A new proposal of Hamiltonians to explain quantum effects

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Abstract: To study the Slonczewski Spin Transfer Torque Effect in the quantum limit, a new model of Hamiltonian is needed. In recent years, it has been found that the requirement of Hermitian Hamiltonians can be replaced by a weaker condition that is the $\mathcal{PT}$ symmetry. This new theory allows a whole new branch of Hamiltonians to be accepted by the quantum theory. It is believed that these Hamiltonians could help to explain unstable systems and dissipative effects. This work aims to study a purposed $\mathcal{PT}$ symmetric Hamiltonian, which explains the Slonczewski STT effect, to see whether the rules of Quantum Mechanics can be applied or not.

I. INTRODUCTION

It is a well known fact that Quantum Mechanics is based on various postulates that cannot be proved. In spite of this, the postulates have been tested many times in diverse experiments that are considered to be unquestionable.

However, this view is challenged by many studies that received little attention until recently such as [5]. These studies state that the condition of self-adjointness can be replaced by the weaker condition of $\mathcal{PT}$ symmetry. Considering this, one can obtain new forms of Hamiltonians whose spectra is real for some parameters.

New results show that non-Hermitian $\mathcal{PT}$ symmetric Hamiltonians have two different regimes. The first is the regime of unbroken symmetry, where all the eigenvalues of the Hamiltonian are real. However, $\mathcal{PT}$ symmetric Hamiltonian eventually breaks the $\mathcal{PT}$ symmetry regime and some eigenvalues of the Hamiltonian become complex. The understanding of the transition between these two regimes is very important for the understanding of many instabilities.

The non-Hermitian Hamiltonians are $\mathcal{PT}$ symmetric, and, therefore they are invariant under the simultaneous action of parity and time reversal ($\vec{x} \to -\vec{x}, t \to -t, i \to -i$). This is due to the $\mathcal{PT}$ symmetric Hamiltonians commute with the antilinear operator $\mathcal{PT}$ and because of it, their eigenvalues are guaranteed to appear in complex conjugate pairs.

In this work the focus is placed on the description of Slonczewski Spin Transfer Torque, using a $\mathcal{PT}$ symmetric Hamiltonian provided by [1], who discuss the effect of the Hamiltonian in the limit of large spin. Instead of the limit of large spins, we focus on the Quantum Mechanics involved with the Hamiltonian. First, it is questioned whether it is possible or not for a particle to tunnel, and if in this case the perturbation theory would work. In addition, we tried to find the probability of transition using the instanton model [4], but we found unexpected results that until now we have not been able to explain. Later, a possible interpretation for the complex spectrum is presented, though we lack of experimental results to see if it is correct. Finally, the correspondence between the results obtained and the results found for the limit of large spin [1] are studied.

At the beginning the aim of this study was to compute the dissipation effect that would emerge from a Hamiltonian $H = \frac{-k_z S_z^2 + k_x S_x^2}{1 - i\alpha}$, which is the same transformation used in [1]. However, we found it really difficult to transform the Hamiltonian H to a $\mathcal{PT}$ symmetric one, and thus the topic was modified and it became the explained previously.

II. MODEL

This study wants to find a model for the quantum behaviour of the Slonczewski Spin Transfer Torque. A simple setup preparation for this experiment is a ferromagnetic cylinder placed on a magnetic field H; the direction of H is considered to be in the x axis. Then, an electric current J is polarized in the direction y, which passes through a non-magnetic metallic spacer and induces torque.

To describe this mechanism a non-Hermitian Hamiltonian for a single spin operator is introduced

$$\mathcal{H} = \frac{-k_z S_z^2 + H_x S_x + ijS_y}{1 - i\alpha} \tag{1}$$

where the anisotropy term has been restricted to the second order for simplicity, jS is considered to be the spin-angular momentum deposited per second in the direction S_y and $\alpha > 0$ a phenomenological constant.

In the limit of small α and taking the spin polarized current $j = \gamma H_0 \beta$, the Hamiltonian (1) can be transformed into the following $\mathcal{PT}$ symmetric Hamiltonian,

$$\mathcal{H}_{\mathcal{PT}} = \gamma H_0(-k_z S_z^2 + h_x S_x + i\beta S_y), \tag{2}$$

where h_x is the applied magnetic field measured in units of some characteristic magnetic field H_0 and β is a di-

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mensionless Spin Transfer Torque parameter, determining (relative to S) the amount of angular momentum transferred on time ($\tau = (\gamma H_0)^{-1}$).

