# Two dimensional spin systems in honeycomb lattices

Author: Núria Velasco Falguera
*Facultat de Física, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain.**

Advisor: Bruno Juliá-Díaz

**Abstract:** In this project we study and solve a 2D quantum system that consists of spins located in a honeycomb lattice. We first solve some particular simple cases, both analytically and numerically, and study their spectral properties. Then we show that we can map it into a fermionic system, and study this one.

## I. INTRODUCTION

Being able to solve particular systems can be useful to understand properties of some materials. Their energy levels, which we find when we solve the hamiltonian, determine the conductivity and resistivity of the material, and also have impact on its optical preperties, as well as other characteristics. [1] Therefore it is interesting to find ways of analytically solving them, so the results obtained can be accurate enough to describe the properties of the material.

In this work we consider the model proposed by Kitaev [2]. This model is very interesting as it hosts anyons, which are defined as particles that do not obey bosonic or fermionic statistics. Besides, Kitaev managed to map it into a fermionic system and solve it.

Anyons were first developed in a theoretical level, and then it was observed that they could exist in some excited levels of some specific systems.[2] Studying systems where there are anyons is intrinsically interesting, as we can work out some properties of these particles that only show in determinate circumstances. Furthermore, anyons were considered to be potentially useful to develop quantum computation in the context of topological quantum computation. [3]

The work is structured as follows, first, in Sec II we present the hamiltonian of the system and discuss the different terms. In Sec III we focus on the spectral properties of the system, first considering a subset and then the full unit cell of the honeycomb lattice. In Sec IV we present the mapping devised by Kitaev and explain how it is constructed. In Sec V we follow the steps that Kitaev makes in order to find an analytical solution to the system, and finally, in Sec VI we discuss the conclusions of this work.

## II. THE PHYSICAL SYSTEM

The system studied is a system of spins located in the vertices of a 2D honeycomb lattice. We consider that the spins have nearest neighbour interaction, with different strength depending on the direction of the link, as showed in Fig 1.

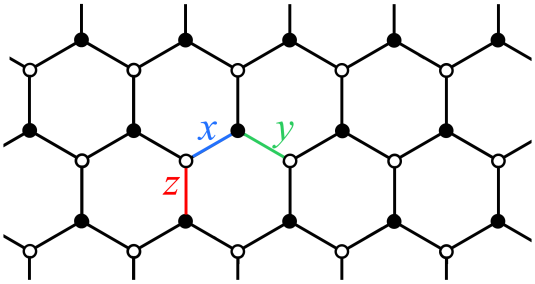


FIG. 1: A representation of the system studied, a 2D honeycomb lattice. We consider three directions, each one marked in a different color in the figure: $x$ in blue, $y$ in green and $z$ in red. We consider two sublattices, one marked by black sites, and one marked with white sites.

The system can be described by the following hamiltonian:

$$H = -J_x \sum_{x-\text{links}} \sigma_j^x \sigma_k^x - J_y \sum_{y-\text{links}} \sigma_j^y \sigma_k^y - J_z \sum_{z-\text{links}} \sigma_j^z \sigma_k^z, \tag{1}$$

where $\sigma^x$, $\sigma^y$ and $\sigma^z$ are the Pauli matrices, and the lower indices refer to which spin are we considering. $J_i$, $i = x, y, z$, are the strength constants of the interaction in the direction $i$. [2] We use the eigenstates of $\sigma^z$ as our base: $|\uparrow\rangle$ and $|\downarrow\rangle$, with $\sigma^z |\uparrow\rangle = |\uparrow\rangle$ and $\sigma^z |\downarrow\rangle = |\downarrow\rangle$.

### A. A simple example

In order to have a better understanding of the hamiltonian, we present the simple case of a 2-spin system connected by a $z$-link.

Particularizing the expression (1) the hamiltonian becomes:

$$H_{2s} = -J_z \sigma_1^z \sigma_2^z. \tag{2}$$

We obtain two energy levels, each one double degenerated: a ground state, formed by parallel spins, that is, $|\uparrow\rangle |\uparrow\rangle$ or $|\downarrow\rangle |\downarrow\rangle$, with energy $E = -J_x$, and a 1st excita-

*Electronic address: tfgac@ub.edu

tion state, formed by antiparallel spins, that is, $|\uparrow\rangle|\downarrow\rangle$ or $|\downarrow\rangle|\uparrow\rangle$, with energy $E = +J_x$.

