

Introduction to the Hubbard Model

Author: Juan Luis Díaz Jiménez

Facultat de Física, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain.

Advisor: Maria dels Àngels Garcia Bach

Abstract: The Hubbard model is very important for the study of magnetic phenomena and strongly correlated electron systems. This work serves as an introduction to the Hubbard model and a presentation of the elements necessary to reach it. Here it is applied to a simple case to see how you work with it.

I. INTRODUCTION

John Hubbard, at the beginning of 1960, proposed in a series of articles a model to describe electrons in transition metal monoxides and electron correlation in narrow energy bands. Due to the complexity of the study of these systems given the vast amount of bounds and continuum electron energy levels, Hubbard proposed to reduce the study to a single localized orbital level per site. This model opens the door to study the interactions between electrons, giving rise to insulating, magnetic, and even novel superconducting effects in a solid.

But before talking about the Hubbard model it is necessary to introduce Bloch's theorem used for delocalised studies.

II. THE BLOCH'S THEOREM

A. Schrödinger's equation

To describe the steady states of all the particles of a solid we use Schrödinger's equation

$$H\Psi = E\Psi \quad (1)$$

where H is the hamiltonian of the solid, Ψ is the wave function of the steady state and E is the energy of the solid in this state.

The Hamiltonian is the sum of the operators of kinetic energy and potential energy.

$$H = K + U, \quad K = K_e + K_n, \quad U = U_{ee} + U_{nn} + U_{en} \quad (2)$$

K_e and K_i are the kinetic operators for the electrons and ions respectively. U_{ee}, U_{ii}, U_{ei} are the potential operators for interactions between electrons, ions and electron and ion.

Due to the number of variables that we have in the equation, it is necessary to make some approximations.

1. Valence approximation. We assume that the electrons in the inner layers are attached to the nucleus forming an ion. Therefore we only take into account the most external electrons, the valence electrons, to work with the solid Hamiltonian.

$$K_n \approx K_i, \quad U_{nn} \approx U_{ii}, \quad U_{en} \approx U_{ei}$$

2. Born-Oppenheimer approximation: We assume that the ions in their equilibrium position are at rest. We can do this approximation because the mass of the ions is larger than the mass of the electrons, therefore the speed of the electrons will be much greater than that of the ions.

$$K_i \approx 0, \quad U_{ii} \approx \text{constant (negligible)}, \quad U_{ei} \approx U_{ei}^0$$

3. Independent electron approximation: We approximate the interaction energy as the sum of the interaction energies of the valence electrons.

$$U_{ee} + U_{ei}^0 \approx \sum_i (U_i(\mathbf{r}_i) + W_i(\mathbf{r}_i)) = \sum_i V_i(\mathbf{r}_i) \quad (3)$$

$U_i(\mathbf{r}_i)$ is the average potential energy created by the ions on the electron i and $W_i(\mathbf{r}_i)$ is the interaction energy of the electron i with the effective field created by the rest of electrons, in which each electron moves independently.

With all these approaches the Hamiltonian of the solid has been reduced to the Hamiltonian for the valence electrons in the solid, as seen as independent particles. From now on, H is understood in this sense.

$$H = \sum_j H_j = \sum_j K_j + V_j = \sum_j -\frac{\hbar^2}{2m} \nabla_j^2 + (U_j(\mathbf{r}_j) + W_j(\mathbf{r}_j)) = \sum_j h_j \quad (4)$$

The solution to the Schrödinger's equation associated with this Hamiltonian can be written as an antisymmetrized product of monoelectric wave functions $\varphi_i(\mathbf{r}_i)$, where $\Phi = \varphi_1(\mathbf{r}_1)\varphi_2(\mathbf{r}_2)\dots\varphi_N(\mathbf{r}_N)$

$$h_i\varphi_i = \epsilon_i\varphi_i \quad (5)$$

The Hamiltonian is independent of spin. The solutions of H give us the part of the space of the wave function. The function of the electron will be $\varphi \otimes \sigma$ where σ is the spin. To refer to the spatial part we use φ and to refer to the function of the electron considering also the spin we use Φ .

The energy of the solid is the sum of all ϵ_i , $E = \sum_i \epsilon_i$.

