The reevaluation of a modern physics course using a numerical simulation of a quantum controlled – not gate

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Abstract: In order to synthesize the knowledge of one semester advanced physics course for engineers in electronics and communications, we propose that the final project will have to make the connection with research. We also believe that this course should be available not only to engineers in electronics and communications, but also to all the electronics and mechatronics careers. The students will intellectually grow up very much if they can be involved in this type of process. The quantum computation process that we propose to be part of the final project takes in account that the students will also have to apply their knowledge of advanced linear algebra in order to understand and describe a process of non- resonant effects on four – spin molecules at room temperature. The four nuclear spins in each molecule represent a four – qubit complex. The interaction between the the qubits will be represented through an Ising type interaction. The modern physics course usually don't include the work with Hamiltonians, which is an important part of quantum mechanics. Introducing this project to the students we can achieve an extended and advanced presentation of the Zeeman effect with applications in quantum computation and also a close review of all the previous mathematics and physics courses. In this way we assure the connection between the academic part and the research process. The paper presents our proposal for this type of final project for the modern physics course, which will allow us to give a supplementary vision to the course and to the students.

Key words: - Research Academics Connection, Modern Physics Course, Engineering Careers in Electronics and Mechatronics

1 Introduction

Tecnológico de Monterrey is a system that has the mission to develop high level professionals, internationally competitive, in order to be an agent of change for the society. The mission of the university includes the involvement of the students in research relevant for the economic and politic development of the country [1]. Our university has a great interest in developing high trained students. We believe that this goal can be achieved also by using the final project of the modern physics course as a connection to research subjects. The modern physics course is addressed to students from the 4th semester for the career of engineer in electronics and communications. The aim of the course, based on the physics book of Raymond Serway and Robert Beichner [2], is to introduce the fundamentals of the special theory or relativity, quantum mechanics and statistical mechanics. Likewise, the fundamentals of solid physics and p-n union modeling are introduced. This is a theoretical course that is very useful for understanding the physical phenomena that underlie the electronics industry.

2 Problem Formulation

We believe that is very important for the students to become aware that they have to dominate very well the principles of the mathematics and physics courses in order to be able to work in a very demanding environment, which are the electronics and mechatronics industries. Many students are taking in account the fact that the mathematics and physics courses are just basic ones for their career; sometimes they do not see that this is the base for their future profession. We believe that these courses serve a lot in understanding processes, equipment functioning or in solving complex industry problems. Many times these mathematics and physics courses are not having a direct connection with industry or

research, the students are not able to see how the concepts of these courses are used at research and industry level, in order to solve complex, real problems.
Another problem we see is that the modern physics course is available just for engineers in electronics and communications.

3 Problem Solution

We believe that the modern physics course should be accessible for all type of engineering careers, or at least for all the careers in electronics and mechatronics, as it requires a synthesis of the knowledge of all mathematics and physics courses from the first 4 semesters. This course is also presenting a different vision of the physics and mathematics development in the XX century and makes the connection with present research problems. As future professionals, we believe that our students should be aware of this modern vision of science in general.
Nowadays, one of the very interesting subjects, among so many others, with direct applications in the future of the electronic industry is quantum computation. A lot of work has been done in this domain, but a lot of work remains to be done also [3], [4], [5]. We based the project for the modern physics course in an extended research work regarding numerical simulation of a quantum controlled - not gate process developed for a certain type of molecules at room temperature [6].
The students will learn how to define one qubit, which is the base of quantum computation, as a superposition of two basic states $|0\rangle$ and $|1\rangle$, instead of bits with values of "0" and "1" (which is the base of our present computation processes), as we can see from equation (1).

