to show (by means of numerical simulations) that the nonlinear coupling between the spin and the classical particle (CP) induces spin transitions between the ‘up’ and ‘down’ states and (2) to ascertain the role played by the UP-invariant as these transitions take place.

The paper is organized as follows: in section 2 we present (i) the Hamiltonian to be studied, (ii) the nonlinear semiquantum equations of motion, (iii) the obtainment of expressions for the mean values $\langle \hat{\sigma}_x \rangle(t)$, $\langle \hat{\sigma}_y \rangle(t)$, and $\langle \hat{\sigma}_z \rangle(t)$, via the maximum entropy principle (MEP) density operator $\hat{\rho}$, (iv) two invariants that the system displays (they are necessary to properly choose the system’s initial conditions without violating neither energy conservation nor the UP), and (v) the discussion of how the transition probabilities (TP) between the two level system’s states are related to the temporal evolution of the mean value $\langle \hat{\sigma}_i \rangle(t)$ (readers unfamiliar with the MEP procedure are referred to appendix A, where we briefly summarize its main tools, and it can also be consulted in Refs [12, 27, 28] to understand how the MEP density operator $\hat{\rho}$ is obtained). In section 3 we present our numerical simulations with the obtained results. In section 4 we draw some conclusions and envisage future work. Finally, we present an appendix A with MEP tools and how to obtain the generalized UP.

2. Model and equations of motion

The Hamiltonian considered here is [6, 7]

$$\hat{H} = B\hat{\sigma}_z + Cq\hat{\sigma}_x + \frac{p^2}{2m} + D\frac{q^4}{4} - F\frac{q^2}{2},$$

(2)

where $\hat{\sigma}_z$ and $\hat{\sigma}_x$ are the $x$ and $z$ components of the $\frac{1}{2}$ spin, respectively. $B$, $C$, $m$, $D$, and $F$ are positive constants. The Hamiltonian given by eq. (2) represents a $\frac{1}{2}$ spin quantum particle in the presence of an external static magnetic field oriented in the $+z$ direction (whose Hamiltonian is given by the term $B\hat{\sigma}_z$, while the constant $B$ is related to the spin precession frequency around the magnetic field). Furthermore, the spin interacts with a CPm $m$ (through the term $Cq\hat{\sigma}_x$), where $C$ is the coupling constant. The spin is confined to a double well potential $V(q) = D\frac{q^4}{4} - F\frac{q^2}{2}$ originated by the (CP). $q$ and $p$ are classical canonical conjugated variables of position and momentum, respectively, corresponding to the CP, while $\frac{p^2}{2m}$ is the CP’s kinetic energy.

The interest to study and understand this type of Hamiltonian’s dynamics arises within the framework of modeling the quantum confinement phenomenon. This phenomenon has been of great interest in the last years due to the confinement of a $1/2$ spin particle (such as the electron) in a potential well so that this phenomenon has potential applications in the development of nanotechnology.

It is easy to see that the Hamiltonian (2) may be considered as a linear superposition of the generators of the SU(2) Lie algebra: $\{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$ fulfill the commutation rule $[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\sum_{l=1}^3 \epsilon_{ijkl} \hat{\sigma}_l$. Notice that the classical terms may be considered as $\left(\frac{p^2}{2m} + D\frac{q^4}{4} - F\frac{q^2}{2}\right)\hat{I}$, with $\hat{I}$ the identity operator, so that the set of operators $\{\hat{I}, \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$ becomes a relevant one for this system and closes a partial Lie algebra under commutation with the Hamiltonian through the closure condition [28] (see appendix A):

$$[\hat{H}(t), \hat{O}] = i\hbar \sum_{r=0}^N g_{ij}(q) \hat{O}_r,$$

(3)

with $g_{ij}(q)$ the coefficients of such linear superposition. The $g_{ij}(q)$ terms in eq. (3) may eventually involve the system’s classical degrees of freedom. Since the identity operator commutes with the Hamiltonian, the classical term does not appear in the final result of the quantum commutation operation given by eq. (3) [27]. This fact has two important consequences: (1) the Ehrenfest’s theorem of Ref. [29]:

$$\frac{\partial \langle \hat{O}_j \rangle}{\partial t} = \sum_{r=0}^N g_{ij}(q) \langle \hat{O}_r \rangle(t), \quad j = 1, \ldots, N,$$

(4)

can still help in obtaining the evolution equations for the quantum variables’ mean values, (2) the system’s entropy remains a constant of the motion, and the MEP density operator $\hat{\rho}$ can also be constructed for the semiquantum case. To obtain the equations of motion for the classical variables we proceed, as classical mechanics prescribes [12, 18]:

$$\frac{dq}{dt} = \frac{\partial \langle \hat{H} \rangle}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial \langle \hat{H} \rangle}{\partial q},$$