III. TUNNEL SPLITTING

The aim of this section is to find a way to perform a perturbation theory for a $\mathcal{PT}$ symmetric Hamiltonian and to explore if it is in accordance with the diagonalization of the matrix associated to it. To do so, all the steps of the perturbation theory will be applied consecutively and we will realize where the corrections should be done.

If we consider the Hamiltonian expressed in equation (2) provided by [1], since the S_z does not commute with the Hamiltonian, it is to be expected that m is no longer a conserved quantum number. Therefore, the magnetic moment of a nanoparticle initially put in a state m can now tunnel. We know that this happens for a Hermitian Hamiltonian, and we want to test it for a $\mathcal{PT}$ symmetric one and see if it is in accordance with the results of perturbation theory.

If we take $h_x = 0$ and small β, the problem of tunnelling between m and $-m$ becomes a two-state problem whose solution using perturbation theory [3] is well known. In this case and for a large variety of spins ($S = 1, 2, 3, 4, 5, 6, 7, 8$), it has been found that the eigenvectors of the equation (2) allow tunnelling between the states m and $-m$.

The resulting Hamiltonian is $\mathcal{H}_{\mathcal{PT}} = \gamma H_0(-k_z S_z^2 + i\beta S_y)$. The tunnelling splits the degenerate levels in $\varepsilon_{m,\pm} = \varepsilon_m \pm \frac{\Delta}{2}$, with its correspondent eigenstates $\psi_{m,\pm} = \frac{1}{\sqrt{2}}(|m\rangle \mp |-m\rangle)$. Then, if we take into account that $S_y = \frac{1}{2i}(S_+ - S_-)$, the Hamiltonian becomes $\mathcal{H}_{\mathcal{PT}} = \gamma H_0(-k_z S_z^2 + \frac{\beta}{2}(S_+ - S_-))$. The Δ_m can now be computed with the $2|m|$-th order of the perturbation theory,

$$\Delta_m = 2V_{m,m+1}\frac{1}{\varepsilon_{m+1} - \varepsilon_m}V_{m+1,m+2}\cdots V_{-m-1,-m}, \quad (3)$$

where Δ is the tunnel splitting, ε_m is the unperturbed energy of the m-th level and $V_{m,m+1} = |\langle m|i\beta S_y|m+1\rangle|$ that fulfils,

$$V_{m,m+1} = V_{m+1,m} = \frac{\beta}{2}\sqrt{S(S+1) - m(m+1)}. \quad (4)$$

Here, it should be noticed that the expression for a Hermitian Hamiltonian is $V_{m,m+1} = \langle m|i\beta S_y|m+1\rangle$, though in our case, in order to correct the theory for the $\mathcal{PT}$ symmetry an absolute value is needed.

Therefore, with the substitution and some arrangements, it is found the following expression for the tunnel splitting Δ_m considering $m < 0$,

$$\Delta_m = \frac{2k_z\gamma H_0}{((-2m-1)!)^2}\frac{(S-m)!}{(S+m)!}\left(\frac{\beta}{2k_z}\right)^{2|m|} \quad (5)$$

if $\beta = k_z\beta'$, then we get the following expression.

$$\frac{\Delta_m}{k_z\gamma H_0} = \frac{2}{((-2m-1)!)^2}\frac{(S-m)!}{(S+m)!}\left(\frac{\beta'}{2}\right)^{2|m|} \quad (6)$$

Now, to see if it gives a good approximation to the real tunnel splitting, the matrix associated to $\mathcal{H}_{PT}$ should be diagonalized in order to confirm if the tunnel splitting resembles with the energy levels.

Supposing the work is done with nanoparticles with spin S, then the energy levels will be $\varepsilon_1, \ldots, \varepsilon_{2S+1}$, but these will be paired two by two excepting one of them. To find the tunnel splitting of these paired energy values ($\Delta_{d,m}$),

$$\Delta_{d,m} = |\varepsilon_i - \varepsilon_j|, \quad (7)$$

supposing that the energy i and j are paired.

