Mott Transition in Strongly Correlated Fermionic Systems: Hubbard Model Review

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ABSTRACT **:** --The Hubbard model is one of the lattice models that enables successful treatment of problems of electronic correlations in quantum materials. The centrality of the Hubbard model in the quantum statistical mechanics of interacting fermions is comparable with the Ising model in classical mechanics. The constant expansion of Hubbard Hamiltonians indicates the great interest in the physics related to the Hubbard model. The present paper reviews this important model which plays a major role in the study of strong correlated fermionic systems. Starting with the basic approach of the model (the one-band model), we introduce others aspects, such as the multi-band and the extended Hubbard model. Due to presence of the repulsive Coulomb interaction, Mott insulators are different from the conventional insulators, and they are one of the strongest correlated fermionic systems. Mott insulators have been analyzed as well as the metal-insulator transition (MIT) in the perspective of the Hubbard model. The Mott transition addresses directly the competition between the kinetic energy and correlation energy, that is the wavelike and the particle character of electrons in the solid. Thus, the Hubbard model turns out to be appropriate in the study of such phase transition, this is the reason why it is still called Mott-Hubbard transition.

KEYWORDS: **Hubbard model, local Coulomb interaction, Mott insulator, metal-insulator transition, correlated fermionic systems, second quantization**

1. Introduction

Electronic transport mechanisms in materials always attract more attention of the scientists since the discovery of the electron by Sir Joseph John Thomson in 1897. Three years after that discovery, Paul Drude was the first physicist to present a microscopic theory to explain the transport properties of electron in materials (especially metals) [1- 4].

Drude model provides a classical mechanics approach to describing conductivity in metals. This model makes several key assumptions. Here are two of them:

- Electrons in metal behave much like particles in an ideal gas (no Coulomb interaction and no collisions between particles). This is called the independent electron approximation.
- Positive charges are located on immobile ions. The electrons do not experience Coulomb interaction with the ions (free electron approximation), but they do collide with the ions and can change direction and velocity. The so-called free electrons are ruled by the Maxwell-Boltzmann statistics.

The conductivity of metal (solid) is computed by the formula below:

$$\sigma = \frac{ne^2\tau}{m} \qquad (1)$$

with τ called relaxation time, n is the number of free electrons per volume (the density), e is the charge of an electron and m the mass of an electron.

The electronic velocity distribution, like that of an ordinary classical gas of density n is given in equilibrium at temperature T by Maxwell-Boltzmann distribution:

$$f_{MB}(v) = n\left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-\frac{mv^2}{2k_B T}} \qquad (2)$$

where v is the electronic velocity and k_B is the Boltzmann's constant.
This simplistic model is pre-quantum mechanical semi-classical model which is still roughly applicable for simple alkaline metals.

Arnold Sommerfeld was the first physicist to successfully apply quantum mechanics to the physics of transport in solids. Shortly after the discovery that the Pauli exclusion principle was needed to account the bound electronic states of atoms, Sommerfeld applied the same principle to the free electrons gas of metals [1]. In accordance with the Pauli exclusion principle, the classical Maxwell-Boltzmann velocity distribution was replaced by a new distribution, named Fermi-Dirac distribution and expressed as follows:

$$f_{FD}(v) = \frac{(m/\hbar)^3}{4\pi^3} \frac{1}{\exp[(\frac{mv^2}{2} - k_B T_0)/k_B T]+1} \qquad (3)$$

where $\hbar$ is the Planck's constant divided par 2π and T_0 is temperature determined by the normalized condition. The density of states ($D(\varepsilon)=\alpha\sqrt{\varepsilon}$) of conduction electrons in 3D systems indicates that the electron states are fully occupied below the Fermi energy ε_F (Fermi-Dirac statistics) [4]. The conductivity has the same form, but the relaxation time is now a function of energy Fermi $(\tau(\varepsilon_F))$. This energy dependence on the relaxation time has little significant effect on the most of quantities of interest in a metal [1].

Although the free electron model has recorded interesting results, it has however experienced many failures. The conventional theory of solids has emerged as being able to overcome some of these failures. This theory is based on the quantum mechanics of single electrons moving in periodic potentials and it has provided an excellent description of substances ranging from semiconducting silicon to superconducting aluminum [5]. Unfortunately, the conventional theory has also experienced limitations due to the electronic correlations present in certain substances.

The present review aims to show, on the one hand, the importance of Hubbard model in the attempt of probing electronic properties of strong correlated fermionic systems, and on another hand, how the strong repulsive Coulomb interaction affects the behavior of these systems. This paper is organized as follows: in section 2, the basic approach of

the Hubbard model (one-band model) is presented, and also the multi-band and extended versions of the Hubbard Hamiltonian. Section 3 is devoted to describing the metal-insulator transition (MIT) and the Mott insulators (Mott-Hubbard- and charge-transfer insulators). Conclusions are presented in section 4.