(5)

where $\langle \hat{H} \rangle = Tr(\hat{\rho}\hat{H})$ is the Hamiltonian function. The development of this semiquantum formalism has already been detailed in previous publications (interested readers can see a brief summary in appendix A and consult Refs [11, 12, 27]). However, we are going to take advantage of them with the purpose of obtaining the TP via the MEP density operator $\hat{\rho}$. Semiquantum formalism takes advantage of the fact that the term containing the classical variables can be considered as $\left(\frac{p^2}{2m} + D\frac{q^4}{4} - F\frac{q^2}{2}\right)\hat{I}$, where $\hat{I}$ is the identity operator and, and because $[\hat{H}, \hat{I}] = 0$, the closure condition given by eq. (3) still holds and it is possible to obtain the MEP density operator $\hat{\rho}$ as prescribed in Ref. [28] for the full quantum case.
Making use of eqs (4) and (5), we obtain a semi-quantum differential equations of motion:

$$\frac{d \langle \hat{\sigma}_z \rangle}{dt} = -2B \langle \hat{\sigma}_x \rangle,$$

(6)

$$\frac{d \langle \hat{\sigma}_y \rangle}{dt} = 2B \langle \hat{\sigma}_z \rangle - 2Cq \langle \hat{\sigma}_y \rangle,$$

(7)

$$\frac{d \langle \hat{\sigma}_x \rangle}{dt} = 2Cq \langle \hat{\sigma}_x \rangle,$$

(8)

$$\frac{dq}{dt} = \frac{p}{m},$$

(9)

$$\frac{dp}{dt} = -C \langle \hat{\sigma}_x \rangle - Dq^3 + Fq.$$  

(10)

It is worth noting that if the coupling constant $C = 0$, the well known equations corresponding to the spin precession around the magnetic field (Larmor precession) are recovered, while the spin does not perform any transition between the ‘up’ and ‘down’ states because $\langle \hat{\sigma}_z \rangle_{(0)} = \langle \hat{\sigma}_z \rangle_{(0)}$ remains a constant of the motion and $\langle \hat{\sigma}_x \rangle_{(0)}$ evolves according to:

$$\langle \hat{\sigma}_x \rangle_{(0)} = \langle \hat{\sigma}_x \rangle_{(0)} \cos(2Bt) - \langle \hat{\sigma}_x \rangle_{(0)} \sin(2Bt),$$

while $\langle \hat{\sigma}_y \rangle_{(0)}$ does according to:

$$\langle \hat{\sigma}_y \rangle_{(0)} = \langle \hat{\sigma}_y \rangle_{(0)} \cos(2Bt) + \langle \hat{\sigma}_y \rangle_{(0)} \sin(2Bt).$$

As for the MEP density operator, from Refs [12, 27, 28, 30, 31] we see that it can be expressed as (see appendix A)

$$\hat{\rho} = \exp\left(-\lambda_0 \hat{I} - \lambda_x \hat{\sigma}_x - \lambda_y \hat{\sigma}_y - \lambda_z \hat{\sigma}_z\right)$$

$$= \frac{1}{2} \left( \hat{I} + \frac{\tanh |\alpha|}{|\alpha|} \hat{\alpha} \cdot \hat{\sigma} \right),$$

(11)

with $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$, $\alpha = (\lambda_x(t), \lambda_y(t), \lambda_z(t))$, and $\lambda_0 = \ln(2\cosh|\alpha|)$ (see Ref. [12] for more details). $\lambda_0(t)$, $\lambda_x(t)$, $\lambda_y(t)$, and $\lambda_z(t)$ are the Lagrange multipliers associated with the relevant set $\{\hat{I}, \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$ used in order to construct $\hat{\rho}$ [28] (the set-members evolve in time).

Taking into account the orthonormal basis $\{|+\rangle = |0\rangle, -|\rangle = |1\rangle\}$ of $\hat{\sigma}_z$ eigenstates, the density operator given by eq. (11) may also be written as

$$\hat{\rho} = \frac{1}{2} \left\{ |0\rangle \langle 0| + |1\rangle \langle 1| - \frac{\tanh |\alpha|}{|\alpha|} [\lambda_z |0\rangle \langle 0| - \lambda_z |1\rangle \langle 1|] + (\lambda_x - i\lambda_y) |0\rangle \langle 1| + (\lambda_x + i\lambda_y) |1\rangle \langle 0| \right\}.$$

(12)

