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Computational Reproduction of Resonant Magnetization Tunneling in High-Spin Molecules and its visualization through an App

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Summary

1 Introduction

First of all, I would like to highlight that I have been involved within a group conformed by Dr. Carles Calero (associate professor of the UB and IN2UB researcher) who has been my tutor, Dr. Bruno Julià (full professor of the UB and ICCUB researcher) and Marc Farreras (a fellow student) that I am very pleased to have worked with.

We were involved in the project *ServiPartícules* created by the ICCUB with the aim to disseminate concepts about quantum mechanics, atomic physics of ultracold gases, Bose-Einstein condensates and solitons via games and demonstration apps (you can find all this programs in clasicallabUB, quantumlabUB and ultracoldUB). The concepts that will be discussed along this report are mainly contained in the realm of quantum physics, so is logical to think that my project, which is Spin Tunneling, is particularly located in the quantumlabUB branch.

When you visit the Spin Tunneling GitHub you realize that there is another project of Spin Tunneling by Laura Guerra. It might seem that I kind of followed her steps, however, this was not tested enough, and it just worked to too low spin in order to be realistic and it was not general enough, so I barely started from scratch. That is why I restarted this exciting project, to solve its leaks and establish a strong basis to the following one who could enhance the animation and make a game to finally popularize so many interesting concepts and explain the experiment performed partly in the University of Barcelona (UB).

2 Goals

The main goal is to reproduce experimental results obtained in a series of experiments which made obvious the spin tunneling phenomena and set up a basis for the study of quantum properties in macroscopic systems. As it is already said, some experiments were partly developed in the UB [1] and this is why this project is so important, to make visible an important event that occurred in the Faculty of Physics that we are studying, apart from teaching and physics dissemination to the new generations thus they get engaged to this fascinating science branch. Moreover, we wanted to plot them in a way that we can visually understand different concepts underlined from the experiment. Steps to follow:

1. Solving time dependent Schrödinger equation for an arbitrary spin (we assume that exchange interaction within the molecule are so large that it can be treated as s=10 object, thus we are looking to specifically solve the s=10 case, although molecules with s=6 can also show this kind of behaviour).

2. Coding a Python program that is able to solve the system of coupled differential equations via RK4.

3. Ensuring that the result is correct via comparison with solutions of lower integer spin (for instance s=1) using a trusted RK4, a Python function (scipy.integrate.solve_ivp) and Laura Guerra's results.

4. Linking the probabilities obtained with other relevant magnitudes relevant to the experiment.

5. Creating a Kivy app to show the experiment results and physics concepts.

3 Methodology

Firstly, it is important to remind that we were a 4 people team where two of them are university professors and professional researchers, and two of them, 3rd year Physics students each of them developing independent projects which were tutored by the researchers (Marc's project was related with solitons, and mine, as I explained, is about Spin Tunneling).

In order to learn how a research group works, we arranged online meetings twice a week where both students had to present their respective current results, discussing with the group if there were some errors in what we did, and specifying the following goals in order to keep progressing in our respective projects. This lasted the whole July and September.

Most of times Marc and I learned from each other's project due to the fact that physical concepts were completely different, which therefore enhanced our knowledge and allowed us to learn and execute different working methods.

Another determining fact was that we, both, were doing scientific research for our first time, so we had similar mistakes in terms of our scope when developing our respective project, such as not investigating enough where our problems or errors were coming from or assuming things as true or fully working without being fully tested and proved. Then our tutors taught how science must be done, and what's more, how to a longtime project should be structured and developed to keep progressing efficiently.

Finally, I consider that hard work, effort and long hours in front of a screen lead me to an experience which really helped me to be more rigorous and structured from a company perspective that I could not learned from my daily student live, while at the same time, it awoke my eagerness to learn in the scientific community which is also hard to see these so many things that are going on in the research world, whilst being a student.

To sum up, it delivered me a higher grade of discipline and organization skills because I had to present results in an understandable way twice a week. Furthermore, it improved my communication and social skills which provided me insights of how to present within a research group.

4 Physics and mathematical resolution

4.1 Spin tunneling

As we have already explained the main goal is to reproduce experimental results and concepts from [1]. This study was based and motivated by previous experiments, such as the ones explained at [2]. One of the firs indices was find in 1986 explained at [3], meanwhile, the explanation was trying to be explained [4].

In the following section the most fundamental physics concepts will be explained in order to understand how the experiment was carried on and how to reproduce its mainly results (by solving the problem). An accurate way to do the calculation of spin tunneling effects in the presence of an applied magnetic field is detailed at [5], another way using a semiclassical limit can be found at [6].

4.1.1 Hamiltonian proposed

There are several Hamiltonians that can be used, an accurate analysis is explained at [7]. A simple and functional one according by [1], which in the end is the one we want to reproduce, is

$$\mathcal{H}_0 = -D\,\mathbf{S}_z^2 - g\mu_B\,\mathbf{S}\cdot\mathbf{H} \tag{1}$$

where D represents the anisotropy energy that breaks the zero-field Zeeman degeneracy, g is the Landé g-factor, μ_B is the Bohr magneton, S_z^2 and $\mathbf{S} = (S_x, S_y, S_z)$ are spin operators, and $\mathbf{H}$ is the magnetic field. In this case $\mathbf{H}$ is applied along the easy axis which we assume it is along Z-axis, and we suppose that it is directly proportional with time t: $\mathbf{H}(t) = (0, 0, H_z\,t)$ where H_z is a constant of proportionality. Therefore, tunneling can not happen in this evolution frame as Hamiltonian (1) commutes with $\mathbf{S}_z$; except a perturbation term is included, i. e. transverse anisotropy or a small off-axis component of magnetic field $\mathbf{H}$. During this paper both cases will be considered, as we will simulate both results. Taking into account this consideration the correct Hamiltonian to reproduce the experiment must have the following shape: $\mathcal{H} = \mathcal{H}_0 + \delta\mathcal{H}$. Apart from that, another important property is derived from equation (1) commutation: the eigenstates of its operators are $|s, m\rangle$ where s stands for total spin and m for the magnetic quantum number.

Although we do not actually know which is this additional perturbing term, the one we propose is a transverse anisotropy perturbation based on theoretical and practical letter where analyses molecular nanomagnets [8], $\delta\mathcal{H}_1 = B\,(\mathbf{S}_x^2 - \mathbf{S}_y^2)$ where B is the anisotropy energy in the perpendicular direction of which spins are defined and it should be much lower than D. Finally, this leads to the Hamiltonian

$$\mathcal{H} = -D\,\mathbf{S}_z^2 - g\mu_B\,H_z\,t\,S_z + B\,(\mathbf{S}_x^2 - \mathbf{S}_y^2). \tag{2}$$

4.1.2 Fundamental concepts

A starting point to understand how spin tunneling works is considering the case that there is no magnetic field $H = 0$. In this case 2 degenerate ground states, $|s, s\rangle$ and $|s, -s\rangle$ (i. e. parallel and antiparallel states to easy axis) are separated by an anisotropy barrier (D). It remains this way until symmetry is broken by means of magnetic field introduction, this means that one state becomes the true ground state, we take as reference $|s, s\rangle$. Once this metastable state becomes resonant (i. e. that both energies coincide) with an excited level $|s, -s + n\rangle$, being $n \in \mathbb{N}$, resonance tunneling occurs. Then, in a rush from the excited level $|s, -s + n\rangle$ spontaneously decays into the metastable ground state $|s, -s\rangle$ due to there is no anisotropy barrier and can interact with the phonons field so instantaneously goes to the true ground state $|s, s\rangle$.