## III. SPECTRAL PROPERTIES OF THE 3 AND 6 SPIN SYSTEM

We can compute the hamiltonian by calculating the tensor products between the pauli matrices that appear in the expression (1). We have a tensor product of Hilbert spaces, one for each spin. Therefore, when we write the tensor products, the sites where there is not a pauli matrix acting, there should be the identity matrix. For example, in the 3-spin case:

$$\sigma_1^x \sigma_2^x \equiv \sigma_1^x \otimes \sigma_2^x \otimes I_3.$$

Using this we calculate every term and sum them to obtain the hamiltonian. Then, diagonalizing it we obtain the eigenvalues and eigenvectors of the system. We do this both analytically and numerically, programming with python.

### A. 3-spin case

In this case, the expression (1) reduces to:

$$H_{3s} = -J_x \sigma_2^x \sigma_3^x - J_z \sigma_1^z \sigma_2^z, \tag{3}$$

and we use the following base: $|\uparrow\uparrow\uparrow\rangle$, $|\uparrow\uparrow\downarrow\rangle$, $|\uparrow\downarrow\uparrow\rangle$, $|\uparrow\downarrow\downarrow\rangle$, $|\downarrow\uparrow\uparrow\rangle$, $|\downarrow\downarrow\uparrow\rangle$, $|\downarrow\uparrow\downarrow\rangle$, $|\downarrow\downarrow\downarrow\rangle$. In this representation the hamiltonian is:

$$H_{3s} = \begin{pmatrix} J_z & 0 & 0 & J_x & 0 & 0 & 0 & 0 \\ 0 & J_z & J_x & 0 & 0 & 0 & 0 & 0 \\ 0 & J_x & -J_z & 0 & 0 & 0 & 0 & 0 \\ J_x & 0 & 0 & -J_z & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -J_z & 0 & 0 & J_x \\ 0 & 0 & 0 & 0 & 0 & J_z & J_x & 0 \\ 0 & 0 & 0 & 0 & 0 & J_x & -J_z & 0 \\ 0 & 0 & 0 & 0 & J_x & 0 & 0 & J_z \end{pmatrix}. \tag{4}$$

We obtain two energy levels, each one with degeneration 4: the ground state, with energy $-\sqrt{J_x^2 + J_z^2}$, and the 1st excitation, with energy $+\sqrt{J_x^2 + J_z^2}$.

We can examine the behaviour of the system as a function of the parameter $J_x$, represented in Fig 2. We observe two eigenvalues, a ground state and an excited state, which have a symmetrical behaviour with respect to zero. The ground state has value $-1$ when $J_x = 0$ and decreases linealy as $J_x$ increases, following $\lambda = -J_x$. The excited state is $+1$ for $J_x = 0$ and increases lineally as we increase the constant, following $\lambda = J_x$. This behaviour observed corresponds to the expected if we analyse the solutions we have just found. The two eigenvalues found analytically are $\pm\sqrt{J_x^2 + J_z^2}$. Therefore, when $J_x \longrightarrow 0$, the eigenvalues tend to $\lambda/J_z = 1$. On the other hand, when $J_x \gg J_z$ we can neglect the contribution of $J_z^2$ to the value of the eigenvalues, and therefore $\lambda = \pm J_x$, as observed in Fig 2.

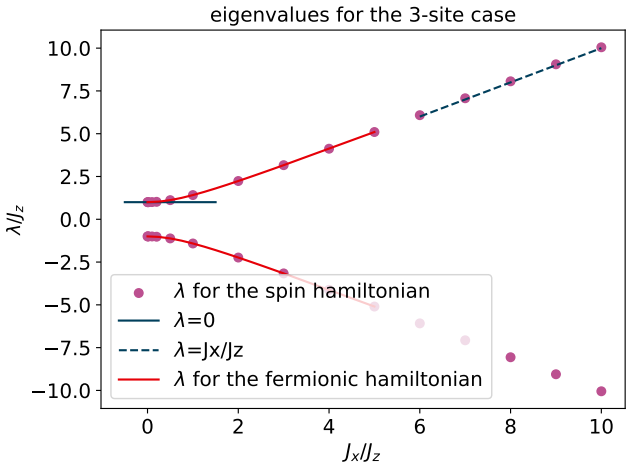


FIG. 2: Representation of the eigenvalues $\lambda/J_z$ as a function of the coefficient $J_x/J_z$. In purple dots we depic the eigenvalues of the spin hamiltonian, and in red lines, the eigenvalues of the fermionic hamiltonian. We also depic the two limit conditions: $\lambda = 0$ for $J_x \longrightarrow 0$ and $\lambda = J_x/J_z$ for $J_x \gg J_z$. We are using $J_z$ as the energy unit.