The quantum observables’ mean values are obtained by means of $\langle \hat{\sigma}_x \rangle = \text{Tr} (\hat{\rho} \hat{\sigma}_x) = -\frac{\partial \rho}{\partial \lambda_0}$ [28], and we obtain (see Ref. [12] for more details):

$$\langle \hat{\sigma}_x \rangle = -\frac{\tanh |\alpha|}{|\alpha|} \lambda_x,$$

(13)

$$\langle \hat{\sigma}_y \rangle = -\frac{\tanh |\alpha|}{|\alpha|} \lambda_y,$$

(14)

$$\langle \hat{\sigma}_z \rangle = -\frac{\tanh |\alpha|}{|\alpha|} \lambda_z,$$

(15)

with $|\alpha| = \sqrt{\lambda_x^2(t) + \lambda_y^2(t) + \lambda_z^2(t)}$ a constant of motion whose value is determined by the initial conditions [12]. Equations (13)–(15) are the mean values’ expressions, noting that the Lagrange multipliers $\lambda_x$, $\lambda_y$, and $\lambda_z$ also evolve in time according to the following nonlinear equations, given by the MEP formalism (see appendix A and [28]):

$$\frac{d\lambda_j}{dt} = \sum_{r=0}^{N} g_{jr}(q)\lambda_r, \quad j = 1, \ldots, N.$$  

(16)

Thus, making use of eq. (16), we obtain:

$$\frac{d\lambda_x}{dt} = 2B\lambda_y,$$

(17)

$$\frac{d\lambda_y}{dt} = -2B\lambda_x + C\lambda_z,$$

(18)

$$\frac{d\lambda_z}{dt} = -2C\lambda_y.$$  

(19)

So as to obtain $\langle \hat{\sigma}_i \rangle_{(0)}$, the system of eqs (17)–(19) should be numerically tackled (they form a nonlinear system). Nevertheless, eqs (13)–(15) are very useful to calculate the spin transition-probabilities between ‘up’ and ‘down’ states (i.e., between $|0\rangle$ and $|1\rangle$ states). Indeed, if we call $P_0$ and $P_1$ the probabilities for quantum state to collapse to the eigenstates $|0\rangle$ and $|1\rangle$, respectively, we have [32]:

$$P_0 = \text{Tr} (\hat{\rho} \hat{P}_0), \quad P_1 = \text{Tr} (\hat{\rho} \hat{P}_1),$$

where $\hat{P}_0 = |0\rangle \langle 0|$ and $\hat{P}_1 = |1\rangle \langle 1|$ are the projectors onto $|0\rangle$ and $|1\rangle$ eigenstates, respectively. Now, using eqs (12) and (15) we obtain

$$P_0 = \frac{1}{2} \left\{ 1 - \frac{\tanh |\alpha|}{|\alpha|} \lambda_z \right\} = \frac{1}{2} \left\{ 1 + \langle \hat{\sigma}_z \rangle_{(0)} \right\},$$

(20)

$$P_1 = \frac{1}{2} \left\{ 1 + \frac{\tanh |\alpha|}{|\alpha|} \lambda_z \right\} = \frac{1}{2} \left\{ 1 - \langle \hat{\sigma}_z \rangle_{(0)} \right\}.$$  

(21)
From eqs (20) and (21) we see that the TP also evolve in time. To obtain them we need \( \langle \dot{\hat{q}}_{z} \rangle_{0} \). If the coupling constant is \( C = 0 \), \( \langle \dot{\hat{q}}_{z} \rangle_{0} = \langle \dot{\hat{q}}_{x} \rangle_{0} \), there are no transitions and the constant-value probabilities are \( p_{0} = \frac{1}{2} \{ 1 + \langle \dot{\hat{q}}_{z} \rangle_{0} \} \) and \( p_{1} = \frac{1}{2} \{ 1 - \langle \dot{\hat{q}}_{z} \rangle_{0} \} \) (they represent the probability that, when measuring the observable \( \hat{q}_{z} \), the state of the system will collapse onto the eigenstates \( |0\rangle \) or \( |1\rangle \), respectively). On the other hand, if the coupling constant is \( C \neq 0 \), \( \langle \dot{\hat{q}}_{z} \rangle_{0} \) is no longer a constant of motion and, in order to obtain \( \langle \dot{\hat{q}}_{z} \rangle_{0} \), the nonlinear systems (6)–(10) must be numerically solved. Thus, from eqs (20) and (21), we conclude that the temporal evolution of \( \langle \dot{\hat{q}}_{z} \rangle_{0} \) accounts for the fact that there are (on average) transitions between the two levels of the quantum subsystem (the spin). These transitions are induced by the nonlinear coupling between the spin and the classical mass \( m \), since the spinning particle is confined within a double well potential.