This can be explained by the Hamiltonian presented before (1). From this we can rapidly answer why the steps are even

$$H_{s,-s+n} = -D\frac{n}{g\mu_B} \tag{3}$$

where $H_{s,-s+n}$ is the magnetic field when there is two resonant states $|s, s\rangle$ and $|s, -s + n\rangle$, both quantum magnetic numbers n are indexed; the other constants and n has already been defined.

Next we will demonstrate how (3) is deduced from Hamiltonian (1) with $H_z \equiv H_{s,-s+n}$, by applying it to both eigenstates $|s, s\rangle$ and $|s, -s\rangle$.

$$\mathcal{H}_0 \, |s, s\rangle = \left[-D\, s^2 - g\mu_b \, H_{s,-s+n} \, s\right] |s, s\rangle \tag{4}$$

$$\mathcal{H}_0 \, |s, -s + n\rangle = \left[-D(-s + n)^2 - g\mu_b \, H_{s,-s+n} \, (-s + n)\right] |s, -s + n\rangle \tag{5}$$

Once we have applied the Hamiltonian we have obtained its associated eigenvalues. As we already know that resonance is produced when these are equal

$$-\, D\, s^2 - g\mu_b \, H_{s,-s+n} \, s = -D(-s + n)^2 - g\mu_b \, H_{s,-s+n} \, (-s + n) \tag{6}$$

eventually we end up obtaining (3) by isolating $H_{s,-s+n}$ from this equality in (6)

$$H_{s,-s+n} = -D\frac{n}{g\mu_B}.$$

In terms of what concerns to what we did before, (3) could be written taking into account that we assumed magnetic field varying proportionally with time and defining $h_z = g\mu_B \, H_z$ where in this case H_z can be defined as $H_{s,-s+n}$, we can obtain

$$h_z \, t_{s,-s+n} = -D\, n \tag{7}$$

which allows us to estimate when the transitions should occur

$$t_{s,-s+n} = -\frac{D}{h_z} n \tag{8}$$

According with [1] this theoretical result (3) fits well with experimental results, even steps of 0.46T . Regarding with this result, [1] pointed that magnetic fields where the steps were produced coincide with the ones where tunneling resonance happens. Moreover, in this study they estimated that the expected number of steps they had to measure esperimentally was 21.6, whilst theoretically we obtain that the number of steps is $2s + 1$, which is 21 in the case of $s = 10$, from $n = 0 \longrightarrow 20$ (last step corresponds to elimination barrier). They could not measure these whole steps due to measure till step 19 they estimated that a 10mK temperature should have been reached, despite they arrived till 1.7K as the minimum temperature.

In regards of what we have already mentioned, the model predicts that multiple level crossings at each resonant field can occur, therefore all levels can tunnel simultaneously. To sum up, this is a model of field-tuned, thermally assisted resonant tunneling out of a metastable spin state.

In conclusion, when field is reduced from saturation no step is observed because states are in true ground state so no tunneling can happen. In contrast with when it is reduced to 0 or reversed that

states are in a metastable state that when become resonant produce the steps. The reason why these steps happen is that resonant transition cause an increase of transition rate. Another interesting feature is that the higher the step is, the easier it is to be observed, as the dip is more pronounced. We can lean its explanation on the fact that the magnetic relaxation time increases with the step because anisotropy barrier is lower as the magnetic field is higher.

Despite the fact that this is a proper way to explain how spin tunneling works we have to take into account that experimentally the initial state ought to be the true ground state and then at some point when crosses H(t)=0 will become to be the metastable state and resonance with other states can happen. That's why in some points of the hysteresis cycle there are steps and in others there are not. So this is what we aim to reproduce.

4.1.3 Another magnetic field dependency on time

Changing how the magnetic field depends on time means a change in the Hamiltonian, the new magnetic field

$$H(t) = H_0 - \alpha\, t \quad (t > 0) \tag{9}$$

where H_0 is a sufficiently high magnetic field where magnetization is already saturated when experiment starts and α is the magnetic field velocity of change.

In contrast with last magnetic field proposed, this one just considers time starting from 0 (positive times). Therefore if both constants are positive it will represent a decrease from high magnetic fields to lower magnetic fields, and vice versa when it comes to consider both negative constants. Therefore, $H(t) = 0$ can be found not only at $t = 0$ as the first magnetic field proposed, but at whatever time depending on the constants, so it may be more useful at the time to make hysteresis cycle. Firstly, we start with $H(t = 0) = H_0$ arrive until $H(t_1) = -H_0$ and then change the sign of α to increase the magnetic field $H(t) = -H_0 + \alpha\, t \quad (t_1 > 0)$ until we get again $H(t_f) = H_0$.

Once analysed this term, it fits in the Hamiltonian as

$$\mathcal{H} = -D\, \mathbf{S}_z^2 + (H_0 - \alpha\, t)\, S_z + B\, (\mathbf{S}_x^2 - \mathbf{S}_y^2) \tag{10}$$

which will allow us to test if the magnetic field term is working properly. Apart from that, we have to recalculate times where

$$H_0 - \alpha\, t_{s,-s+n} = D\, n \tag{11}$$

which allows us to estimate when the transitions should occur

$$t_{s,-s+n} = -\frac{D}{\alpha} n + \frac{H_0}{\alpha}. \tag{12}$$

4.2 Differential equations solution

Firstly, the Hamiltonian used to simulate the experiment is applied into the Schrödinger equation in order to obtain the coupled differential equation system that define the evolution of the states probabilities along time. Secondly, this result is compared with an specific case, in order to show the validity of the solution, spin s=1 is considered. Finally, the numerical resolution is explained which makes use of a computational method, a suitable one is Runge-Kutta 4 (RK4) which is the one we will code to solve this problem, apart from a Python solver to prove that everything works as expected and to test different ways and pick the best one.

4.2.1 States probabilities along time

We start considering the particle general wave function which ensembles the whole eigenstates set of spin s

$$|\phi\rangle\,(t) = \sum_{m=-s}^{s} a_m(t)\, |s, m\rangle \tag{13}$$

which verifies the orthonormal property

$$\langle \phi | \phi \rangle = \sum_{m=-s}^{s} |a_m(t)|^2 = 1 \quad \forall t. \tag{14}$$

Once we have everything defined it's time to find out how the coefficients evolve with time by applying the already known Schrödinger law

$$i\hbar\, \partial_t \, |\phi(t)\rangle = \mathcal{H} \, |\phi(t)\rangle \, . \tag{15}$$