B. Bloch functions

To find the Bloch functions it is necessary to solve (5).

We must bear in mind that if the ionic nuclei are distributed periodically and regularly we can assume that the potential $V(\mathbf{r})$ has the periodicity of the Bravais lattice. Therefore we can develop $V(\mathbf{r})$ in Fourier series

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}$$

$$V_{\mathbf{G}} = \frac{1}{V_c} \int_{cell} V(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r} \quad (6)$$

Where \mathbf{G} are the vectors of the reciprocal lattice and V_c is the volume of the cell.

Since $V(\mathbf{r})$ has the periodicity of the Bravais lattice, the probability density of the stationary states must also have this probability. The wave functions associated with these states that meet this condition are of the form:

$$\varphi(\mathbf{r}) = e^{if(\mathbf{r})} u(\mathbf{r}) \quad (7)$$

$u(\mathbf{r})$ have the periodicity of the lattice and $f(\mathbf{r} + \mathbf{R}) = f(\mathbf{r}) + f(\mathbf{R})$, where $f(\mathbf{R}) = \mathbf{k} \cdot \mathbf{R}$. This

$$\mathbf{k} = \sum_{i=1}^3 \frac{n_i}{N_i} \mathbf{b}_i \quad (8)$$

is a constant vector where \mathbf{b}_i are the vectors of the base of the reciprocal lattice and N_i are the numbers of cells of the direct lattice in the direction i .

Bloch's theorem says that the value of a Bloch function subjected to a translation \mathbf{R} in the lattice of Bravais differs in a phase $e^{i\mathbf{k}\cdot\mathbf{R}}$. The probability density is a real value.

$$\varphi(\mathbf{r} + \mathbf{R}) = e^{if(\mathbf{r}+\mathbf{R})} u(\mathbf{r} + \mathbf{R}) = e^{if(\mathbf{R})} e^{if(\mathbf{r})} u(\mathbf{r}) = e^{if(\mathbf{R})} \varphi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{R}} \varphi(\mathbf{r}) \quad (9)$$

The Bloch functions are

$$\varphi(\mathbf{k}, \mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u(\mathbf{r}) \quad (10)$$

III. WANNIER FUCTIONS

The Bloch functions are periodic in \mathbf{k} -space. Therefore they have a Fourier series in plane waves in the reciprocal of the reciprocal space, that is in the direct space. φ_n can be written like this:

$$\varphi_n(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{N}} \sum_j W_n(\mathbf{R}_j, \mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{R}_j}, \quad (11)$$

The functions $W_n(\mathbf{R}_j, \mathbf{r})$ are the Wannier functions. They can be calculated from the Bloch functions

$$W_n(\mathbf{R}_j, \mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \varphi_n(\mathbf{k}, \mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{R}_j} \quad (12)$$

The summation is over all \mathbf{k} -vectors in a Brillouin zone.

Each Wannier function is centered at the midpoint of the cell. In addition, Wannier functions form an orthonormal complete basis

$$\int W_n^*(\mathbf{R}_i, \mathbf{r}) W_m(\mathbf{R}_j, \mathbf{r}) d\mathbf{r} = \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} e^{i\mathbf{k}\cdot\mathbf{R}_i - i\mathbf{k}'\cdot\mathbf{R}_j} \int \varphi_n^*(\mathbf{k}, \mathbf{r}) \varphi_m(\mathbf{k}', \mathbf{r}) d\mathbf{r} = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \delta_{nm} = \delta_{nm} \delta_{ij} \quad (13)$$

As it is a complete base

$$\mathbf{I} = \sum_i |W_n(\mathbf{R}_i, \mathbf{r})\rangle \langle W_n(\mathbf{R}_i, \mathbf{r})| \quad (14)$$

Therefore we can say that Wannier functions are localized orthonormal functions about individual points in the lattice. In other hand, Bloch functions are extended functions. The transformation between both functions is a unitary transformation, i.e. the Hilbert space generated by both is the same. Thanks to this we can work with one or other according to our needs.

The Wannier functions are a great tool to work in situations where the spatial position of electrons plays an important role. The most important areas of application are:

1. Attempt to derive a transport theory for Bloch electrons.
2. Phenomena involving localized electronic levels.
3. Magnetic phenomena.