Additionally this system exhibits two dynamic invariants:

1. **The energy**: As the Hamiltonian does not explicitly depend on time, the system’s energy \( \langle H \rangle = \text{Tr}(\hat{p}\hat{H}) \) remains a constant of the motion:

\[
\langle \hat{H} \rangle = B\langle \hat{q}_{z} \rangle + Cg\langle \hat{q}_{x} \rangle + \frac{p^{2}}{2m} + D\frac{q^{4}}{4} - F\frac{q^{2}}{2}. \tag{22}
\]

From eq. (22) it is possible to obtain the equations of motion for the classical variables \( p \) and \( q \) (see eqs (9) and (10)), according to the classical mechanics prescription given by eq. (5).

2. **The UP**: In Refs [12, 26, 27] we have derived an expression for the generalized UP which must be fulfilled by a set of relevant operators closing a partial semi-Lie algebra under commutation with the system’s Hamiltonian, via the closure condition given by eq. (3) (we briefly outline the procedure in appendix A). We have already stated the conditions for constancy of the motion. In the SU(2) Lie algebra case, this invariant, \( \langle \dot{\hat{p}} \rangle^{2} \), acquires the form:

\[
0 < \langle \dot{\hat{q}}_{x} \rangle^{2} + \langle \dot{\hat{q}}_{y} \rangle^{2} + \langle \dot{\hat{q}}_{z} \rangle^{2} < 1, \tag{23}
\]

defining the well-known Bloch sphere of the system \( \langle \dot{\hat{p}} \rangle^{2} = \langle \dot{\hat{q}}_{x} \rangle^{2} + \langle \dot{\hat{q}}_{y} \rangle^{2} + \langle \dot{\hat{q}}_{z} \rangle^{2} \). This invariant can only adopt values belonging to the interval \((0, 1]\). As we previously stated, these two invariants are very useful to choose the system’s initial conditions without violating neither energy constancy nor uncertainty. Our invariants also help in dealing with the nonlinear semiquantum system given by eqs (6)–(10).

### 3. Numerical simulations and results

Several numerical simulations were performed to study how the TP \( p_{0} \) and \( p_{1} \) (for ‘the same’ initial conditions) evolve in time, combining different values of the coupling strength, \( C \), and the UP-invariant, \( \langle \dot{\hat{p}} \rangle \). We wish to highlight the roles of these parameters while analyzing our results. The energy values in eq. (22), and the rest of the parameters’ values in eqs (6)–(10), remain fixed throughout all our simulations.

We set: \( \langle H \rangle = 1.1, m = 1, B = 2, D = 5.1822658, \) and \( F = 7.4624624, \) and consider five different values for \( C: 0.1, 0.5, 1, 5 \) and 10, chosen so that, at least, two orders of magnitude of the coupling strength are encompassed. Thus, five graphs are displayed corresponding to all these \( C \)-value. Each figure exhibits the following:

(a) a Poincaré surface of section in classical variables, \( q \) and \( p \), for the hyperplane \( \langle \hat{q}_{z} \rangle = 0 \);

(b) a Poincaré surface of section in quantum variables, \( \langle \hat{q}_{x} \rangle, \langle \hat{q}_{y} \rangle \) and \( \langle \hat{q}_{z} \rangle \) (Bloch sphere), for the hyperplane \( p = 0 \); and

(c) the time evolution for the TP \( p_{0} \) and \( p_{1} \).

At a given time, each sub-figure is divided into six panels, labeled: I–VI, according to six decreasing values of \( \langle \dot{\hat{p}} \rangle \) belonging to the validity interval \((0, 1]\).

For each \( \langle \dot{\hat{p}} \rangle \)-value, the initial conditions \( \{ \langle \hat{q}_{x} \rangle_{0}, \langle \hat{q}_{y} \rangle_{0}, \langle \hat{q}_{z} \rangle_{0}, q_{0}, p_{0} \} \) are used so as to describe the situation. They are the same in all the cases, which entails that the quantum coordinates are located at unvarying places on the pertinent Bloch sphere. This entails setting:

\[
\langle \hat{q}_{x} \rangle_{0} = \langle \hat{q}_{y} \rangle_{0} = \langle \hat{q}_{z} \rangle_{0} = \langle \hat{p} \rangle / \sqrt{3}. \tag{24}
\]

The remaining initial coordinates are \( q_{0} = -0.5 \), while \( p_{0} \) is obtained from the energy conservation condition of eq. (22). Thus, for the six panels one has

<table>
<thead>
<tr>
<th>Panel</th>
<th>( \langle \dot{\hat{p}} \rangle )</th>
<th>( \langle \hat{q}_{x} \rangle )</th>
<th>( \langle \hat{q}_{y} \rangle )</th>
<th>( \langle \hat{q}_{z} \rangle )</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>( 0.99 )</td>
<td>( 0.5715767, i = x, y, z )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>II</td>
<td>( 0.80 )</td>
<td>( 0.4618802, i = x, y, z )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>III</td>
<td>( 0.60 )</td>
<td>( 0.3464101, i = x, y, z )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IV</td>
<td>( 0.40 )</td>
<td>( 0.3041143, i = x, y, z )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>( 0.20 )</td>
<td>( 0.11547, i = x, y, z )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VI</td>
<td>( 0.01 )</td>
<td>( 5.7735 \times 10^{-3}, i = x, y, z )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The first thing to be observed in figures 1–5 is that the system described by eqs (6)–(10) may display both chaotic and regular dynamics.