For the sake of simplicity, from now on we will consider atomic units where $e = m_e = \hbar = 1$ (dimensionless), simplifying most equations. It means that longitude will be measured with Bohr radius $a_0 = \frac{\hbar^2}{m_e e^2} = 0.529177210903(80) \cdot 10^{-10}$m; Energy is measured with Hartree energy $E_h = \frac{m_e e^4}{\hbar^2} = 27.211386245988(53)$ eV; and time is measured with $t_0 = \frac{\hbar^3}{m_e e^4} \approx 2.419 \cdot 10^{-17} s$. Then we define $h_z = -g\mu_B \, H_z$ and we substitute equation (13) to (15), multiply by $\langle s, k|$, where as per usual s, k are the spin particle and the quantum magnetic moment, respectively, and isolate derived time-dependent coefficients

$$\dot{a}_k(t) = -i \sum_{m=-s}^{s} a_m(t) \, \langle s, k | \mathcal{H} | s, m \rangle \tag{16}$$

where k values vary from $-s$ to s, by means of this operations we have obtained the system of coupled differential equations to solve by apply the corresponding Hamiltonian. As this is a tough path we will show how the Hamiltonian is applied first[1]

$$\begin{aligned}
\mathcal{H} \, |s, m\rangle &= -D \, \mathbf{S}_z^2 \, |s, m\rangle - h_z \, t \, S_z \, |s, m\rangle + B \, \left(\mathbf{S}_x^2 - \mathbf{S}_y^2 \right) |s, m\rangle \\
&= -D \, m^2 \, |s, m\rangle - h_z \, t \, m \, |s, m\rangle + \frac{B}{2} \Big[N_+(m) \, N_+(m+1) \, |s, m+2\rangle + N_-(m) \, N_-(m-1) \, |s, m-2\rangle \Big],
\end{aligned}$$

where operators are defined in the **Appendix** section, then this is multiplied by $\langle s, k|$

$$\langle s, k | \mathcal{H} | s, m \rangle = -D \, m^2 \delta_{k,m} - h_z \, t \, m \delta_{k,m} + \frac{B}{2} \Big[N_+(m) \, N_+(m+1) \delta_{k,m+2} + N_-(m) \, N_-(m-1) \delta_{k,m-2} \Big] \tag{17}$$

when substituted to (16) we finally get how coefficients behave along time evolution in the frame of the currently Hamiltonian considered

$$\begin{aligned}
\dot{a}_k(t) = -i \Big\{ a_k(t)(-D \, k^2 - h_z \, t \, k) + \sum_{m=-s}^{s} a_m(t) \frac{B}{2} \Big[& N_+(m) \, N_+(m+1) \delta_{k,m+2} \\
& + N_-(m) \, N_-(m-1) \delta_{k,m-2} \Big] \Big\}.
\end{aligned} \tag{18}$$

4.2.2 Spin 1 example

In order to show that the solution obtained in the previous section an example will be performed. An easy one is s=1 due to how the eigenstates $\{|-1\rangle, |0\rangle, |1\rangle\}$ of S_z and S_z^2 interact with the Hamiltonian we have proposed (2).

On the one hand, we apply the Hamiltonian by an straight forward application of the spin 1 operators[2]

$$\begin{aligned}
\mathcal{H} \, |-1\rangle &= -D \, |-1\rangle + h_z \, t \, |-1\rangle + B \, |1\rangle \\
\mathcal{H} \, |0\rangle &= 0 \\
\mathcal{H} \, |1\rangle &= -D \, |1\rangle - h_z \, t \, |1\rangle + B \, |-1\rangle
\end{aligned}$$

when substituted in (16) derived coefficients result to be

[1] Consider taking a look to how spin operators work at Appendix section A. Rotational Generators (where we can change J by the spin operator S).

[2] Consider taking a look to how spin 1 operators work at Appendix section B. Spin 1 Operators.

$$\dot{a}_{-1}(t) = -i\left[a_{-1}(t)\left(-D + h_z\, t\right) + a_1(t)B\right] \tag{19}$$

$$\dot{a}_0(t) = 0 \tag{20}$$

$$\dot{a}_1(t) = -i\left[a_1(t)\left(-D - h_z\, t\right) + a_{-1}(t)B\right] \tag{21}$$

On the other hand, we apply to the recently general solutions found

$$\begin{aligned}\dot{a}_{-1}(t) &= -i\left[a_{-1}(t)(-D + h_z\, t) + a_1(t)\frac{B}{2}N_-(1)N_-(0)\right] \\ &= -i\left[a_{-1}(t)(-D + h_z\, t) + a_1(t)B\right]\end{aligned}$$

$$\dot{a}_0(t) = 0$$

$$\begin{aligned}\dot{a}_1(t) &= -i\left[a_1(t)(-D - h_z\, t) + a_{-1}(t)\frac{B}{2}N_+(-1)N_+(0)\right] \\ &= -i\left[a_1(t)(-D - h_z\, t) + a_{-1}(t)B\right]\end{aligned}$$

note that obviously when either $m = 1$ or $m = -1$ reach raising and lowering operator, respectively, $N_+(1)$ and $N_-(-1)$ must be 0. Moreover, given this specific s=1 case, all others $N_\pm(m)$ are $\sqrt{2}$ as $s(s+1) = 2$ and second term inside square root of $N_\pm(m)$ vanish due to its definition. As this consideration is applied we can see that results are equal in both cases.

4.2.3 Another perturbing term

Another term to use would imply an off-axis magnetic field component for the sake of simplicity $\delta\mathcal{H}_2 = -h_x\, S_x$ will be used, where S_x is an operator defined at Appendix section A and h_x is a small magnetic constant (we suppose it does not vary along time). By substituting this perturbing term in exchange with the first one to (2), this ends up leading to the new Hamiltonian

$$\mathcal{H} = -D\,\mathbf{S}_z^2 - h_z t\, S_z - h_x\, S_x \tag{22}$$

which applied to Schrödinger equation leads to the same derivative coefficients equation (16) as before.

So what differs from the previous solution is when Hamiltonian is applied

$$\begin{aligned}\mathcal{H}\,|s,m\rangle &= -D\,\mathbf{S}_z^2\,|s,m\rangle - h_z\, t\, S_z\,|s,m\rangle - h_x\, S_x\,|s,m\rangle \\ &= -D\,m^2\,|s,m\rangle - h_z\, t\, m\,|s,m\rangle - \frac{h_x}{2}\Big[N_+(m)\,|s,m+1\rangle + N_-(m)\,|s,m-1\rangle\Big]\end{aligned}$$

multiplied by $\langle s,k|$

$$\langle s,k|\mathcal{H}|s,m\rangle = -D\,m^2\delta_{k,m} - h_z\, t\, m\delta_{k,m} - \frac{h_x}{2}\Big[N_+(m)\delta_{k,m+1} + N_-(m)\delta_{k,m-1}\Big] \tag{23}$$

when substituted to (16) we finally get how coefficients behave along time evolution in the frame of the currently Hamiltonian considered which differs from the first one.

$$\dot{a}_k(t) = -i\Big\{a_k(t)(-D\,k^2 - h_z\, t\, k) - \sum_{m=-s}^{s} a_m(t)\frac{h_x}{2}\Big[N_+(m)\delta_{k,m+1} + N_-(m)\delta_{k,m-1}\Big]\Big\}. \tag{24}$$

Note that for computing times where resonances are produced we have not used the perturbing time so the results are the same as before.