$\lvert m \rvert$	Δ_m	$\Delta_{d,m}$	e
5	$5.38228 \cdot 10^{-18}$	$5.38428 \cdot 10^{-18}$	$2.0026 \cdot 10^{-21}$
4	$1.11607 \cdot 10^{-12}$	$1.11555 \cdot 10^{-12}$	$5.1900 \cdot 10^{-16}$
3	$4.375 \cdot 10^{-8}$	$4.38365 \cdot 10^{-8}$	$8.646 \cdot 10^{-11}$
2	$2.9167 \cdot 10^{-4}$	$2.94016 \cdot 10^{-4}$	$2.346 \cdot 10^{-6}$
1	$1.5 \cdot 10^{-1}$	$1.788 \cdot 10^{-1}$	$2.88 \cdot 10^{-2}$

TABLE I: Perturbation tunnel splitting, Diagonalized tunnel splitting, and absolute error for $S = 5$ and $\beta = 0.1k_z$.

The results of TABLE I have been obtained using Wolfram Mathematica 11.2 for the diagonalization of the matrix, and considering nanoparticles with spin $S = 5$ and a current $\beta = 0.1k_z$. As it can be seen, the perturbation results predict correctly the tunnel splitting for large $|m|$, and the error increases for smaller $|m|$ as it was expected.

The same calculations have been run for larger S and the results are the same, having great accordance with the perturbation theory.

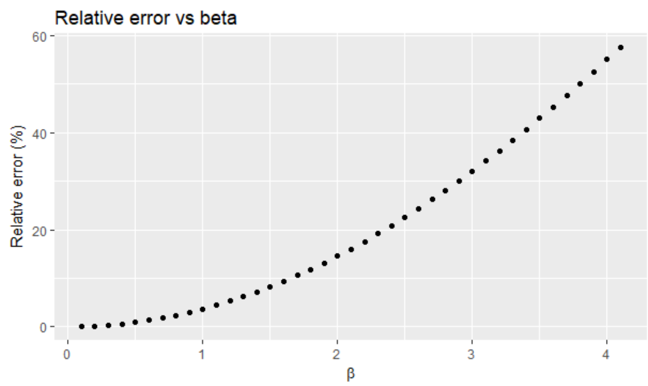

FIG. 1: Relative error of using the perturbation theory instead of the diagonalization of the Hamiltonian (2) for $h_x = 0$, $S = 5$, considering $\beta = \beta' k_z$ and the tunnel slpitting is measured using $|m| = 5$, Δ_{-5}.

In figure 1 can be seen the relative error of Δ_{-5} in function of β considering $h_x = 0$, and $S = 5$.

As it was expected, the perturbation theory reproduces the results very well for small β, but when β is increased it fails in describing the value of the tunnel splitting. That result is the same that should be expected from the usual quantum theory.

IV. ENERGY SPECTRUM

One of the interesting facts of the $\mathcal{PT}$ symmetric Hamiltonians is that it has been proved that they allow to study dissipative effects and dynamic phase transitions out of equilibrium systems in the continuous approximation.

The aim of this section is to develop a few quantum tools to use during the symmetry breaking and see if they are in agreement with the results of [1] and the behaviour of a Slonczewski Spin Transfer Torque (STT) effect.

A. Finding complex Energy values

As it has been seen in the previous section that, considering once again the $\mathcal{PT}$ symmetric Hamiltonian on [1] for small β all the energy spectrum is real. Thus, it is in clear correspondence with the usual Quantum Theory [2]. However, when the current β is increased above certain value, a pair of complex conjugate energies appears in the energy spectrum.

$$\begin{cases} \varepsilon_1 = -1 \\ \varepsilon_2 = -0.5 + 0.33166i \\ \varepsilon_3 = -0.5 - 0.33166i \end{cases} \tag{8}$$

In example (8) the energy spectrum for the $\frac{\mathcal{H}_{\mathcal{PT}}}{\gamma H_0 k_z} = -S_z^2 + h'_x S_x + i\beta' S_y$, where $h_x = 0$, $\beta = 0.6k_z$ and $S = 1$ can be seen.

It can also be seen that the complex spectrum is paired with complex conjugates. Moreover, it is easy to see that all the complex eigenvalues will be paired complex conjugates. The Hamiltonian in [1] can be rewritten as $\frac{\mathcal{H}_{\mathcal{PT}}}{\gamma H_0 k_z} = -S_z^2 + h'_x S_x + \frac{\beta'}{2}(S_+ - S_-)$, and this ensures that all the coefficients in the associated matrix will be real and the characteristic polynomial will have real coefficients. That is, the only way to have complex roots is if they come as paired complex conjugates.