Since the Wannier functions are located on the lattice knots, they can be written as a linear combination of atomic functions. As we only take into account the valence electrons of each atom, we can assume that often each Wannier function can be approximated by an atomic function or an specific linear combination of (quasi-)degenerated atomic functions determined by the atoms with which we are working. For example if we are studying a copper lattice the Wannier function could be $W \sim \chi_{3d_x^2-y^2}$.

When approximate Wannier functions by atomic functions we lose the property of orthogonality between Wannier functions centered on different cells because the atomic functions can overlap with the functions of the neighboring atoms (and the atomic functions are not orthogonal unlike the Wannier functions) as we can see in Fig.(1).

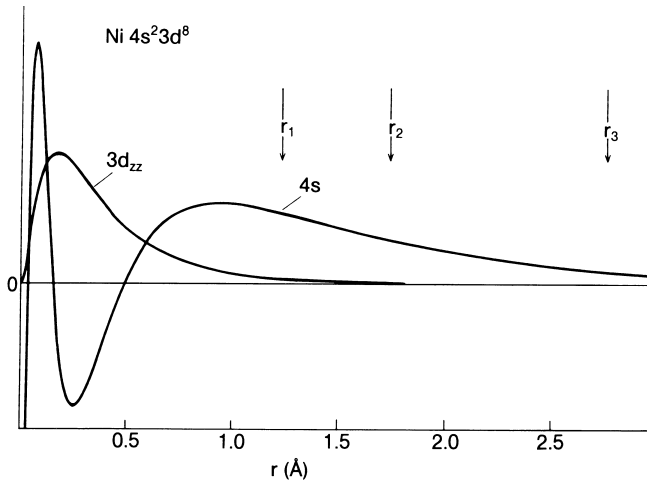


FIG. 1: Interaction of two atomic functions depending on the semidistance. r_1 , r_2 and r_3 they are the semidistance to the first, second and third neighbor. We can see that the 4s function is much more extended than the 3d function, therefore it will overlap with more functions.

If the Wannier functions with which we are going to work can be approximated by little extended atomic functions then we can suppose that the orthonormality is a good approximation, since we are only interested in interactions with first neighbors.

IV. THE HUBBARD MODEL

Let's recover the associated Hamiltonian to the solid $H = K_e + U_{ee} + U_{ei}^0 + U_{ii}^0 + U_{medium} - U_{medium}$. Therefore

$$K_e + U_{ei}^0 + U_{ii}^0 + U_{medium} \equiv \sum_j h_j$$

$$U_{ee} - U_{medium} \equiv \frac{1}{2} \sum_{ij} g(\mathbf{r}_i, \mathbf{r}_j)$$

$$H = \sum_j h_j + \frac{1}{2} \sum_{ij} g(\mathbf{r}_i, \mathbf{r}_j) \quad (15)$$

Where $g(\mathbf{r}_i, \mathbf{r}_j) = \frac{e^2}{4\pi\epsilon_0} |\mathbf{r}_i - \mathbf{r}_j|$.

Now we can rewrite the Hamiltonian through the Wannier functions and the creation and destruction operators.

A. Creation and destruction operators

The operator $c_{m\sigma}^+$ creates a electron in a state $W_m(\mathbf{R}_i, \mathbf{r})$ with spin $\sigma \in \{\alpha, \beta\}$ (where α is for spin up and β is for spin down). This is the creation operator.

The operator $c_{m\sigma}$ destroys a electron in a state $W_m(\mathbf{R}_i, \mathbf{r})$ with spin $\sigma \in \{\alpha, \beta\}$. This is the destruction operator.