2. Hubbard model

Lacking a working *ab-initio* theory, strongly-correlated systems have been studied for a long time through low-energy model Hamiltonians. The minimal model to describe a system with a narrow band at the Fermi level is the Hubbard model [6] and is one of the fundamental models in condensed matter physics. The centrality of the Hubbard model in the quantum statistical mechanics of interacting fermions is comparable with the Ising model in classical mechanics [7]. It offers one of the most simple ways to get insight into how the interactions between electrons give rise to insulating, magnetic, and even novel superconducting effects in a solid [8]. This model was introduced independently by J. Hubbard, M. C. Gutzwiller and J. Kanomori around the same period [9 -13]. It was written down in the early 1960's and initially applied to understanding the behavior of the transition metal monoxides (FeO, NiO, CoO). This compounds exhibit antiferromagnetic insulator behavior, while they were predicted to be metallic by studies which do not deal with strongest electronic interactions [8].

The Hubbard model describes the fundamental dichotomy between itinerancy and locality for correlated electrons on a lattice [6]. This Hubbard Hamiltonian is expressed in a real-space second quantization formalism which is ideally suited to describe systems with electrons localized at the atomic orbital [14].

2.1- One-band Hubbard model

A conventional starting point for the study of strongly correlated electron systems is the single-band version of the Hubbard Hamiltonian [6] written as follows:

$$H = -t \sum_{\langle ij\rangle,\sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + \mathbf{h.c.}\right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (4)$$

where $\langle ij\rangle$ denotes the nearest-neighbor atomic sites, $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) is the fermion creation operator (fermion annihilation operator) at site i with spin $\sigma \in \{\uparrow, \downarrow\}$, $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$ is the density of fermions with spin σ, t parameterizes the hopping amplitude, the so-called Hubbard U is the on-site Coulomb interaction and **h**. **c**. denotes the Hermitian conjugate. The hopping parameter t for the kinetic energy of the electrons is determined by the overlap of atomic wave functions on neighboring sites [15]. Imada *et al.* [16] in their important study of Metal-Insulator Transitions (MIT) have expressed the hopping integral *t:*

$$t = \int d\mathbf{r} \varphi^{*}_{i\sigma}(\mathbf{r}) \frac{1}{2m} \nabla^2 \varphi_{j\sigma}(\mathbf{r}) \qquad (5)$$

where $\varphi_{i\sigma}(\mathbf{r})$ and $\varphi_{j\sigma}(\mathbf{r})$ are two atomic Wannier orbitals on sites i and j respectively, m is the electron mass and the Planck constant $\hbar$ is set to unity.

The Hubbard U means the repulsive Coulomb interaction between electrons on the same lattice site. The term $Un_{i\uparrow}n_{i\downarrow}$ represents an energy cost U for the site i has two electrons and describes a local repulsion between electrons [15]. U is also an integral calculated in the following equation [16]:

$$U = \int d\mathbf{r} d\mathbf{r'} \varphi^{*}_{i\sigma}(\mathbf{r}) \varphi_{i\sigma}(\mathbf{r}) \frac{e^2}{|\mathbf{r}-\mathbf{r'}|} \varphi^{*}_{i-\sigma}(\mathbf{r'}) \varphi_{i-\sigma}(\mathbf{r'}) \qquad (6)$$

The hopping amplitude and the on-site Coulomb repulsion represent the minimal set of parameters necessary to capture the physics of Mott insulators. A schematic picture of the Hubbard model is shown in the Fig.1.

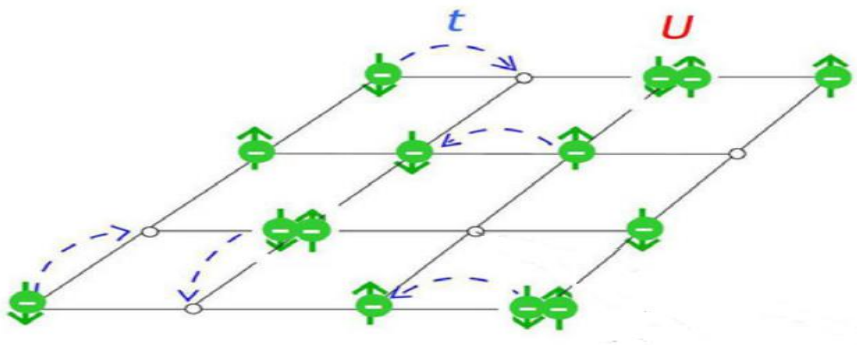

Fig. 1. Pictorial representation of the terms in the Hubbard Hamiltonian [17].