It is reasonable to wonder whether there is a complex energy spectrum of all S or there are some nanoparticles with a concrete spin that does not allow the spectrum to become complex. This study has numerically analysed particles of spin $S = \frac{1}{2}, 1, 2, 3, 4, 5, 6, 7, 8$ and all of them developed a complex energy spectrum. Moreover, the study [1] considers a spin $S \longrightarrow \infty$ and it also finds complex eigenvalues. So there is no evidence that supports the theory that for certain spins there are no complex eigenvalues.

Another interesting question is whether when β increases there are new pairs of complex energy appear or the system only develops a pair of them. The answer is that all the systems analysed develop new pairs of complex energy levels with increasing β. The results of the Hamiltonian (2) with $h_x = 0$ and increasing β for $S = 3$ can be found in table II.

	$\beta'_1 = 0.2$	$\beta'_2 = 0.3$	$\beta'_3 = 1.5$	$\beta'_4 = 3$
ε_1	-8.989	-8.973	-8.338	$-1.22 + 8.57i$
ε_2	-8.989	-8.973	-8.318	$-1.22 - 8.57i$
ε_3	-3.979	-3.953	$-0.96 + 4.01i$	-7.000
ε_4	-3.978	-3.950	$-0.96 - 4.01i$	$-3.50 + 4.87i$
ε_5	-1.033	-1.076	-3.758	$-3.50 - 4.87i$
ε_6	-0.674	$-0.53 + 0.51i$	$-2.83 + 1.67i$	$-5.77 + 1.51i$
ε_7	-0.359	$-0.53 - 0.51i$	$-2.83 - 1.67i$	$-5.77 - 1.51i$

TABLE II: Energy spectrum of the Hamiltonian (2) with $S = 3$, $h_x = 0$ and different $\beta = \beta' k_z$.

Another property that must be taken into account is that for $S \in \mathbb{N}$ there has to be a real energy value, due to there are $2S + 1$ different values, and the complex values must be paired.

The next steps provide an interpretation on these complex energy values.

B. Interpretation of the Energy Spectrum

It is known from the Shröndinguer equation [2], that if the Hamiltonian is time independent, then exists the following time evolution operator

$$U(t) = e^{\frac{iHt}{\hbar}} \tag{9}$$

In this study, the time evolution operator is used with a complex energy spectrum. This leads either to an increase or a decrease of the probability of finding the particle in certain states.

Considering a nanoparticle with spin S, $|\psi'_1\rangle, \ldots, |\psi'_{2S+1}\rangle$ the eigenvectors of the Hamiltonian (2) for a given β and supposing there is only a pair of complex eigenvalues which are $\varepsilon_{2S} = a + bi$ and $\varepsilon_{2S+1} = a - bi$ and a normalized initial state $|\psi\rangle(0) = \sum_{i=1}^{2S+1} c_i |\psi'_i\rangle$, with $\sum_{i=1}^{2S+1} |c_i|^2 = 1$, the usual time evolution operator leads to the following expression,

$$|\psi\rangle(t) = \sum_{i=1}^{2S+1} c_i e^{\frac{-i\varepsilon_i t}{\hbar}} |\psi'_i\rangle \tag{10}$$

which is clearly not normalized, since

$$|\psi\rangle(t) = \sum_{i=1}^{2S-1} c_i e^{\frac{-i\varepsilon_i t}{\hbar}} |\psi'_i\rangle + c_{2S} e^{\frac{-iat+bt}{\hbar}} |\psi'_{2S}\rangle + c_{2S+1} e^{\frac{-iat-bt}{\hbar}} |\psi'_{2S}\rangle \tag{11}$$

If this expression is expected to have a physic interpretation, $|\psi\rangle(t)$ must be renormalized after the application of the time evolution operator. This is new and it is only needed in the non-Hermitian $\mathcal{PT}$ symmetric Hamiltonian due to in the Hermitian ones the function is still normalized after the application of the time evolution operator. To express $|\psi\rangle(t)$ with compact notation, the sum from $i = 1$ to $i = 2S + 1$ will be used, but it is important to bear in mind that for $i = 2S$ and $i = 2S + 1$ there is a real term in the exponential.

$$|\psi\rangle(t) = \frac{\sum_{i=1}^{2S+1} c_i e^{\frac{-i\varepsilon_i t}{\hbar}} |\psi_i'\rangle}{\sqrt{1 + (e^{\frac{2bt}{\hbar}} - 1)|c_{2S}|^2 + (e^{\frac{-2bt}{\hbar}} - 1)|c_{2S+1}|^2}} \tag{12}$$

So as it can be seen in (12) if $t \to \infty$ and $c_{2S} \neq 0$ then, $\psi(t \to \infty) = |\psi_{2S}'\rangle$.