4.2.4 Numerical resolution: RK4

The coupled differential equation system has already been found, so the next step is solving it by means of an adequate computational method. A popular and powerful one is RK4 due to the fact that local order precision is h^5 achieving a great balance between computational time and precision. This is a multi-step method which aims to find a high order approximation of $y(x_0 + h)$ where h is the step. Considering one RK algorithm the more precision we need, the more steps we will perform, so the lower will be h value as it is defined as $h = (x_f - x_0)/\#steps$. If the precision needed to our problem exceeds the capacity of the RK proposed, we should consider moving forward to the next RK algorithm. Eventually, if we are already using a high RK and it is not working properly we might need to find another method. In this case, RK4 is the one proposed and the algorithm works as follows

$$\mathbf{y}_1 = \mathbf{y}_0 + \frac{h}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4) \tag{25}$$

$$\mathbf{k}_1 = \mathbf{f}(x_0, \mathbf{y}_0)$$

$$\mathbf{k}_2 = \mathbf{f}(x_0 + \frac{h}{2}, \mathbf{y}_0 + \frac{h}{2}\mathbf{k}_1)$$

$$\mathbf{k}_3 = \mathbf{f}(x_0 + \frac{h}{2}, \mathbf{y}_0 + \frac{h}{2}\mathbf{k}_2)$$

$$\mathbf{k}_4 = \mathbf{f}(x_0 + h, \mathbf{y}_0 + h\mathbf{k}_3)$$

5 Application development

5.1 Preliminary code

First of all, what will be developing is a program able to solve the coupled differential equation system with a function from scipy modules, RK4 and with the operators due to the fact that we will first consider s=1. All these procedures will be done in order to get the probabilities spectrum to find the molecule in a specific spin in a determined time. Ensuring that the norm is conserved will be a must, apart from testing different implementations and getting the same results.

5.1.1 Testing method

As we described in the past section, in order to progress adequately firstly we have to solve a particular case, i. e. spin 1. So the very first program is focused on solving the coupled differential equations system composed by (19), (20) and (21). It mainly implements function `solve_ivp` in module `scipy.integrate` which is aimed to solve this kind of problems involving complex numbers. It enables us to compare different paths and reach a tested general solution ensuring that it is actually the correct one. Some facts to take under consideration before coding are Hamiltonian parameters: $D = 1\frac{J}{[\hbar^2]}$, $h_z = 0.1\frac{J}{t\,[\hbar^2]}$ and $B = 0.1$; initial conditions of coefficients $a_{-1}(t_0) = 1$ and 0 for all other states; and starting and final times: -10 s and 10 s, respectively. The results obtained from the development of this initial program are found in Fig. 1.

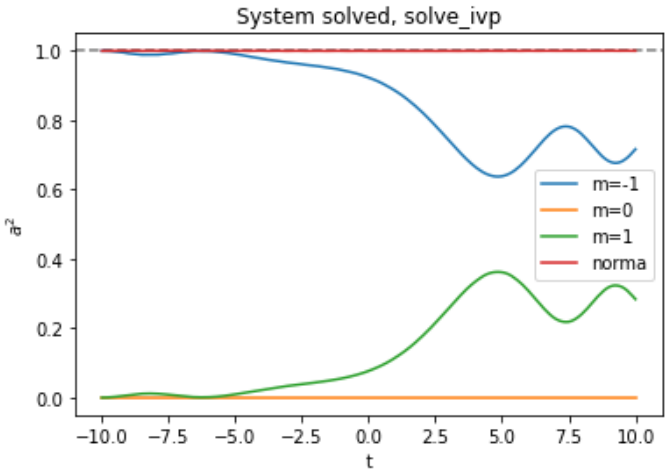

Fig. 1: Computational solution plot of coefficients states of a spin 1 system, to the power of 2 (state probability) in front of time evolution which is delimited between [-10, 10]s. This is the specific case given certain initial conditions and a certain spin tunneling Hamiltonian. This evolution comes from coupled differential equation system derived from Schrödinger equation appliance which in this case are solved by means of a Python program which implements function 'solve_ivp'.

Maintaining the same conditions and Hamiltonian we apply the straight forward method (using the corresponding base and operators for spin 1) at equation (16). Straightaway, we solve the system by means of RK4 algorithm used in 20000 steps. Finally, we obtain the result in Fig. 3, that we can clearly see it is not completely equal to Fig. 1 as RK4 accrues error from each step and `solve_ivp` works with the most optimal algorithm it can use. However, in order to be sure that our RK4 algorithm works properly, we have performed a test example consisting in a simple pendulum of $g = 10\,m/s^2$, $l = 0.1\,m$, $\theta_0 = \pi/4$ rad and $\dot{\theta}_0 = 2$ rad/s. We used 2000 steps for implementing RK4 and its result is plotted in Fig. 2, which we know is correct as we already knew the solution before we performed this test.

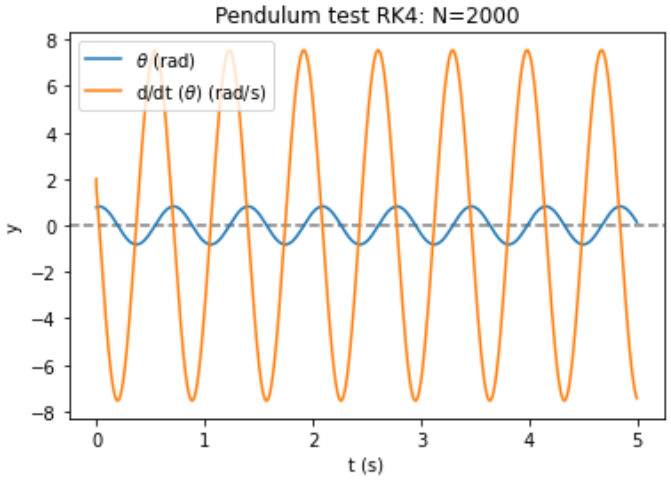

Fig. 2: Computational solution plot of angle pendulum respect the equilibrium axis θ and angular velocity $\dot{\theta}$, in front of time evolution which is delimited between [0, 5]s. This evolution comes from simple pendulum equation appliance which in this case are solved by means of a Python program which implements RK4 algorithm in N=2000 steps.

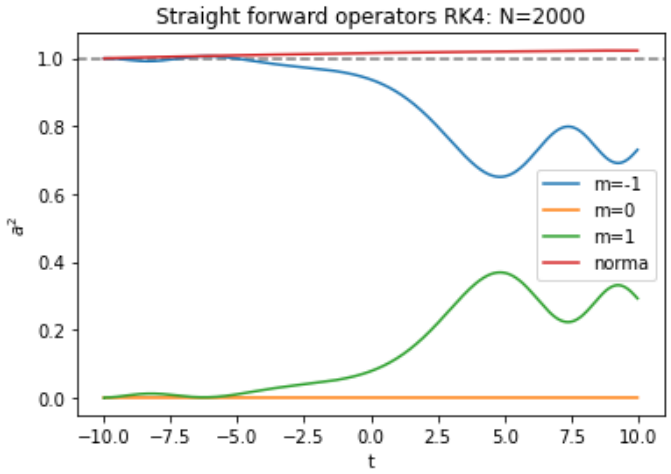

Fig. 3: Computational solution plot of coefficients states of spin 1 particle to the power of 2 (state probability) in front of time evolution which is delimited between [-10, 10]s. This is the specific case given certain initial conditions and a certain spin tunneling Hamiltonian. This evolution comes from coupled differential equation system derived from Schrödinger equation appliance which in this case are solved by means of a Python program which implements RK4 algorithm in N=20000 steps.

In the end we have obtained the same result from two different trusted paths so we ought to obtain the same result from applying (24). This is going to be solved by the optimal function mentioned before to achieve a great processing performance in contrast with implementing RK4 algorithm and a large number of steps. As it is expected we finally obtain Fig. 4 which is completely equal to Fig. 1 .