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \tag{1}$$

We should also emphasize the origin of quantum computation and the connection with the experiments of nuclear magnetic resonance (NMR) at room temperature [7]. It has to be introduced also the vision of some of the most important dynamics aspects, which is the influence of non – resonant interactions, arising from the time dependent Hamiltonian (H). The students will become familiar with the use of the Hamiltonian, as a powerful tool for describing the interaction between the molecules and electromagnetic field using the Zeeman effect, which is a subject of the modern physics course. Thus, the Zeeman effect will be presented in a complex theoretical and experimental way. It would be also emphasized the numerical influence of non – resonant effects on the dynamics of a single π pulse quantum controlled – not (CN) gate for a four - spin molecules, at room temperature. The interaction between the spins was assumed to be of the Ising type. The students would have to establish the region of parameters in which a single – pulse quantum CN gate can function at room temperature using the NMR technique. The method to be used, the one developed previously [6], the so- called "2πk method", consists in selecting the value of Rabi frequency (Ω_α) in order to suppress the unwanted transitions among various levels in the system. This method would be studied for the more complex case of four – spin molecules, at room temperature.
The students would have to set the conditions of the theoretical experiment and to work by themselves to find these conditions, as follows:

$$T \approx 300\,K \tag{2}$$

$$k_B T >> \hbar\omega_0 \tag{3}$$

The typical transition frequency:

$$\frac{\omega_0}{2\pi} \approx 10^8\,Hz \tag{4}$$

The typical condition for the spins:

$$\frac{\hbar\omega_0}{k_B T} \approx 10^{-5} \tag{5}$$

The Hamiltonian in the case of Ising interaction type should be defined as follows:

$$\mathrm{H} = -\sum_{\alpha=0}^{3} \vec{\mu}_\alpha \cdot \vec{B} - 2\hbar \sum_{\alpha=0}^{3} \sum_{\beta>\alpha} J_{\alpha\beta} I_\alpha{}^z I_\beta{}^z \tag{6}$$

The Hamiltonian that describes the dynamics of the four- spins molecule is:

$$H = H_0 + V \tag{7}$$

$$H_0 = -\hbar \sum_{\alpha=0}^{3} \left[\omega_\alpha I_\alpha{}^z + 2 \sum_{\beta>\alpha} J_{\alpha\beta} I_\alpha{}^z I_\beta{}^z \right] \qquad (8)$$

$$V = -\frac{\hbar}{2} \sum_{\alpha=0}^{3} \Omega_\alpha \left(e^{i\omega t} I_\alpha{}^+ + e^{-i\omega t} I_\alpha{}^- \right) \qquad (9)$$

The evolution equation of the density matrix for the tour-spines type molecules is the following:

$$i\hbar \left(\frac{d\rho}{dt} \right) = [H, \rho] \qquad (10)$$

It will be defined the density matrix for pure states (11), (12), (13), (14):

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)| \qquad (11)$$

$$\rho_{nm}(t) = \langle u_m | \rho(t) | u_n \rangle = \langle u_m | \psi(t) \rangle \langle \psi(t) | u_n \rangle \qquad (12)$$

$$\rho_{nm}(t) = c_m c^*{}_n \qquad (13)$$

$$i\hbar \rho = [H, \rho] \qquad (14)$$

For a set of states, the density matrix has the following expression (15):

$$\rho = \frac{e^{-\beta \hat{H}}}{tr\left(e^{-\beta \hat{H}}\right)} \qquad (15)$$

With the condition $E_k / k_B T << 1$, the density matrix becomes:

$$\rho = \frac{1}{N}\left(1 - \beta \hat{H}\right) \qquad (16)$$

The reduced density matrix will have the following expression:

$$\rho_r = \frac{\beta \hat{H}}{N} \qquad (17)$$

For the reduced density matrix, it has to be used the following condition (18):

$$tr(\rho_r) = 0 \qquad (18)$$

The application of the "$2\pi k$ method" will allow the students to obtain, after different other results, as can be observed in fig.1, the optimal conditions for errors suppression, as it is presented in fig.2, graph 4.