Moreover, the theory explained above will be tested considering that the system can be described as [1] and follows the Hamiltonian (2). In addition, nanoparticles with spin $S = 5$ and with a preparation that fulfils $|\psi\rangle(0) = |5\;5\rangle$ are used. Since in this system m is not a good quantum number, there will be some mixture of eigenvectors of the Hamiltonian (2) and the equation (12) will have to be applied. Then, a numerical expression for $|\psi\rangle(t)$ will be generated. To finish, a study of $\langle S_z\rangle(t)$ will be performed to discover if this theory is in concordance with the Slonczewski STT effect.

As it is known, if the state $\psi(t) = \sum_{m=-S}^{S} c_m|m\rangle$ where m is the projection of the spin in the third axis and $\phi(t)$ is normalized, then $\langle S_z\rangle = \sum_{m=-S}^{S} |c_m|^2 m$. To find an expected value that could describe a real system, $\langle S_z\rangle(t)$ is required to be at least continuous, and then the validity of its results can be discussed.

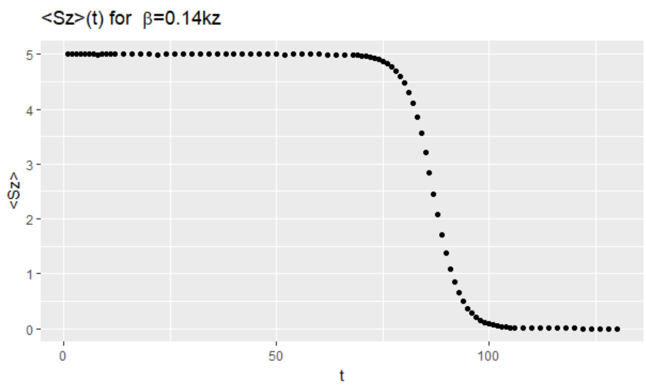

FIG. 2: $\langle S_z\rangle(t)$ for the resolution of the Schrdinger equation for Hamiltonian (2) with $h_x = 0$ and $\beta = 0.14k_z$ and for $S = 5$ with $|\psi\rangle(0) = |5\rangle$.

First of all, it should be said that for $S = 5$ and $h_x = 0$, the first complex pair of eigenvalues appear for $\beta = 0.135k_z$. This means that in the case of figure 2, the diagonalization of $\mathcal{H}_{\mathcal{PT}}$ has complex eigenvalues.

As it can be seen, the evolution of $\langle S_z\rangle(t)$ begins with a value near 5, then it begins a transition from 5 to 0 and it stabilizes in $\langle S_z\rangle = 0$. This could mean an alienation of the spin with the direction of the current β.

The next step is to see how does the $\langle S_z\rangle(t)$ change when the electric current β is increased. It does also mean that there will be more than one pair of complex eigenvalues of the Hamiltonian (2). So it is important to see if the expected value will still be continuous or it will have any discontinuity.

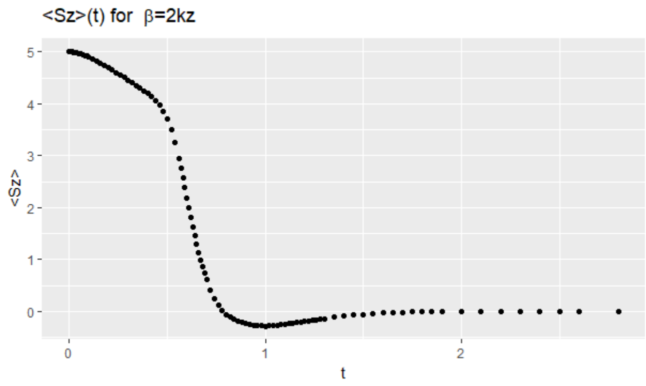

FIG. 3: $\langle S_z\rangle(t)$ for the resolution of the Schrdinger equation for Hamiltonian (2) with $h_x = 0$, $\beta = 2k_z$ and for $S = 5$ with $|\psi\rangle(0) = |5\rangle$.