### B. 6-spin case

Let us now consider a more realistic case: a 6-spin case, which is the main unit of the honeycomb lattice. The hamiltonian is:

$$H = -J_x(\sigma_1^x\sigma_2^x + \sigma_4^x\sigma_5^x) - J_y(\sigma_2^y\sigma_3^y + \sigma_5^y\sigma_6^y) - J_z(\sigma_3^z\sigma_4^z + \sigma_6^z\sigma_1^z). \tag{5}$$

We consider $J_z$ as the energy unit. The behaviour of the system as a function of the coefficient $J_x/J_y$ is studied, and can be seen in Fig 3.

We can see that nine eigenvalues are obtained, and the behaviour of two limit cases can be analysed: $J_x \longrightarrow 0$

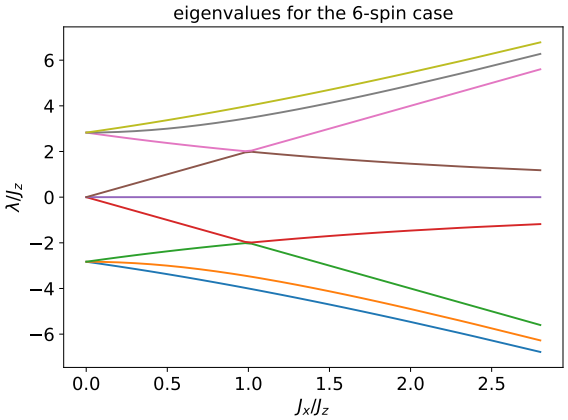


FIG. 3: Representation of the eigenvalues for the 6-spin case as a function of $J_x$, imposing $J_y = J_z$.

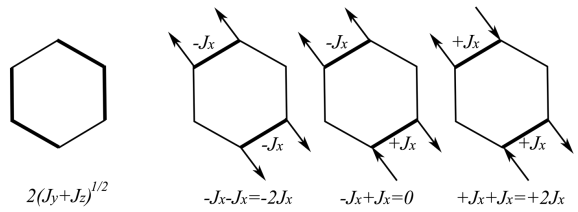


FIG. 4: Representation of the behaviour of the links in the limit cases of a 6-spin case. The relevant links in the interaction are represented with bold lines. The limit case $J_x \longrightarrow 0$ is the one on the left, and the possibilities for the limit $J_x >> J_y, J_z$, on the right.

and $J_x \gg J_y, J_z$.

For $J_x \longrightarrow 0$, the different eigenvalues converge around 3 values, $\lambda = -2\sqrt{2}, 0, 2\sqrt{2}$, see Fig 3. We can consider that there is no link in the direction $x$, as we can see in Fig 4 left, so the system can be considered as two independent 3-spin links. As we know the eigenvalues for a 3-spin case, found in section III A, we can add them up and obtain the following eigenvalues: $\lambda_- = \lambda_-^{(1)} + \lambda_-^{(2)} = -2\sqrt{2}$, $\lambda_0 = \lambda_-^{(1)} + \lambda_+^{(2)} = 0$ and $\lambda_+ = \lambda_+^{(1)} + \lambda_+^{(2)} = +2\sqrt{2}$, which correspond to the values observed in Fig 3.

We can see that the degeneration of the eigenvalues split when we increase $J_x$, because the $x$-links begin to take rellevance. For $J_x = J_y = J_z = 1$ two of the values coincide and we only have 7 different eigenvalues.

As we keep increasing $J_x$, the eigenvalues converge into only 3 lineal behaviours: one around 0 and the other ones symmetric, following $\lambda = \pm 2J_x$, see Fig 3. When $J_x \gg J_y, J_z$, the $x$-link has significatively more rellevance than the other two links, so, in a first approximation, we only have links in the $x$ direction. This will lead to these 3 possible behaviours, depicted in Fig 4, in the right.