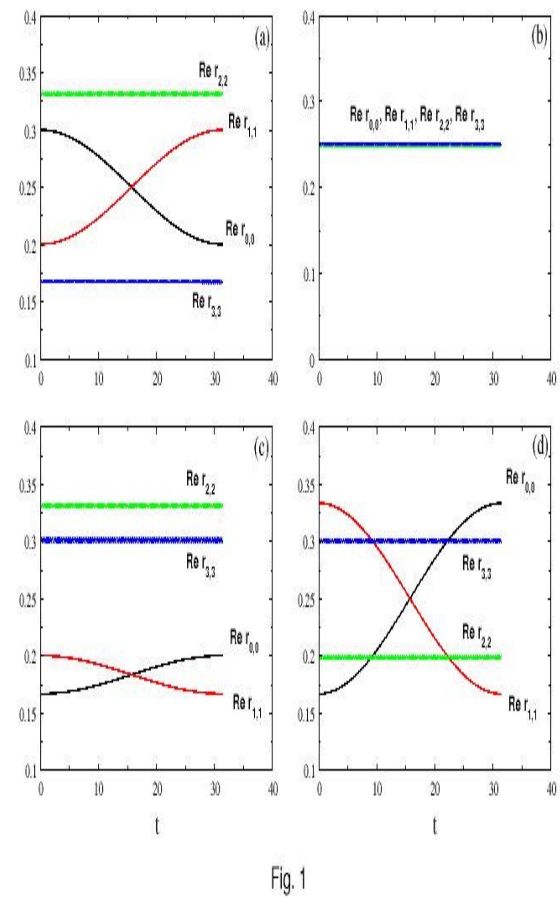

Fig.1 – The evolution of the first 4 diagonal, real elements of the reduced density matrix under the action of a π pulse.

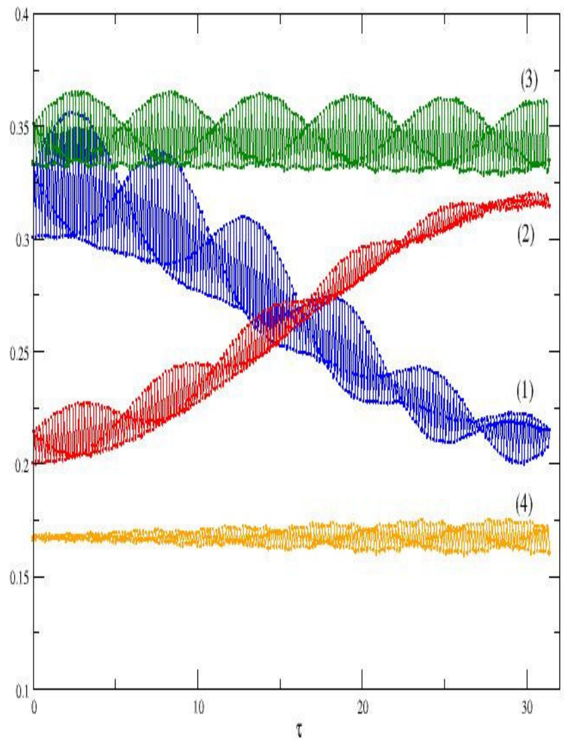

Fig.2 - Evolution of the reduced density matrix's real part (1): r00, (2): r11, (3): r22, y (4): r33 for $\Omega = 0.1$, $J+=J-=10$, $J=10$ y $J'=20$. From the graph 4 we can observe that the errors were successfully suppressed.

The process of numerical simulations showed in fig.1, using the $2\pi k$ method with different coupling constants, succeed to suppress the errors due to non – resonant transition for a quantum CN gate. This is a complex process during which the students will realize that of course other types of errors need to be taken in account, as the errors suppressed with this method are not the only one that can occur. The students will realize that this method can be applied for k – spin molecules, where k is higher than 4.

4 Conclusion

The modern physics course is an appropriate tool for emphasizing the importance of mathematics and physics basic courses. The involvement of the students in a research process during the modern physics course will give them the possibility to synthesize and develop all the knowledge of mathematics and physics courses of the first semesters. We believe that the quantum computation is an appropriate subject in order to emphasize the knowledge development and modern applications of quantum mechanics in general.

This course should be available to all engineering careers, as we see it as an important and powerful toll for developing the professional abilities of the students.

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