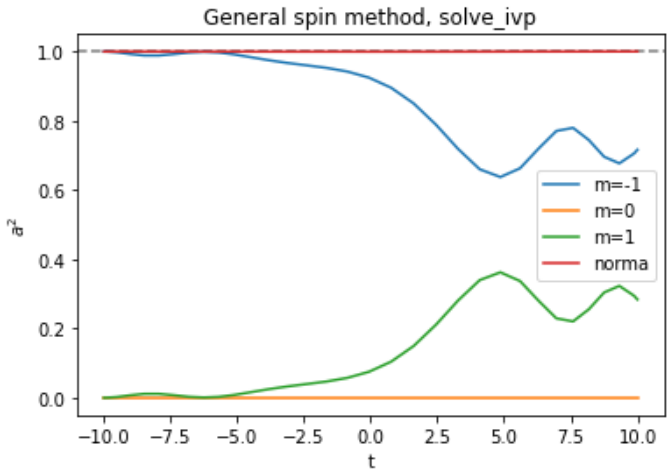

Fig. 4: Computational solution plot of coefficients states of spin 1 particle to the power of 2 (state probability) in front of time evolution which is delimited between [-10, 10]s. This is the specific case given certain initial conditions and a certain spin tunneling Hamiltonian. This evolution comes from coupled differential equation system derived from Schrödinger equation appliance which in this case are solved by means of a Python program which implements 'solve_ivp'. Although the figure plotted is equal to Fig. 1, the code used to generate this figure contains do not just solve the coupled differential equations system, it can derive and solve the problem for arbitrary spin.

Moreover, to be completely sure that everything goes on well we applied our RK4 with $N = 20000$, results can be seen in Fig. 5, which as it was expected results to be the same as Fig. 3.

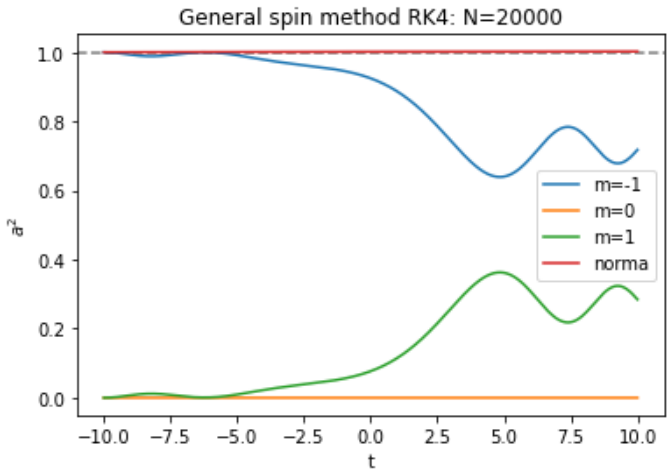

Fig. 5: Computational solution plot of coefficients states of spin 1 particle to the power of 2 (state probability) in front of time evolution which is delimited between [-10, 10]s. This is the specific case given certain initial conditions and a certain spin tunneling Hamiltonian. This evolution comes from coupled differential equation system derived from Schrödinger equation appliance which in this case are solved by means of a Python program which implements RK4 algorithm in N=20000 steps. Although the figure plotted is equal to Fig. 3, the code used to generate this figure contains its generalization to arbitrary spin as the one in Fig. 4.

Finally, an interesting feature to take into account is that code to generate both 20000 steps of RK4 and the same image do not spend the same amount of time to run. The one using the straight forward application of operators lasts approximately 37.5 s, whereas the one that has implemented the arbitrary spin solution lasts approximately 12 s, which means a huge improvement from the preliminary version. Despite of this, the method used will be the one using `solve_ivp` as the result is immediately plotted.

5.1.2 States energies, resonances times and starting cycle

Once the method is tested and proved that works properly, next step is trying to find its resonance times and the magnetization which is defined as $M(t) = \sum_{i=1}^{s} m_i |a_i(t)|^2$. By plotting energies we realize that the previous values were starting with a metastable state and that is not what we want. In fact, we consider that the initial state is the true ground state (because of the experiment construction), and at some point, where $H(t) = 0$, it becomes degenerate and there are two ground states which become resonat. Then the remaining part of this resonance process of the new metastable state will continue to have resonances with other states. In the case of the Hamiltonian (2) resonances are produced from steps of two due to the form of its perturbing term as it can be see in Fig. 6 and Fig. 7 . Another interesting fact is that norm is not correctly conserved, so it will mean that an analysis of parameters that this occurs is needed, and we sould try to find a solution

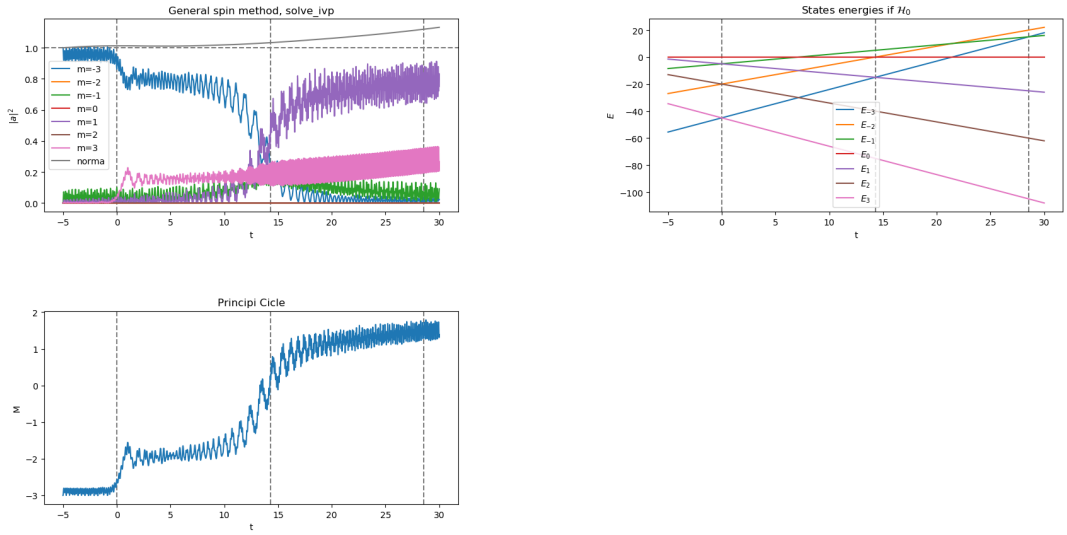

Fig. 6: First attempt to solve the coupled differential equations system. It can be seen that the transitions are correct, but norm is not conserved.