Since these operators work with electrons (which are fermions) and wave functions must be antisymmetric,

they must comply with the anticommutation relations of two operators.

$$\{c_{i\sigma}, c_{j\sigma'}^+\} = \delta_{ij}\delta_{\sigma\sigma'}, \{c_{i\sigma}^+, c_{j\sigma'}^+\} = 0, \{c_{i\sigma}, c_{j\sigma'}\} = 0 \quad (16)$$

Let's see an example of how these operators work: If we have the state $|\alpha, \beta, \alpha, \beta\rangle$ and the operators $c_{1\beta}^+, c_{1\alpha}^+, c_{1\alpha}, c_{2\beta}, c_{2\alpha}^+$ then

$$c_{1\beta}^+ |\alpha, \beta, \alpha, \beta\rangle = |\beta\alpha, \beta, \alpha, \beta\rangle$$

$$c_{1\alpha}^+ |\alpha, \beta, \alpha, \beta\rangle = 0$$

$$c_{1\beta}^+ c_{2\beta} |\alpha, \beta, \alpha, \beta\rangle = |\alpha\beta, 0, \alpha, \beta\rangle$$

$$c_{1\alpha} c_{2\alpha}^+ |\alpha\beta, 0, \alpha, \beta\rangle = |\beta, \alpha, \alpha, \beta\rangle \quad (17)$$

B. Representation of the Hamiltonian according to Wannier functions

Now that we have seen how the creation and destruction operators work and some of their properties, we can use them to rewrite the Hamiltonian using the Wannier functions. We want to write the Hamiltonian as a function of the destruction and creation operators. For this we will use that the Wannier functions are a complete base

Taking the Hamiltonian from (15)

$$\sum_j h_j = \mathbf{I} \sum_j h_j \mathbf{I}' =$$

$$\sum_{ni\sigma} |W_{n\sigma}(\mathbf{R}_i, \mathbf{r})\rangle \langle W_{n\sigma}(\mathbf{R}_i, \mathbf{r})| \sum_j h_j$$

$$\sum_{mj\sigma'} |W_{m\sigma'}(\mathbf{R}_j, \mathbf{r})\rangle \langle W_{m\sigma'}(\mathbf{R}_j, \mathbf{r})| \quad (18)$$

$$|W_{n\sigma}(\mathbf{R}_i, \mathbf{r})\rangle \equiv c_{ni\sigma}^+$$

$$\langle W_{m\sigma}(\mathbf{R}_j, \mathbf{r})| \equiv c_{mj\sigma}$$

$$\langle W_{n\sigma}(\mathbf{R}_i, \mathbf{r})| \sum_j h_j |W_{m\sigma}(\mathbf{R}_j, \mathbf{r})\rangle \equiv h_{nmij} \quad (19)$$

$$\sum_j h_j = \sum_{nm} \sum_{ij} \sum_{\sigma} h_{nmij} c_{ni\sigma}^+ |0\rangle \langle 0| c_{mj\sigma} =$$

$$\sum_{nm} \sum_{ij} \sum_{\sigma} h_{nmij} c_{ni\sigma}^+ c_{mj\sigma} \quad (20)$$

Since g is a function of two variables, the identities that we will use will be

$$\mathbf{I} = \sum_{nmij\sigma\sigma'} |W_{n\sigma}(\mathbf{R}_i, \mathbf{r})\rangle \langle W_{m\sigma'}(\mathbf{R}_j, \mathbf{r})| \langle W_{m\sigma'}(\mathbf{R}_j, \mathbf{r})| W_{n\sigma}(\mathbf{R}_i, \mathbf{r})| \quad (21)$$

$$\begin{aligned} \sum_{ij} g(\mathbf{r}_i, \mathbf{r}_j) &= \mathbf{I} \sum_{ij} g(\mathbf{r}_i, \mathbf{r}_j) \mathbf{I}' = \\ \sum_{nmn'm'} \sum_{ijkl} \sum_{\sigma\sigma'} &\langle W_n(\mathbf{R}_i, \mathbf{r}) W_m(\mathbf{R}_j, \mathbf{r}') | \\ &*g(\mathbf{r} - \mathbf{r}') | W_n'(\mathbf{R}_k, \mathbf{r}) W_m'(\mathbf{R}_l, \mathbf{r}') \rangle \\ &*c_{ni\sigma}^+ c_{mj\sigma'}^+ c_{m'l\sigma'} c_{n'k\sigma} \end{aligned} \quad (22)$$