Although we use only one initial condition in each panel, we claim that, for \( \langle \dot{\hat{p}} \rangle \)-values close to 1, the system presents a higher degree of chaoticity than for \( \langle \dot{\hat{p}} \rangle \)-values in the vicinity of 0. This means that, in the first situation, a greater portion of the phase space is occupied by chaotic orbits compared to the periodic ones’ portion. When \( \langle \dot{\hat{p}} \rangle \) is close to 0, the situation is the opposite one.

Secondly, confronting the Poincaré sections in the classical and quantum variables (figures 1–5a and b), one appreciates the strong correlation between the two subsystems, since chaotic or periodic motion in one subsystem corresponds to similar motion in the other.
Figure 1. The coupling strength is $C = 0.1$, and the UP-invariant values listed in the panels are as follows: (I) $\langle \hat{\sigma} \rangle = 0.99$; (II) $\langle \hat{\sigma} \rangle = 0.8$; (III) $\langle \hat{\sigma} \rangle = 0.6$; (IV) $\langle \hat{\sigma} \rangle = 0.4$; (V) $\langle \hat{\sigma} \rangle = 0.2$; (VI) $\langle \hat{\sigma} \rangle = 0.01$. (a) Poincaré’s surface of section in the classical variables $p$ vs $q$ for the hyperplane $\langle \hat{\sigma} \rangle = 0$. (b) Poincaré’s surface of section in the quantum variables $\langle \hat{\sigma}_x \rangle$, $\langle \hat{\sigma}_y \rangle$, $\langle \hat{\sigma}_z \rangle$ for the hyperplane $p = 0$. (c) Time series for the probability transitions $P_0(t)$ (blue) and $P_1(t)$ (red).

Figure 2. The coupling strength is $C = 0.5$, and the UP-invariant values listed in the panels are as follows: (I) $\langle \hat{\sigma} \rangle = 0.99$; (II) $\langle \hat{\sigma} \rangle = 0.8$; (III) $\langle \hat{\sigma} \rangle = 0.6$; (IV) $\langle \hat{\sigma} \rangle = 0.4$; (V) $\langle \hat{\sigma} \rangle = 0.2$; (VI) $\langle \hat{\sigma} \rangle = 0.01$. (a) Poincaré’s surface of section in the classical variables $p$ vs $q$ for the hyperplane $\langle \hat{\sigma} \rangle = 0$. (b) Poincaré’s surface of section in the quantum variables $\langle \hat{\sigma}_x \rangle$, $\langle \hat{\sigma}_y \rangle$, $\langle \hat{\sigma}_z \rangle$ for the hyperplane $p = 0$. (c) Time series of the probability transitions $P_0(t)$ (blue) and $P_1(t)$ (red).

(as it was already reported in [12]). It is worth noting that this correlation does not depend on the magnitude of the coupling strength ($C$). However, this magnitude is related to the portion of space into which a chaotic orbit spreads. To confirm this assertion look at the increasing dotted area in both the $(p, q)$ Poincaré surface and in the Bloch sphere. See, for example, panel I of sub-figures (a) and (b). Not only the chaotic dynamics is influenced
Figure 3. The coupling strength is $C = 1$, and the UP-invariant values in the panels are as follows: 

- (I) $\langle \hat{\sigma} \rangle = 0.99$; 
- (II) $\langle \hat{\sigma} \rangle = 0.8$; 
- (III) $\langle \hat{\sigma} \rangle = 0.6$; 
- (IV) $\langle \hat{\sigma} \rangle = 0.4$; 
- (V) $\langle \hat{\sigma} \rangle = 0.2$; 
- (VI) $\langle \hat{\sigma} \rangle = 0.01$.

(a) Classical variables: $q, p$ 
(b) Quantum variables: $\langle \hat{\sigma}_y \rangle, \langle \hat{\sigma}_x \rangle, \langle \hat{\sigma}_z \rangle$ 
(c) Transition probabilities: $P_0, P_1$

by the value of $C$, but also the regular one, in the sense that, for higher values of $C$, more sophisticated patterns emerge as it may be appreciated in panels IV and V of figures 2a and b. There is always a peculiar relation

Figure 4. The coupling strength is $C = 5$, and the UP-invariant values listed in the panels are as follows: 

- (I) $\langle \hat{\sigma} \rangle = 0.99$; 
- (II) $\langle \hat{\sigma} \rangle = 0.8$; 
- (III) $\langle \hat{\sigma} \rangle = 0.6$; 
- (IV) $\langle \hat{\sigma} \rangle = 0.4$; 
- (V) $\langle \hat{\sigma} \rangle = 0.2$; 
- (VI) $\langle \hat{\sigma} \rangle = 0.01$.