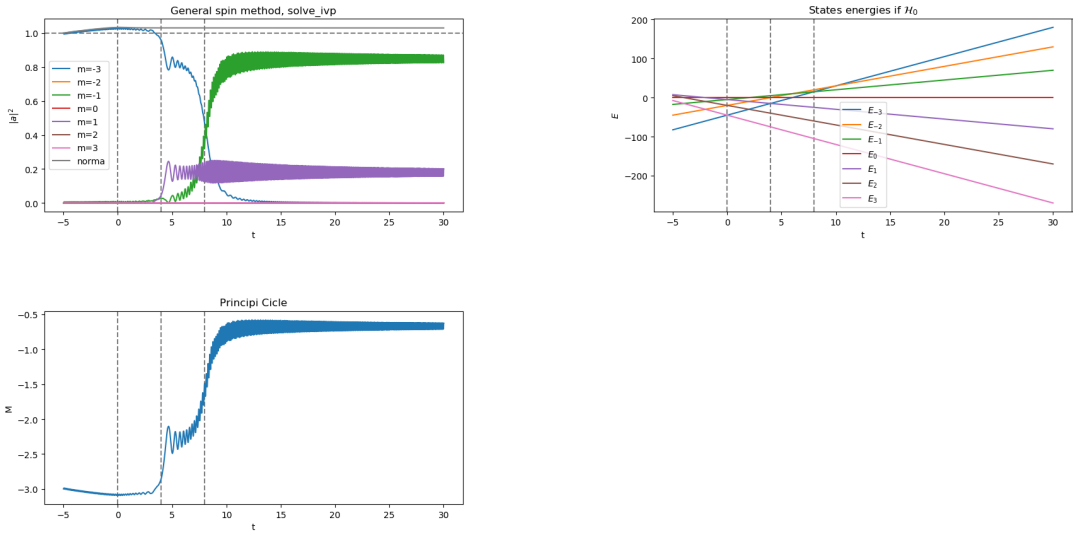

Fig. 7: Analog to 6, but changing parameters to find different transitions.

It is crucial to have the norm conserved, so arguments which control the error from function solve_ivp have to be changed. The parameters are rtol, atol corresponding to relative accuracy (number of correct digits) and absolute accuracy (number of correct decimal places), respectively. Once this is solved, we are ready to make the app and try what happens to different values and if the other perturbing term works as it must do.

5.1.3 Resonances of the other perturbing term

In order to see if something different happens and more than 2 resonances are produced, we analyse the other perturbing term where resonances are produced in steps of 1 s each state, as it is shown in Fig. 8.

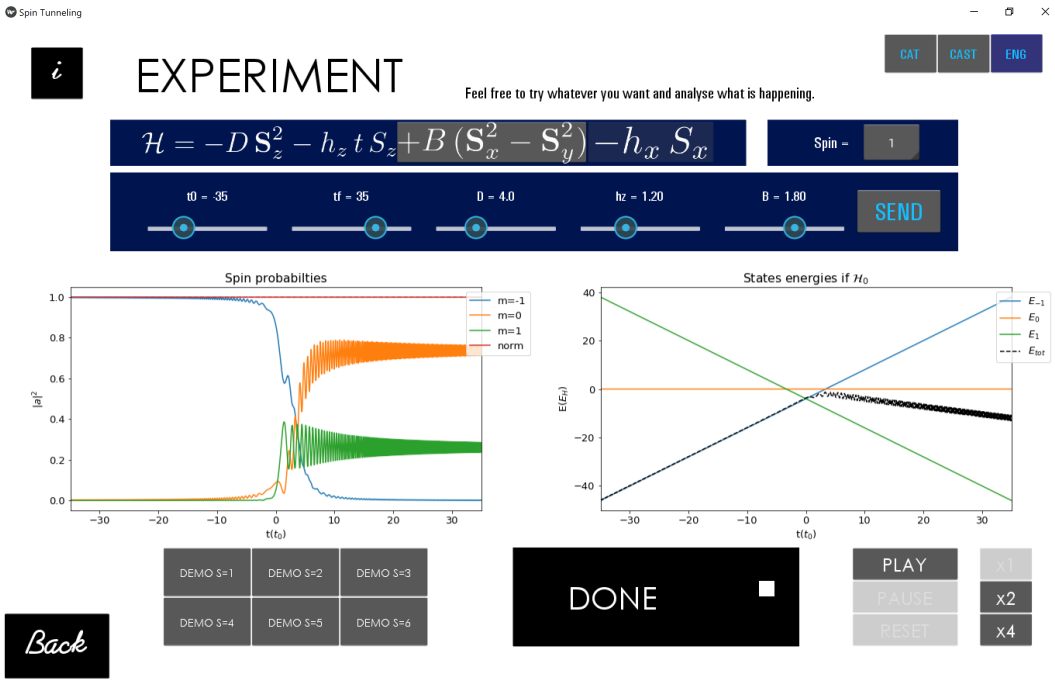

Fig. 8: This is a screenshot of the final app where we can see that the spin tunneling occurs in steps of 1 s as predicted.

6 App UIX and structure

This section introduces a brief explanation of how the final app looks like, what allows the user to do and implicitly it shows its structure and functionalities. It is worth to be reminded that it is been developed using Python and Kivy which implies developing object oriented programming skills.

6.1 Starting Screen

First of all, once the app is started, it is coded in a way that automatically maximize the window app and an starting screen pops up for a few seconds. This starting screen shows the logo application, as it can be seen in Fig. 9. After 3 seconds has passed, the app passes directly to the Menu Screen where we can decide what to do.

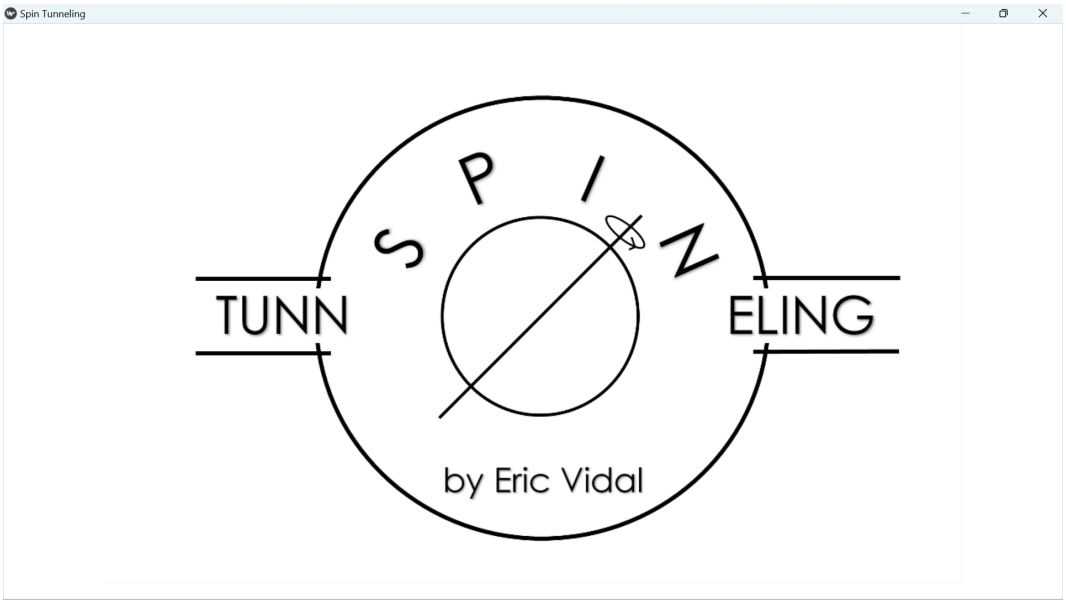

Fig. 9: This is a screenshot where appears the introduction screen (which is showed for 3 seconds), and it is a logo image designed by the author. Then vanishes to enter into the menu.