J. Bünemann, in the study of the Gutzwiller variational theory [6] has presented the single-band Hubbard Hamiltonian in another form:

$$H = \sum_{ij} \sum_{\sigma=\uparrow,\downarrow} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{7}$$

where t_{ij} is a bond-dependent hopping matrix element on near-neighbor sites ⟨ij⟩ [18].

Y. Claveau *et al.* [19] has considered the simplest Hubbard model as the non-degenerate band Hubbard Hamiltonian which is expressed in this way:

$$H = - \sum_{ij\sigma=\uparrow,\downarrow} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{8}$$

And the same authors have defined the term t_{ij} as the translation in the second-quantization language of both the kinetic energy and the crystal-potential energy associated with an electron at site i:

$$t_{ij} = \int d\mathbf{r} \varphi_{i\sigma}^{*}(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})\right) \varphi_{j\sigma}(\mathbf{r}) \tag{9}$$

The term $V(\mathbf{r})$ represents the periodic crystal-potential energy, and $t_{ij}=(t_{ji})^{*}$ because the Hamiltonian is Hermitian. An approximation that is usually employed for the hopping term t_{ij} is to consider it as being different from zero only when i and j are considered to be the nearest-neighbor ($t_{ij}=t$) [19].

Equations (7) and (8) are identical insofar as both terms of itinerancy and locality are present. This two terms demonstrate the interplay between kinetic energy gain and cost of Coulomb interaction. F. Lechermann in his notes of *Model Hamiltonians and Basic Techniques* [20] add another term scaling by the local single-particle level energy ε_0 which is not strictly mandatory:

$$H = - \sum_{ij\sigma=\uparrow,\downarrow} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \varepsilon_0 \sum_{i\sigma} n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{10}$$

. The Fourier transform of t_{ij} is the dispersion relation ε_k [6]. Finally, the Fourier transform of the kinetic energy term involves the dispersion $\varepsilon_{\mathbf{k}}$ and the momentum distribution operator $n_{\mathbf{k}\sigma}$:

$$\sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} \tag{11}$$

Let's remind some useful Fourier transform relations concerning fermion creation and annihilation operators:

$$c^{\dagger}_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N}}\sum_{\mathbf{R_j}} e^{-i\mathbf{k}.\mathbf{R_j}} c^{\dagger}_{\mathbf{R_j}\sigma} \tag{12}$$

$$c_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N}}\sum_{\mathbf{R_j}} e^{i\mathbf{k}.\mathbf{R_j}} c_{\mathbf{R_j}\sigma} \tag{13}$$

The creation operator $c^{\dagger}_{i\sigma}$ and annihilation operator $c_{i\sigma}$ are anticommuting:

$$\left\{c_{i\sigma}, c^{\dagger}_{j\sigma'}\right\} = \delta_{ij}\delta_{\sigma\sigma'} \tag{14}$$

$$\left\{c^{\dagger}_{i\sigma}, c^{\dagger}_{j\sigma'}\right\} = 0 \tag{15}$$

$$\left\{c_{i\sigma}, c_{j\sigma'}\right\} = 0 \tag{16}$$

The change in " basis " from the site indices to momentum indices does not affect the anticommutation relations.

Richard T. Scalettar [8] has presented another formulation of the single-band Hubbard Hamiltonian :

$$H = -t\sum_{\langle ij\rangle,\sigma}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + \mathbf{h.c.}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} - \mu\sum_{i}(n_{i\uparrow}+n_{i\downarrow}) \tag{17}$$

The final term is a chemical potential which controls the filling. The situation where the filling is one electron per site is referred to as 'half-filling' since the lattice contains half as many electrons as the maximum number (two per site) [18]. At the half-filling, $\mu = \frac{U}{2}$. Studies of the Hubbard Hamiltonian (HH) often focus on the half-filled case because it exhibits a lot of interesting phenomena (Mott insulating behavior, anti-ferromagnetic order, etc.) [8]. Therefore, it has been found convenient to rewrite (17) in the following form called PHS-form :

$$H = -t\sum_{\langle ij\rangle,\sigma}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + \mathbf{h.c.}\right) + U\sum_{i}\left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) - \mu\sum_{i}\left(n_{i\uparrow}+n_{i\downarrow}\right) \tag{18}$$

The PHS-form is a Hubbard Hamiltonian version which takes into account the Particle-Hole Symmetry (PHS). The latter is important because it is the basis of very useful mappings between the attractive and repulsive HH and because it plays a crucial role in QMC (Quantum Monte Carlo) simulations.