(a) Poincaré’s surface of section in the classical variables $p$ vs $q$ for the hyperplane $\langle \hat{\sigma}_y \rangle = 0$. 
(b) Poincaré’s surface of section in the quantum variables $\langle \hat{\sigma}_x \rangle, \langle \hat{\sigma}_y \rangle, \langle \hat{\sigma}_z \rangle$ for the hyperplane $p = 0$. 
(c) Time series for the probability transitions $P_0(t)$ (blue) and $P_1(t)$ (red).

between the magnitudes of $C$ and $\langle \hat{\sigma} \rangle$ for the system to exhibit chaotic motions. No matter how large the $C$-value is, a value of $\langle \hat{\sigma} \rangle$ close to 0 ends up impeding the possibility of chaotic dynamics.
The probability transitions \( \langle \sigma \rangle \) in the classical variables and \( \langle \sigma \rangle \) in the quantum variables for the hyperplane \( p = 0 \). We analyze the different behavior of the temporal evolution of the TP, \( P_0(t) \) and \( P_1(t) \) according to the value of both, \( C \) and value of the UP-invariant \( \langle \bar{\sigma} \rangle \). This happens via normalization \((P_0(t) + P_1(t) = 1)\) for any time \( t \), as expected.

Looking at figures 1c–5c, related to time evolution of \( P_0(t) \) (blue color) and \( P_1(t) \) (red color), we see that in the first three (figures 1c–3c), the signals in each panel exhibit an oscillatory form that reflects on the type of motion displayed by the orbit of the same initial condition, as it is seen in the same panel of the corresponding sub-figures (a) and (b). That is, chaotic, quasi-periodic, and periodic orbits correspond to chaotic, quasi-periodic and periodic waveforms of the TP signals, respectively. However, striking differences among the regimes are to be observed when \( C \) grows and the \( \langle \bar{\sigma} \rangle \)-value decreases. This fact is not so clear in the last two graphs (figures 4c and 5c), where the width of the amplitudes of the oscillation ranges of the signals seem to be the only visible difference among them.

We claim that the features described below do not depend on the signal’s sampling length so that a short time window (10 ≤ Δt ≤ 50) is used. Also, we enlarge the ordinate axis in all the panels labeled with VI, for clarity’s sake.

Consider now figure 1c for \( C = 0.1 \). One sees that the oscillation amplitudes’ intervals of both time series are well separated: the \( P_0(t) \) values are always larger than the \( P_1(t) \) values. This fact seems to be independent of (1) the UP-value \( \langle \bar{\sigma} \rangle \) and (2) whether the orbit generated by the chosen initial condition is chaotic (panels I and II) or regular one (panels III–VI).

Pass now to figure 2c. For \( C = 0.5 \) one sees that the ranges of oscillation-amplitudes for both series begin to spread, with their widths, related to \( \langle \bar{\sigma} \rangle \), becoming smaller and smaller as \( \langle \bar{\sigma} \rangle \rightarrow 0 \). It is also seen that the amplitude-ranges approach each other, and the number of oscillations within any sub-interval \( \Delta t \) grows compared to the case depicted in figure 1c.

In figure 3c, the value of the coupling parameter is increased to \( C = 1 \). The oscillations’ rapidity increases compared to those of the previous two figures. It is observed that \( P_0(t) \) reaches values close to 1, and symmetrically, \( P_1(t) \) approaches 0, for \( \langle \bar{\sigma} \rangle \rightarrow 1 \). The amplitude ranges of both signals overlap more and more in this process. In all panels one sees that the number of times the signals cross each other also increases both for chaotic and regular orbits. The mean of the crosses are approximately the same in both regimes, but the \( t \)-values where they take place come in a regular fashion for periodic orbits, as expected.

The situation in figures 4c and 5c, where \( C = 5 \) and \( C = 10 \), respectively, is very different. The oscillation amplitudes-ranges coincide in all cases, the overlap is almost unity, and this happens regardless of the value.
of \( \langle \hat{\sigma} \rangle \). The signals display rapid oscillations so that a shorter time window \( (\Delta t = 10) \) must be taken in order for them to be appreciated, even if \( \mathcal{P}_1(t) \) values approach unity and \( \mathcal{P}_0(t) \) values tend to 0. For these \( C \)-values it is already difficult to distinguish if the signal is chaotic or not.