6.2 Menu Screen

Once the app is initialized and it has already gone to the menu, the menu screen should look like Fig. 10 . Here, we can see the logo again, at the top left corner, then then the app's name and welcoming sentence, and at the top right corner a 'Language Menu' that is not working as the 'Tutorial' and 'Game' buttons. However, I left these in case that someone is willing to continue this project and finally make a game.

Below the title it is supposed to be a brief summary of what the game consists and what can the user do in the application, although now there is a disclaimer that reminds that this is not entirely finished, and advises where to enter because it is actually properly working ('Resonance' and 'Experiment' sections). Another thing to take into account in case that there is another, is that would be nice that if it is wanted the user to do the Tutorial before playing the Game, the programmer should disable the Game button and explain in this space that once the tutorial is done, then the Game button will be able.

Finally, we can find the credits to the tutors and the institutions that take part in this project.

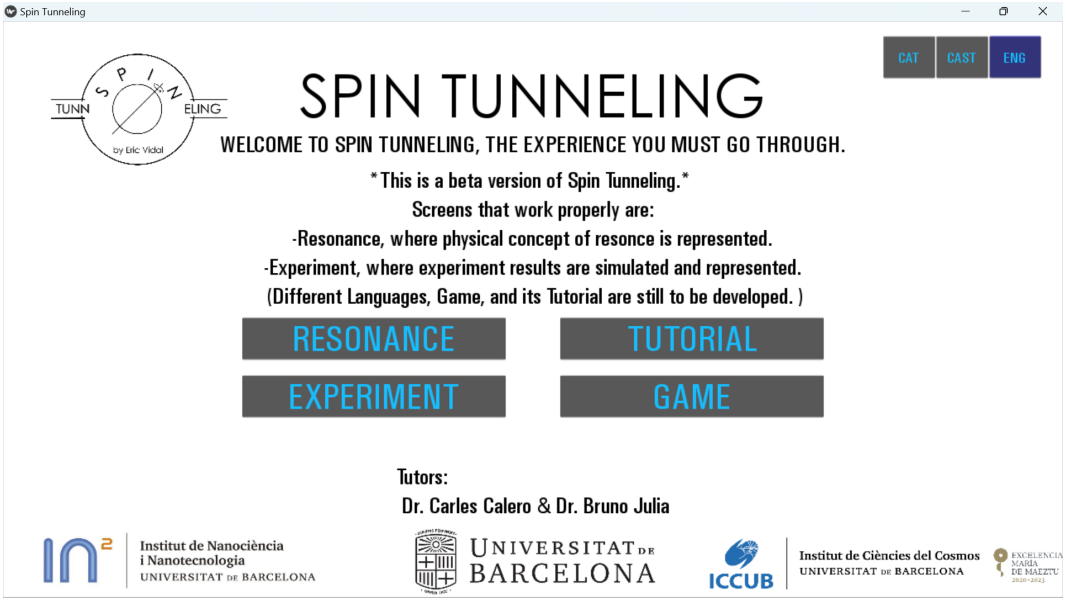

Fig. 10: This is a screenshot where we can see that the menu screen. As it can be seen the languages and game (and tutorial) buttons are left to be used. However the buttons that actually work are Resonance and Experiment. That are actually quite the same, but in Experiment we start the simulation with the real Ground State, and in the experiment with the Metastable state. This will lead to different results and it is easier to see the resonance phenomena if we start with the Metastable state.

6.3 Resonance and Experiment Screen

We have arrived at the working screens where the physics happens. As we can see from Fig. 11, Resonance and Experiment screens just change in which is the initial state, the metastable ground state or the true ground state, respectively. This fact can be easily seen at the Energies graph of each screen, as at the Resonance, the overall energy in a discontinuous black line, starts from top, allowing it to make a lot of transitions so it is easily observed the resonant phenomena. In contrast, the Experiment screen has the overall energy starting from the true ground state so, it correspond to the lowest energy, which is the bottom in the graph, implying much less transitions that the resonant screen one.

In terms of what we can do across the screen. We can see that at the top of the screen we can find, from left to right, the information PopUp (where we can find all the information about the screen), the screen title and slogan and the Language Menu (which is not working).

Below we can find that we can choose the Hamiltonian perturbative term (that we have to remember that each one will produce a different s step), which spin we want the system to have, and different sliders with the initial and final time, and Hamiltonian parameters, such as the anisotropy energy D, the magnetic rate hz and either the magnetic deviation h_x or the anisotropy energy in the perpendicular direction of which spins are defined B, depending of which Hamiltonian perturbation has been chosen.

Then there are the plots of probabilities and energies of the different s states across time.

At the bottom, from left to right, we find the Back button to go back to the Menu; different demos parameters for each spin s, where quite good plots are appreciated; the Loading Box; and the buttons to start, pause and restart the animation, plus the velocity reproduction wanted.

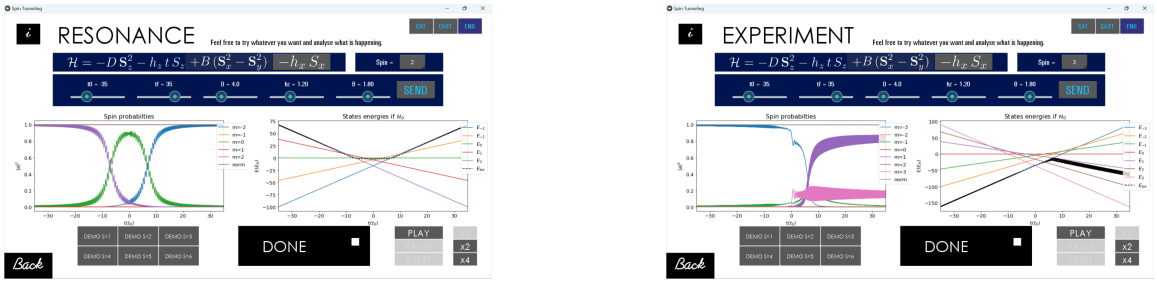

Fig. 11: This is a screenshot where we can see the Resonance and Experiment Screen, respectively. The upper blue boxes contain the buttons and sliders to decide different parameters and compute the solution. In the graphics are plotted the results for these parameters, spin and Hamiltonian perturbative term. At the lower boxes we have some demos with default parameters at the left side, and video player buttons to animate the graphics and understand better how the probability behaves.

6.4 Information PopUp

Finally, we can find out what happens when we click on the Information button, and it is not a surprise that a PopUp appears with all the necessary information to understand what is the physical meaning of the parameters and how the screen works, Fig. 12.

However, it does not pretend how the whole physics works, it is supposed to be a work before starting to use the app, and which is consolidated and understood by the use of it, putting in practice what the user have learned in an interactive and entertaining way.