In figure 3, it can be seen that the transition between $\langle S_z\rangle = 5$ to $\langle S_z\rangle = 0$ happens faster than in figure 2. However, it can be seen that the expected value of the $\langle S_z\rangle$ is inverted for a while; the expected value of the S_z is negative during a short period of time.

It could be relevant to know if there is any current β for which $\langle S_z\rangle$ switches from $|\psi\rangle(0) = S$ to $|\psi\rangle(t) = -S$, although until this moment we have not been able to find it. However, this is an interesting way to follow this study, since it could be important for the development of quantum computers in the future.

V. CORRESPONDENCE PRINCIPLE

The correspondence principle in physics states that the behaviour of systems described by quantum mechanics reproduces classical physics in the limit of large quantum numbers.

To see if the results of this study reproduce the quantum behaviour of nanoparticles in a Slonczewski STT model, the results should be compared with the results in [1]. Using the same values of k_z and h_x, the value of the critical β (which is the current needed for the Hamiltonian (2) in order to develop the first pair of complex conjugate eigenvalues) should be almost the same in [1].

In [1] $S \to \infty$, $k_z S \to \frac{D}{2}$ with $h_x = 1$ and $D = 20$ are used and this finds that $\beta_c \approx 4.5$. If the Hamiltonian (2) is substituted by these values, with $S = 5$, $k_z = \frac{D}{2S} = 2$, then $\mathcal{H}_{\mathcal{PT}} = \gamma H_0(-2S_z^2 + S_x + i\beta S_y) = 2\gamma H_0(-S_z^2 + \frac{1}{2}S_x + i\beta' S_y)$. Some analytical calculations have been run for the Hamiltonian (2) and the results have been $\beta_c' = 0.5175$, $\beta_c = 1.035$. The same calculations have been tested for larger $S = 6, 7$, and it has been found that $\beta_c \approx 1$. The results do not seem to be in agreement with the value found by [1].

Although our results are in accordance with the results found by *E. Chudnovsky* (private correspondence), which have not been published yet, that say that the value $\epsilon_c = \frac{\beta_c}{k_z S}$ should be constant. Since in our experiment $k_z S$ is constant, β_c should be constant as well.

Moreover, the real and imaginary parts of the energy spectrum for $S = 3$ has been plotted in figure 4, and the results compared with [1] are practically the same.

This brings us to conclude that there are some discrepancies between the units used by [1] and the ones we used.

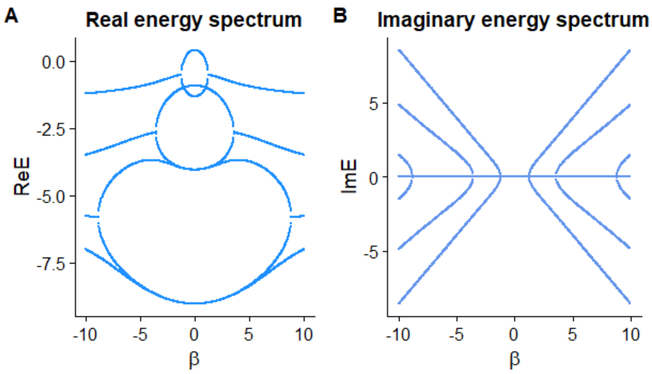

FIG. 4: Real and imaginary spectrum in function of β for the diagonalization of the Hamiltonian $\mathcal{H}_{\mathcal{PT}} = \gamma H_0(-2S_z^2 + S_x + i\beta S_y)$ for $S = 3$.

VI. CONCLUSIONS

- It has been found that the tunnel splitting of the non-Hermitian Hamiltonian (2) is in great accordance with the perturbation theory. As expected, the perturbation theory is almost in full agreement with the energy spectrum of the Hamiltonian for low β, though it is not the case for higher β.

- It has been given a possible interpretation for the complex eigenvalues of the energy spectrum, and how it would affect the expected value of the third projection of the spin. The results shall be compared with experimental tests to see the level of accordance.

- It has been noticed an agreement between our results, Chudnovsky's and [1].

Future steps for this work are to find if there is any way to invert the initial spin. This will be done by using Landau Zener effect and dumping.

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