We note that the last two \( C \)-values considered become very large compared to the rest of the parameter’s values. This fact is even more noticeable for \( C = 10 \) (figure 5c), where an over-coupling of the two subsystems occurs, leading to a situation in which the characteristics mentioned above become accentuated.

4. Conclusions

As previously stated, the nonlinear coupling between the 1/2 spin (in the presence of a constant magnetic field) and the potential generated by a CP, forces the spin to make transitions between its two states ‘up’ \((|0\rangle)\) and ‘down’ \((|1\rangle)\). The TP \( \mathcal{P}_0(t) \) and \( \mathcal{P}_1(t) \) depend upon the time evolution of the \( \hat{\sigma}_z \) spin component’s mean value.

We study the influence, on the \( \mathcal{P}_0(t) \) and \( \mathcal{P}_1(t) \) TP associated time series, of varying the values of two of the system parameters: (1) the coupling constant, \( C \), between the classical and quantum subsystems and (2) the UP-invariant, \( \langle \hat{\sigma} \rangle \).

We observe that for a weak coupling (small \( C \)-values), the oscillation amplitudes intervals’ ranges never overlap while for strong coupling (large \( C \)-values) they always overlap, regardless of whether the system exhibits chaos or not, and regardless of the value of \( \langle \hat{\sigma} \rangle \).

\( \langle \hat{\sigma} \rangle \) mainly influences the amplitude of the TP-probabilities \( \mathcal{P}_0 \) and \( \mathcal{P}_1 \) signals. When the systems behaves in a more classical way (\( \langle \hat{\sigma} \rangle \) tends to 0), the ranges of the oscillation amplitudes drastically decrease, and the TP-values are close to 0.5.

An exhaustive analysis of the time series for the TP \( \mathcal{P}_0(t) \) and \( \mathcal{P}_1(t) \) with the entropy-complexity plane methodology developed in Ref. [33] would be desirable when designing nanotechnological devices and quantum gates in quantum computing.

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Appendix A

A.1 The MEP tools

When describing the quantum state of a system, it is common to resort to the density operator \( \hat{\rho} \). The MEP seeks to find the statistical operator that maximizes entropy \( S \):

\[
S = - \text{Tr} (\hat{\rho} \ln \hat{\rho}),
\]

(A.1)

consistent with a set of given constraints [28]. That is, the statistical operator that allows the system to evolve from a state of maximum entropy to another state of maximum entropy. The set of constraints are generally given by the knowledge of the expectation values of certain operators which are known at the instant \( t = 0 \) as [28]:

\[
\langle \hat{O}_i \rangle = - \text{Tr} (\hat{\rho} \hat{O}_i), \quad i = 0, \ldots, N
\]

(A.2)

(where \( \hat{O}_0 = \hat{I} \) is the identity operator which must be included in the set in order to fulfill the normalization condition \( \text{Tr} (\hat{\rho}) = 1 \)). As demonstrated in [28], the entropy \( S \) remains a constant of motion if the statistical operator \( \hat{\rho} \) is an exact solution of the equation of motion:

\[
\frac{\partial (\ln \hat{\rho})}{\partial t} = \frac{1}{\hbar} \left[ \hat{H}, \ln \hat{\rho} \right],
\]

(A.3)

where \( \hat{H} \) is the system’s Hamiltonian. The constraints required to specify the MEP statistical operator are expressed in the usual way:

\[
\ln \hat{\rho} = - \sum_{i=0}^{N} \lambda_i(t) \hat{O}_i = - \lambda_0 - \sum_{i=1}^{N} \lambda_i(t) \hat{O}_i,
\]

(A.4)

where \( \lambda_0 \) is the Lagrange multiplier associated with the identity operator \( \hat{I} \) and \( \hat{O}_i \) are the operators belonging to the initial set given by eq. (A.2). If we insert eq. (A.4) into eq. (A.3), we obtain:

\[
\sum_{i=1}^{N} \frac{\partial \lambda_i(t)}{\partial t} \hat{O}_i = \frac{1}{\hbar} \sum_{i=1}^{N} \lambda_i(t) [\hat{H}, \hat{O}_i].
\]

(A.5)

Equation (A.5) means that it is possible to exactly solve the evolution eq. (A.3) if and only if the condition:

\[
[\hat{H}, \hat{O}_i] = i\hbar \sum_{r=0}^{N} g_{ri} \hat{O}_r
\]

(A.6)

is fulfilled, where \( g_{ri} \) are coefficients which may depend upon time if the Hamiltonian \( \hat{H} \) is time-dependent.