Clearly, the one-band HH is a simplification that is valid in the strict sense only when the atom has only one *s* orbital, as in hydrogen atom. The next subsection will present the multi-band HH.

2.2- Multi-band Hubbard model

The applicability of the one-band Hubbard model to d or f electron systems is a priori questionable since the partially filled bands correspond to atomic orbitals which are 5-fold and 7-fold degenerate (for each spin direction), respectively. Bands in a lattice are more complicated than orbitals of isolated atoms [6]. The bands that are formed are under the strong influence of anisotropic crystal fields in solids. Because the $3d$ orbital has the total angular momentum $L = 2$, it has fivefold degeneracy ($L_z = 2,1,0,-1,-2$) for each spin and hence a total of tenfold degeneracy including spins. This degeneracy is lifted by the anisotropic crystal field.

Fig. 2 shows an example of the crystal field splitting, where the cubic lattice symmetry leads to a higher energy level of fourfold degenerate e_g orbitals and sixfold degenerate lower orbitals, t_{2g} [16]. The t_{2g} orbitals ($|d_{xy}\rangle, |d_{yz}\rangle, |d_{zx}\rangle$) and the e_g orbitals ($|d_{x^2-y^2}\rangle, |d_{3z^2-r^2}\rangle$) give rise to threefold degenerate and twofold degenerate band respectively [6]. For light elements of transition-metal, such as V and T_i, the Fermi level is on the t_{2g} bands, which are threefold degenerate under the cubic crystal field -as this has been noticed before- with possible weak splitting of this degeneracy under the Jahn-Teller distortion in the perovskite structure ($L_{1-x}Sr_xVO_3$; $R_{1-x}A_xT_iO_3$) . When the Fermi level is on the e_g bands, as in Ni and Cu compounds, the degeneracy is twofold in the absence of the Jahn-Teller

distortion. In the compounds with light transition-metal elements such as Ti, V, Cr,..., only a few bands formed from 3d orbitals are occupied by electrons per atom. By contrast, in transition-metal compounds with heavy transition-metal elements such as Cu and Ni, the t_{2g} band is fully occupied far below the Fermi level [16].

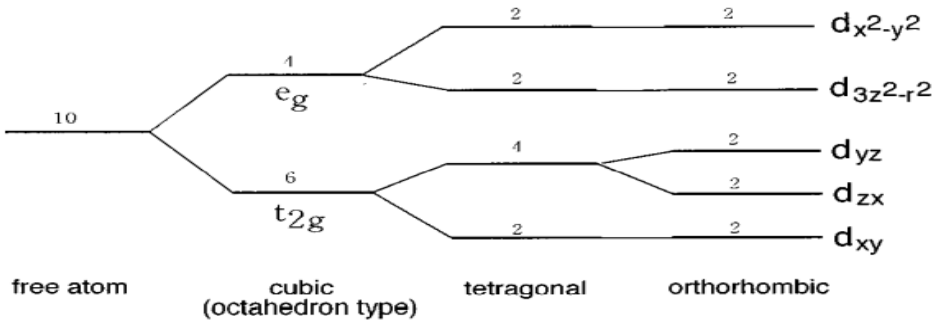

Fig. 2. Crystal-field splitting of $3d$ orbitals under cubic, tetragonal, and orthorhombic symmetries. The numbers cited near the levels are the degeneracy including spins [16].

The Hubbard model in multi-band approach has many forms according to authors' works. E. Pavarini [21] has written the so-called generalized multi-band HH in transition-metal systems:

$$H_{mband} = -\sum_{ii'}\sum_{\sigma}\sum_{mm'} t_{mm'}^{ii'}\, c_{im\sigma}^{\dagger} c_{im'\sigma} + \frac{1}{2}\sum_{i}\sum_{\sigma\sigma'}\sum_{m_\alpha m_\alpha'}\sum_{m_\beta m_\beta'} U_{m_\alpha m_\beta m_\alpha' m_\beta'}\, c_{im_\alpha\sigma}^{\dagger} c_{im_\beta\sigma'}^{\dagger} c_{im_\beta'\sigma'} c_{im_\alpha'\sigma} \qquad (19)$$

Where $c_{im\sigma}^{\dagger}$ creates an electron at site i with spin σ and orbital quantum number m, and the parameter $t_{mm'}^{ii'}$ are the hopping integrals ($i \neq i'$) or the crystal-field splittings ($i = i'$). $U_{m_\alpha m_\beta m_\alpha' m_\beta'}$ is the Coulomb interaction tensor and its elements can be expressed in terms of Slater integrals.