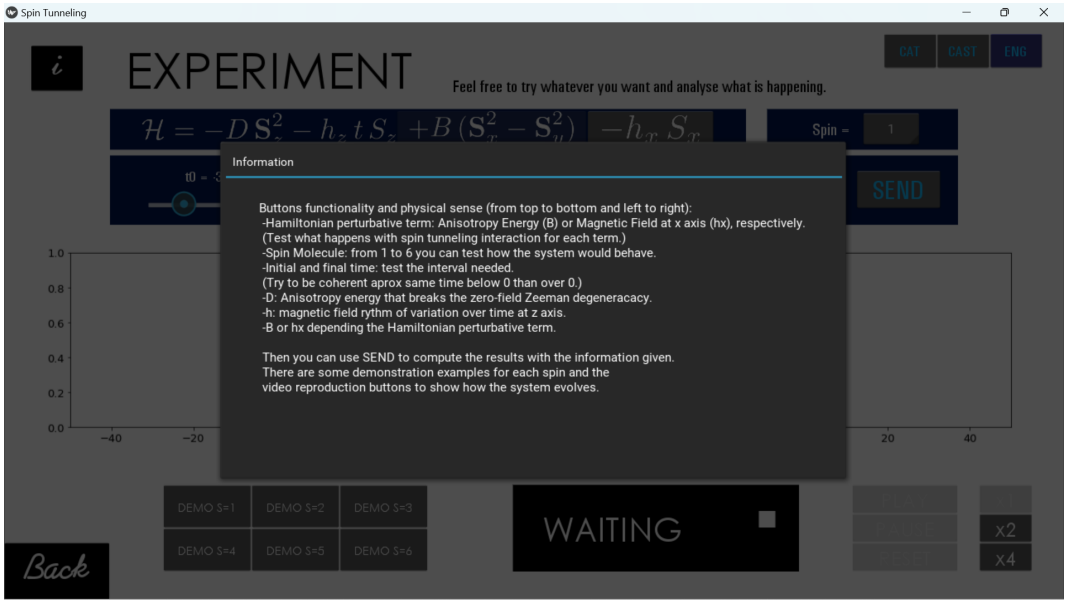

Fig. 12: This is a screenshot where we can see that the popup screen. Here there is all the relevant information related to the eligible parameters and its physical concept.

7 General Conclusions

In overall, we have achieved most goals in terms of recreating the experimental results and making a representation that helps to understand better all the significant physical concepts.

It comes implicit that we have correctly solved the differential equations that show the spin tunneling behaviour for a general s system. Afterwards, these solutions has been plot via matplotlib and I have even generated GIFs using the imageio package (which is not included within the project, so I have installed it separately).

It was easy to realize that the time consumed to solve the equation computationally with Python was larger than expected so in order to effectively teach non-expert users we could limit its maximum

s to 6.

Finally, the app was successfully developed with plenty of feature to experiment with and some PopUps that explain how it works.

7.1 Further steps

Some difficulties due to how Kivy works does not allow to reproduce properly a video inside an app. The only option I found to reproduce a video is to do a video player app and nothing else can be done in there. A solution that I tried was to pass a GIF via matplotlib, but once the GIF is created the folder is not refreshed while using the app. I just find the possibility to reproduce it by shutting the app and reopening it. So what I finally conceived was to with all the data already calculated, creating and plotting the successive images according to a time progression.

In terms of representation using matplotlib in Kivy I do not think that there is much more to do, but some other options that from my point of view are worth to try it would be changing to another app maker. Flutter has a bigger community than Kivy and the widgets are more adaptable. If apart from an experiment representation, someone is interested in making a game, Unity probably is a better choice.

Another thing to take into account is that this project could be continued by trying to implement this code using a compiled language (such as C++) that are faster than interpreted languages (such as Python), in order to see if it could reduce waiting time to compute the solutions.

Finally, my game idea consisted in implement the fact that the measurement in quantum mechanics is probabilistic, thus it could add another concept to disseminate and make clear that although the evolution is deterministic we generally yet do not know in which exact final state will be our system. So it implies studying the behaviour of the probabilities depending the allowed parameters.

Once we know that, the game would consist in proposing time band zones where we should find the molecules in a definite s with a certain probability, and the player would have 3 opportunities to find a certain set of parameters that meet the probabilities required. Then once they think they can success in what is required, they do the measure. By playing this game, the user could learn the system behaviour depending the given parameters and with the help of the professors link it with the physical explanation. For example an increase of the magnetic rate, h, would mean a process more adiabatic alike. They could also discover what means to have a greater anisotropy energy D or magnetic field deviation h_x, to probabilities (states).

This game proposal is in the line of what a fellow student, Francesc Sabater, did with his project, EigenGame, but with the added difficulty that in this case there are not analytical solutions which substantially complicates the process to make the game without bugs and incongruities with the physical concepts that we want to disseminate, that at the end is the most important thing in these kind of projects.

8 Personal Conclusions

I am very glad to have done this internship, as it taught me skills that I could have rarely learn in any other way. The fact that I could have worked online the whole summer studying a topic it is not explained during the Physics degree within a group research environment has been amazing.

The group dynamics has been magnificent with both professors giving me tips to constantly improve. Actually, there were occasions that I did not really see the point of what I had to do or what I was doing until I executed it and finally realized what it was meant for. This helped me a lot to both, follow and respect a determined hierarchy in a working group and also to be self-determined in some manner while developing my personal project.

During this practices I had to be creative and resilient to solve all sort of problems, and find new paths to achieve the results I want it. In regards of teamwork it has been an unrepeatable opportunity that have taught me a knowledge I even could not conceive. One important aspect was developing a parallel project with a fellow student that had nothing to do with mine, and yet being capable of help him and learn from his collaboration. It is also worth to underline that the aspect of learning how I must present results to a research group, by making in an comprehensible way and communicating properly to be understood by the other members of the group.

To sum up, it has been a great experience that have given me a lot, helping me to understand how science must be done, plus the added value that I was developing an app by myself with no previous knowledge. Without doubt it has been tough in some moments, but I have never hesitated in my capability to overcome every problem and I sorted out every difficulty in my path.

I am very thankful to the opportunity that Dr. Carles Calero and Dr. Bruno Julià have brought me and I believe that I have achieved their expectations. I hope they could also learn something from these practices and feel they were as rewarding as I felt it. I also appreciate a lot the help of Marc Farreras and I expect him to have learnt the same or more from my help than I have learnt from his.

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Appendix

A. Rotational Generators

1. $J_z |j,m\rangle = m\hbar |j,m\rangle$
2. $J_z^2 |j,m\rangle = (m\hbar)^2 |j,m\rangle$
3. $J_+ = J_x + iJ_y$
4. $J_- = J_x - iJ_y$
5. $J_x = \frac{J_+ + J_-}{2}$
6. $J_y = i\frac{J_- - J_+}{2}$
7. $J_+ |j,m\rangle = N_+(m) |j,m+1\rangle$
8. $J_- |j,m\rangle = N_-(m) |j,m-1\rangle$
9. $N_\pm(m) = \hbar\sqrt{j(j+1) - m(m\pm 1)}$
10. $J_x^2 = \frac{1}{4}(J_+^2 + J_-^2 + J_-J_+ + J_+J_-)$
11. $J_+^2 |j,m\rangle = N_+(m)N_+(m+1) |j,m+2\rangle$
12. $J_-^2 |j,m\rangle = N_-(m)N_-(m-1) |j,m-2\rangle$
13. $J_+J_- |j,m\rangle = N_+^2(m) |j,m\rangle$
14. $J_-J_+ |j,m\rangle = N_-^2(m) |j,m\rangle$

B. Spin 1 Operators

1. $S_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$
2. $S_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$
3. $S_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
4. $S_x^2 = \frac{\hbar^2}{2}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}$
5. $S_y^2 = \frac{\hbar^2}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}$
6. $S_z^2 = \hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
7. $|-1\rangle_z \equiv |-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$
8. $|0\rangle_z \equiv |0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$
9. $|1\rangle_z \equiv |1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$