Finally, inserting eq. (A.6) into eq. (A.5), we obtain (taking into account that the set \( \{ \hat{I}, \hat{O}_1, \hat{O}_2, \ldots, \hat{O}_N \} \) is a linearly independent one):

\[
\frac{\partial \lambda_i}{\partial t} = \sum_{r=0}^{N} g_{ir} \lambda_r, \quad i = 1, \ldots, N.
\]

(A.7)

So, the evolution equation for the density operator (A.3) has turned into a system of coupled differential equations for the Lagrange multipliers associated with the constraints given by eq. (A.2).
Summing up, eq. (A.6) is the well-known closure condition derived in Ref. [28] and it is our eq. (3). When the closure condition is fulfilled (it is to say, when it is possible to close a semi-Lie algebra under commutation operation with the system’s Hamiltonian) it happens that:

(i) The system’s entropy remains a constant of motion.

(ii) The MEP density operator which makes the system to evolve from one maximum entropy state to another maximum entropy state acquires the following form for all instant:

$$\hat{\rho} = \exp \left( -\lambda_0 - \sum_{i=1}^{N} \lambda_i(t) \hat{O}_i \right). \quad (A.8)$$

(iii) The evolution equation for the density operator given by eq. (A.3), has been converted into the set of coupled differential equations for the Lagrange multipliers given by eq. (A.7).

Finally we pose, what about if it is not possible to close the algebra with the set of constraints we initially know? In this case, we must follow the prescription given in Ref. [28]: we should add as many operators as necessary in order to make the closure condition fulfill.

**A.2. The generalized UP**

It is known that for a given set of, say $N$ non-commuting observable $\{\hat{O}_1, \hat{O}_2, \ldots, \hat{O}_N\}$, they fulfill between two of them the uncertainty relation [26]:

$$\left(\Delta \hat{O}_i\right)^2 \left(\Delta \hat{O}_j\right)^2 - \left[ \langle \hat{L}_{ij} \rangle - \langle \hat{O}_i \rangle \langle \hat{O}_j \rangle \right]^2 \geq -\frac{1}{4} \left( [\hat{O}_i, \hat{O}_j] \right)^2, \quad (A.9)$$

with $\left(\Delta \hat{O}_i\right)^2 = \langle \hat{O}_i^2 \rangle - \langle \hat{O}_i \rangle^2$ and $\langle \hat{L}_{ij} \rangle = \frac{1}{2} \langle \hat{O}_i \hat{O}_j + \hat{O}_j \hat{O}_i \rangle$. If we perform the summation over the whole possible pairs of observables belonging to the set we obtain [26]

$$\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left[ \left(\Delta \hat{O}_i\right)^2 \left(\Delta \hat{O}_j\right)^2 - \left[ \langle \hat{L}_{ij} \rangle - \langle \hat{O}_i \rangle \langle \hat{O}_j \rangle \right]^2 \right] \geq -\frac{1}{4} \sum_{i=1}^{N} \sum_{j=1}^{N} \left( [\hat{O}_i, \hat{O}_j] \right)^2, \quad i \neq j. \quad (A.10)$$

Equation (A.10) is the generalized uncertainty relation principle of Ref. [26]. Now, if we define for $i \neq j$:

$$I = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left[ \left(\Delta \hat{O}_i\right)^2 \left(\Delta \hat{O}_j\right)^2 - \left[ \langle \hat{L}_{ij} \rangle - \langle \hat{O}_i \rangle \langle \hat{O}_j \rangle \right]^2 \right], \quad (A.11)$$

it is possible to demonstrate (with the help of the closure condition given by eq. (A.6)) that the quantity $I$ given by eq. (A.11) is a constant of the motion, i.e. $\frac{dI}{dt} = 0$ (interested readers can see the proof in Ref. [26]).

It is also possible to demonstrate that, when the set of non-commuting observable is composed by the generators of the SU(2) Lie algebra $\{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$, eq. (A.10) adopts the simple form [12, 26]:

$$I = 3 - 2 \left[ \langle \hat{\sigma}_x \rangle^2 + \langle \hat{\sigma}_y \rangle^2 + \langle \hat{\sigma}_z \rangle^2 \right] \geq \langle \hat{\sigma}_x \rangle^2 + \langle \hat{\sigma}_y \rangle^2 + \langle \hat{\sigma}_z \rangle^2. \quad (A.12)$$

If we call $\langle \hat{\sigma}^2 \rangle = \langle \hat{\sigma}_x \rangle^2 + \langle \hat{\sigma}_y \rangle^2 + \langle \hat{\sigma}_z \rangle^2$, then eq. (A.12) leads to the well-known definition of the Bloch sphere:

$$\langle \hat{\sigma}^2 \rangle = \langle \hat{\sigma}_x \rangle^2 + \langle \hat{\sigma}_y \rangle^2 + \langle \hat{\sigma}_z \rangle^2 < 1. \quad (A.13)$$

In Ref. [12], we have justified why in eq. (A.13) the equal sign cannot be valid.

**References**