### C. Avoided crossing

An avoided crossing occurs when the representations of two eigenvalues as a function of a parameter should cross, but due to a symmetry breaking, they do not cross and avoid each other instead. It happens when two parts of a hamiltonian do not commute with each other.[4]

Let us study a simple example of an avoided crossing phenomena to help us understand our case. Consider a lattice with hamiltonian $H(g) = H_0 + gH_1$, where $g$ is a parameter, and let's study the evolution of the eigenvalues as a function of the parameter $g$. In the specific case where $H_0$ and $H_1$ commute with each other, the eigenvectors are independent of $g$, but the eigenvalues of course change in function of $g$. An excited state can lower its value until, for some value $g_0$, the excited state and the ground state have the same energy. Therefore there is a crossing, and what was the ground state becomes the excited state, and viceversa. However, on a more general

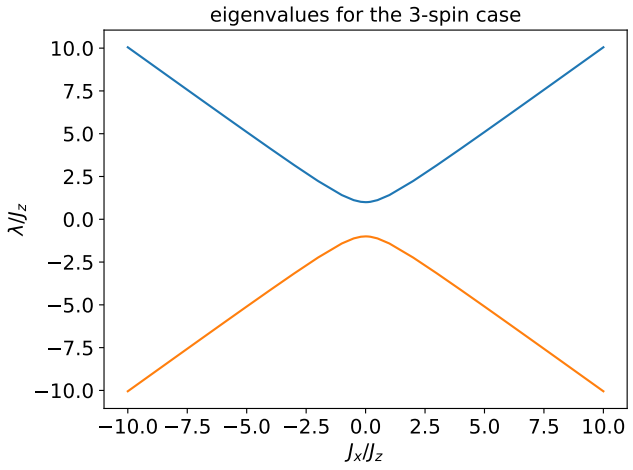


FIG. 5: Representation of the eigenvalues of the 3-spin case as a function of the coefficient $J_x/J_z$.

case where $H_0$ and $H_1$ do not commute, the point $g = g_0$ is not analytical, so what we observe is an avoided crossing. [4] We can now study this phenomena in the two cases we are considering.

#### 1. *Avoided crossing in a 3-spin system*

The hamiltonian in this case was the one in (3), and rewriting it:

$$H = -J_x H_x - H_z. \tag{6}$$

The two parts of this hamiltonian, $H_x$ and $H_z$, do not commute with each other, so there must be an avoided crossing. This is indeed what we observe in Fig 5, where the two eigenvalues of the system seem like they should cross but they do not, there is an avoided crossing.

#### 2. *Avoided crossing in a 6-spin system*

In Fig 3 we observed a crossing between two eigenvalues. Remember that the case considered there is quite symmetric, as $J_y = J_z$. However, if we slightly break this symmetry by imposing, for example, $J_y = 1.1J_z$, depicted in Fig 6, the different parts of the hamiltonian do not commute with each other, and then we observe an avoided crossing.

## IV. MAPPING THE SPINS INTO FERMIONS

The hamiltonian can be mapped into a free fermionic hamiltonian. We now follow the steps needed to make this transformation.

To understand this mapping, we first introduce the creation and annihilation operators: The creation operator,

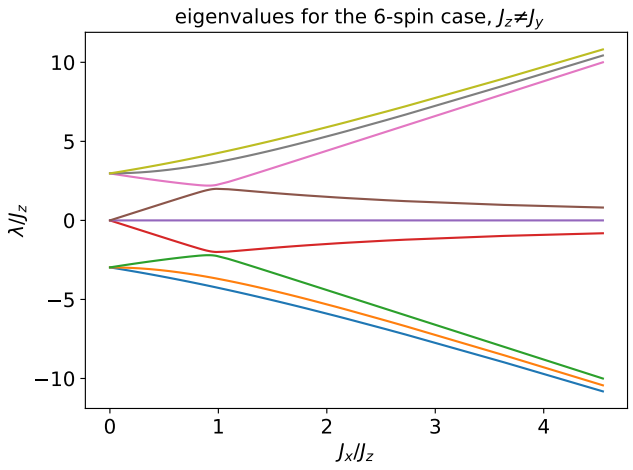


FIG. 6: Representation of the eigenvalues as a function of the coefficient $J_x/J_z$, imposing $J_y = 1.1J_z$ to break the symmetry there is in Fig 3.

named $a_k^\dagger$, creates a particle in the single particle state $k$, whereas the annihilation operator, denoted $a_k$, destroys a particle in the single particle state $k$.[6]

From these operators we can build the Majorana operators [2]:

$$c_{2k-1} = a_k + a_k^\dagger; \tag{7}$$

$$c_{2k} = \frac{a_k - a_k^\dagger}{i}, \tag{8}$$

which obey fermionic anticommutation roules.