We reduce our study to the case of a single band, therefore $m = n = 1$ and

$$h_{ijnm} = h_{ij} = \langle W(\mathbf{R}_i, \mathbf{r}) | h(\mathbf{r}) | W(\mathbf{R}_j, \mathbf{r}') \rangle \quad (23)$$

$$g_{ijkl} = \langle W(\mathbf{R}_i, \mathbf{r}) W(\mathbf{R}_j, \mathbf{r}') | g(\mathbf{r} - \mathbf{r}') | W(\mathbf{R}_k, \mathbf{r}) W(\mathbf{R}_l, \mathbf{r}') \rangle \quad (24)$$

Now our Hamiltonian can be written as

$$H = \sum_{ij} \sum_{\sigma} h_{ij} c_{i\sigma}^+ c_{j\sigma} + \frac{1}{2} \sum_{ijkl} \sum_{\sigma\sigma'} g_{ijkl} c_{i\sigma}^+ c_{j\sigma'}^+ c_{l\sigma'} c_{k\sigma} \quad (25)$$

We use Hubbard's approximations to rewrite h_{ij} and g_{ijkl} .

If $i \neq j$ then $h_{ij} = -t$ when i, j are nearest neighbors, and zero otherwise. This is the hopping term.

For g_{ijkl} , if $i = j = k = l$ then $g_{ijkl} = U$. For the rest of the cases $g_{ijkl} = 0$.

Therefore Hubbard's Hamiltonian is

$$H = -t \sum_{\langle ij \rangle} \sum_{\sigma} c_{i\sigma}^+ c_{j\sigma} + U \sum_i c_{i\alpha}^+ c_{i\beta}^+ c_{i\beta} c_{i\alpha} \quad (26)$$

C. Physical interpretation of Hubbard's Hamiltonian

Due to Born-Oppenheimer approximation the atoms in the lattice are still and the electrons in the last layer move. This is a good approximation for a solid with only one relevant orbital. Each site of the lattice is limited by the Pauli Exclusion Principle, therefore in each one we can only have: an empty site, a one electron with spin up, one electron with spin down or two electrons with spin up and down.

As the electrons can move, they interact through Coulomb interaction. The biggest interaction will be that of two electrons occupying the same site. We will assume that the contribution to the energy is 0 if the site is empty or with only one electron, or U if the site is doubly occupied. With the term $U c_{i\alpha}^+ c_{i\beta}^+ c_{i\beta} c_{i\alpha}$ we express this fact.

To express the kinetic energy of the electrons when moving from one place to another neighbor, we can suppose that one electron is destroyed in the first site and another is created in the next. The energy of this jump is denoted by t and will be determined by the overlapping of two wave functions of the pair of atoms. The approximation that they can only jump to spaces that

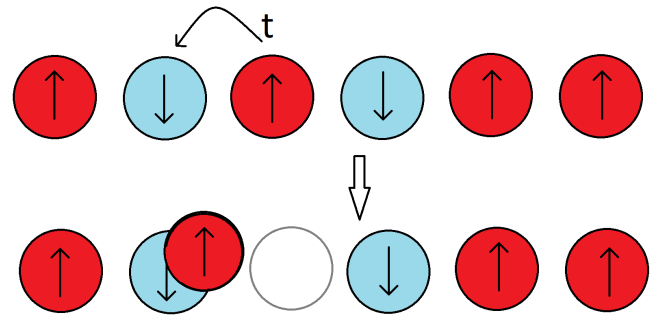


FIG. 2: Pictoric representation of the kinetic term t in the Hubbard Hamiltonian.

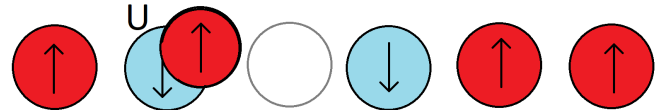


FIG. 3: Pictoric representation of the one site repulsion term U in the Hubbard Hamiltonian.

are first neighbors is due to the wave functions decrease exponentially.

The term U in absence of the t ($U \gg t$) would favor local magnetic moments, since it would suppress the possibility of a second electron at singly occupied sites. In this case, the energy levels are determined by the number of double occupied sites and the number of electrons in relation to the number of sites.

If the term U is the one that is absent ($t \gg U$), this causes the electrons of the system to spread throughout the solid. In this case it will not be necessary to use the Hubbard model and we can study the electrons with the Bloch model, since the functions that describe the electrons will be more extended.