We can create Fock states, $|n_1, n_2, ..., n_m\rangle$, where $n_k$ determines the number of particles in the state $k$. As we work with fermions, $n_k = 0, 1$.

Each spin leads to 2 fermionic levels. So when we map from spin to fermion, in each site where we had a spin we can either have one fermion of type $\uparrow$, one fermion of type $\downarrow$, both of them, or none of them. Therefore, particularizing the operators in Eq. (8), for each site we have the following Majorana operators:

$$b^x := c_1 = a_1 + a_1^\dagger; \tag{9}$$

$$b^y := c_2 = \frac{a_1 - a_1^\dagger}{i}; \tag{10}$$

$$b^z := c_3 = a_2 + a_2^\dagger; \tag{11}$$

$$c := c_4 = \frac{a_2 - a_2^\dagger}{i}. \tag{12}$$

The base we use is the following: in each site we have $|00\rangle, |10\rangle, |01\rangle, |11\rangle$ where the first number indicates the number of fermions of type $\uparrow$, and the second number, the number of fermions of type $\downarrow$.

These operators help us transform the spin system into a fermionic system, with a change proposed in [2] given by:

$$\tilde{\sigma}^x = ib^x c \; ; \; \tilde{\sigma}^y = ib^y c \; ; \; \tilde{\sigma}^z = ib^z c, \tag{13}$$

and $\tilde{\sigma}^i$ act as an extension of the Pauli Matrices extended to the Fock space.

Going back to building the hamiltonian, we can now substitute the Pauli matrices for the operators we have just built in (13), and the hamiltonian becomes:

$$H_f = \sum_{j,k} 2J_{\alpha_{jk}} b_j^\alpha c_j b_k^\alpha c_k = \frac{i}{4} \sum_{j,k} 2J_{\alpha_{jk}} u_{jk} c_j c_k, \tag{14}$$

where we have defined the following operators:

$$u_{jk} = ib_j^{\alpha_{jk}} b_k^{\alpha_{jk}}. \tag{15}$$

The operators $u_{jk}$ commute with the hamiltonian, so we can split the space into eigenspaces [2] of $u_{jk}$ and treat them as numbers, corresponding to their eigenvalues $u_{jk} = \pm i$. This means that we have a sum over all the pairs of sites where we multiply two operators of the 2nd type of fermions ($c_j c_k$) by constants.

This hamiltonian can be solved analytically, as we do in section V. However, let us first consider some easy cases to have a better understanding of the system obtained.

### A. Some particular cases

### B. 2-site case

Let us consider a simple case, using $J_z$ as the energy unit. We obtain $\lambda_{12} = \pm 1$ as eigenvalues, each one with degeneration 8. This value corresponds to $\lambda_{12} = \pm J_z$, which is the same result we obtained using the spin hamiltonian.

### C. 3-site case

In this case the hamiltonian is:

$$H_{3f} = \frac{i}{2}(J_x(u_{12}c_1c_2 + u_{21}c_2c_1) + J_z(u_{23}c_2c_3 + u_{32}c_3c_2)). \tag{16}$$

We have 3 sites, in which we can have 2 types of fermions ($\uparrow$ or $\downarrow$). Therefore, our basis has the form $|n_1 n_2 n_3\rangle$, where $n_i = 0, 1, 2$. However, we can see that as the operators are of the form $c$, they only affect the 2nd type of fermions, so we can use a basis $|n_1 n_2 n_3\rangle$, where $n_i = 0, 1$.

We can study the behaviour of the system as a function of the parameter $J_x$.

As seen in Fig 2, the eigenvalues for this fermionic hamiltonian, depicted in a red line, correspond to the ones obtained for the 3-spin case, depicted in purple dots.

This case can also be solved analytically, writing the hamiltonian and diagonalizing it, and we obtain the same solutions as we did for the spin case.

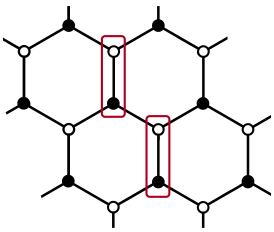

FIG. 7: Representation of the lattice, marking with a rounded rectangle the new considered unit cells. Inside each unit cell, which is determined by the index $s$, there are two types of sites, black and white, distinguished by the index $\lambda$.

## V. FINDING THE ANALYTICAL SOLUTION

Once we have the fermionic hamiltonian, we can find the analytical solution to the complete system.

We work with a new characterization of the sites: we define a unit cell [2], which is formed by two sides linked by a $z$-link. Each site $j$ is represented by the indices $(s, \lambda)$, where $s$ refers to the unit cell and $\lambda$ to the position type inside the cell. This characterization can be seen in Fig 7.

With this new notation, our hamiltonian becomes:

$$H = \frac{i}{4}\sum 2J_{\alpha_{s\lambda,t\mu}} u_{s\lambda,t\mu} c_{s\lambda} c_{t\mu} = \frac{i}{4}\sum A_{\alpha_{s\lambda,t\mu}} c_{s\lambda} c_{t\mu}. \tag{17}$$

We pass this hamiltonian to the momentum representation by using the fourier transform. We use that $J$ and $u$ only depend on $\lambda$, $\mu$ and $t-s$, so we fix $s=0$ and the index $t$ scans the system:

$$\tilde{A_{\lambda\mu}}(\mathbf{q}) = \sum_t e^{i(\mathbf{q},\mathbf{r}_t)} A_{0\lambda,t\mu} \tag{18}$$

In each site we will only sum for the three sites that are nearest neighbors of the site considered, so this sum for all the terms will end up only having 3 terms. We need to find the spectrum of $i\tilde{A}_{\lambda\mu}$, which corresponds to the eigenvalues of the system. To do so, we compute $\tilde{A}_{\lambda\mu}$, which will be a 2x2 matrix. The diagonal terms are 0, because they correspond to the ones occupying the same type of site inside a unit cell, which are never linked. We calculate the two non diagonal terms and we obtain:

$$\begin{aligned} \sum_t e^{i(q,r_t)} 2J_{\alpha_{0\lambda,t\mu}} u^{std}_{0\lambda,t\mu} = \\ 2(e^{i(q,v_1)} J_y u_y + e^{i(q,v_2)} J_x u_x + e^{i(q,v_3)} J_z u_z) = \\ 2(e^{i(q,v_1)} J_y + e^{i(q,v_2)} J_x + J_z), \end{aligned} \tag{19}$$

where we name 1, 2 and 3 the different sites with whom our site interacts. Diagonalizing it, we find that these are the eigenvalues of $i\tilde{A}$, so the result in (19) are the spectrum of the fermionic system.

## VI. CONCLUSIONS

In this work we have studied a particular system consisting of spins situated in a 2D honeycomb lattice. We have been able to solve particular cases, as well as the general case. The conclusions that derive from this work are the following:

We have studied the spectrum of the system as a function of the coupling parameters, which has helped us understand the behaviour of the system. We have also focused on the avoided crossing phenomena, and we have seen that it can occur or not depending on the symmetry of the system.

Following the work of Kitaev, we have also successfully mapped a spin system into a fermionic system, and that has allowed us to analytically solve the problem. As expected, the solutions we have obtained for the fermionic system and the spin system have been the same, and have helped us understand the system considered.

In a further work we would like to analyse the solution found analytically in detail, study the different phases, and in particular we would also like to consider the anyonic phases and their behaviour.

### Acknowledgments

I would like to express my profound gratitude to Bruno Juliá, the supervisor of this work, because his direction and dedication have allowed me to improve my way of working, and I am very thankful for everything he has helped me learn during this semester. I am also deeply grateful to my family and friends, for the support and encouragement they have given me.

[1] C. Kittel, *Introduction to Solid State Physics*, 8th. ed. (John Wiley & Sons, New York, 2005)

[2] A. Kitaev: "Anyons in an exactly solved model and beyond". Annals of Physics **321**, 2, (2006).

[3] H. Bombín, "Topological codes," in Lidar, D. A. and Brun, T. A. (eds) *Quantum Error Correction.* Cambridge University Press, pp. 455–481, (2013).

[4] S. Sachdev, *Quantum phase transitions*, 2nd. ed. (Cambridge University Press, Cambridge, 1999).

[5] J.M. Leinaas, J. Myrheim, "On the theory of identical particles". Nuovo Cim B **37**, 1–23 (1977).

[6] B. Juliá-Díaz, "Mecánica cuántica de N cuerpos y sistemas ultrafríos", Notes of the subject, unpublished.