When both terms are present, despite the simplicity of the model, the analytical study is quite complicated.

Normally U and t are calculated with a molecular cluster model or are deduced from experimental values.

D. Diagonalization of the 4-site Hubbard Hamiltonian

Because the most common diagonalization that we find in the literature is for the Hamiltonian with 2-sites, here I present the work method for the Hamiltonian of 4-sites. The objective will be to calculate the energy as an eigenvalue of the Hubbard matrix and study how this varies with t and U . It consists of a one-dimensional lattice with four sites occupied by four electrons, two with spin up and two with spin down. The lowest energy states are those with each site occupied by only one electron (This configuration is a degenerated state of energy 0).

As we have said before we assume that electrons can only interact with first neighbors. Also, as a first approx-

imation, we will also assume that there can only be one site doubly occupied.

The first thing we will do is create a base in the Hilbert space with the occupation numbers. The first 6 elements of the base that we take are the neutral states

$$\begin{aligned} |\alpha, \beta, \alpha, \beta\rangle &= e_1, |\alpha, \alpha, \beta, \beta\rangle = e_2, \\ |\beta, \alpha, \beta, \alpha\rangle &= e_3, |\alpha, \beta, \beta, \alpha\rangle = e_4, \\ |\beta, \beta, \alpha, \alpha\rangle &= e_5, |\beta, \alpha, \alpha, \beta\rangle = e_6, \end{aligned}$$

Applying the Hamiltonian to e_i we find other possible combinations of these four electrons.

The total number of combinations (with the above restrictions) between the four electrons is 30, that is, our Hilbert space has dimension 30 and is made up of 30 components. We apply H to e_1 :

$$\begin{aligned} H|\alpha, \beta, \alpha, \beta\rangle &= -t|0, \alpha\beta, \alpha, \beta\rangle - t|\alpha\beta, 0, \alpha, \beta\rangle \\ &+ t|\alpha, 0, \alpha\beta, \beta\rangle + t|\alpha, \alpha\beta, 0, \beta\rangle - t|\alpha, \beta, 0, \alpha\beta\rangle - \\ &\quad t|\alpha, \beta, \alpha\beta, 0\rangle = \\ &-te_7 - te_8 + te_9 + te_{10} - te_{11} - te_{12} \end{aligned} \quad (27)$$

Realizing this same calculation for the remaining elements of the base we obtain the matrix of the Fig. (4).

FIG. 4: Matrix for the 4-site Hubbard Hamiltonian.

If we allow two doubly occupied sites, we just have to add five more elements to the base, the $2U$ terms would appear on the diagonal and the terms t would have to be calculated.

To calculate the energy we must calculate the eigenvalues of the matrix. For this we take $t = \lambda U$ and $U = 1$. We vary the value of λ .

Note that in small t , the fundamental state is dominated by the neutral states (states in which there is only one electron in each knot). When growing t the weight of the ionic states (states in which one knot is empty and another has two electrons) is increased, indicating a mobility of the electrons and the possible transition to a conducting state (Mott transition), with a state dominated by delocalized electrons.

| t | E_0 | neutral weight | ionic weight |
|-----|-----------|----------------|--------------|
| 0.1 | -0.088742 | 0.921662 | 0.078338 |
| 0.5 | -1.230997 | 0.568828 | 0.431172 |
| 0.7 | -1.907582 | 0.509556 | 0.490444 |
| 1.1 | -3.293969 | 0.452992 | 0.547008 |

TABLE I: Energy values of the ground state, the weight of neutral states and ionic states for different λ s.

V. CONCLUSIONS

In this paper we have seen how to introduce the Wannier functions as a unitary transformation of the Bloch functions. We have also seen how to rewrite the Hamiltonian of the solid using the Wannier functions getting to express the Hamiltonian using the creation destruction operators. This Hamiltonian is called Hubbard's Hamiltonian.

Finally, we have calculated its associated matrix for the Hamiltonian Hubbard case of 4 sites. This model allows us to study the passage of the insulating material to the conductive material (Mott transition) or to use the perturbation theory for small t to find the Hamiltonian of Heisenberg. These are some examples of the many utilities that the Hubbard model has.

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