Another formulation of the multi-band Hubbard Hamiltonian called generalized rotationally invariant multi-band Hubbard Hamiltonian is given in [20]. This Hubbard model is derived from the rotationally invariant slave boson (RISB) theory [22], an elaborate generalization of original ideas for manifest multi-orbital problems:

$$H_{mband} = \sum_{ij,mm',\sigma} t_{ij}^{mm'} c_{im\sigma}^{\dagger} c_{jm'\sigma} + U\sum_{im} n_{im\uparrow} n_{im\downarrow} + \frac{1}{2}\sum_{i,m\neq m',\sigma}\left[U' n_{im\sigma} n_{im'\bar{\sigma}} + U'' n_{im\sigma} n_{im'\sigma}\right]$$

$$+ \frac{1}{2}\sum_{i,m\neq m',\sigma}\left[J c_{im\sigma}^{\dagger} c_{im'\bar{\sigma}}^{\dagger} c_{im\bar{\sigma}} c_{im'\sigma} + J_C c_{im\sigma}^{\dagger} c_{im\bar{\sigma}}^{\dagger} c_{im'\bar{\sigma}} c_{im'\sigma}\right] \qquad (20)$$

where m, m' are here either t_{2g} or e_g states, $U_{mm'mm'} = U_{m,m'} = U - 2J(1-\delta_{m,m'})$ and, for $m \neq m'$, $U_{mm'm'm} = J_{m,m'} = J$.

Y. Claveau *et al.* [19] have underlined in the study of multi-orbital Hubbard Hamiltonian that several intra-atomic Coulomb terms appear, depending on whether intra-orbital ($U_{m,m'}$ with $m=m'$) or inter-orbital ($U_{m,m'}$ with $m\neq m'$) Coulomb repulsion is concerned. And the Hund's exchange term J for ($m \neq m'$) also appears because of the multi-dimensional orbital of the degree of freedom. B. Himmetoglu *et al.* [23], M. Cococcioni [14] and R. Eder [8] have expressed the interactions parameters in terms of the Slater Condon parameters F^k and the products of Gaunt coefficients a^k and b^k:

$$U_{m,m'} = \sum_{k\epsilon\{0,2,4\}} a^k(m,m') F^k \;\; ; \;\; J_{m,m'} = \sum_{k\epsilon\{0,2,4\}} b^k(m,m') F^k \qquad (21)$$

For more information about these coefficients and parameters, one can be referred to [8] and[14].

J. Büneman has proposed another version of multi-band Hubbard Hamiltonian by distinguishing *localized* orbitals and *delocalized* orbitals. And he observed that localized orbitals require more sophisticated treatment of the local Coulomb interaction [14]. More precisely, multi-band Hubbard models are those where several atomic species are present; not all characterized by the same Hubbard *U* [19].

In the following subsection, another formulation of Hubbard model taking into account off-site interaction will be analyzed.

2.3- Extended Hubbard model

The centrality of the Hubbard model in describing in the most basic way strongly correlated materials is well known. This model exhibits phenomena such as magnetism and metal-insulator transitions with or without magnetic transitions. However, particularly due to neglecting nonlocal interaction, the Hubbard model can be quite far from describing real materials whenever nonlocal interactions are not efficiently screened [24].

The interest of the extended Hubbard model has been revamped in the last decades by the discovery of high T_c superconductors and the intense research activity focusing around them [25]. Several numerical studies suggest that the inter-site interaction plays indeed an important role [26] and superconductivity is predicted in a regime with repulsive on-site ($U > 0$) and attractive inter-site ($V < 0$) couplings [25]. In low-dimensional systems, especially quasi-1D compounds, the nearest-neighbor (NN) Coulomb integral V is often relevant at specific fillings to drive e.g. charge – density-wave (CDW) or spin-density-wave (SDW) instabilities [20]. M. Schüler *et al.* have used in their study of the first-order metal-insulator transition with the extended Hubbard model this formulation [24]:

$$H_{exhub} = -t \sum_{\langle ij\rangle,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{i \neq j} V_{ij} n_i n_j \qquad (22)$$

with U the local interaction (on-site Coulomb interaction) and V_{ij} the nonlocal interaction (inter-site Coulomb interaction) between electrons at sites i and j.

F. Dolcini and his colleague [27], investigating the integrable extended Hubbard Hamiltonians from symmetric group equations, have considered the most general form of extended Hubbard model, invariant under spin-flip and conserving the total number of electrons and the magnetization:

$$H_{exhub} = -\sum_{\langle ij\rangle,\sigma} \left[t - X\left(n_{i,-\sigma} + n_{j,-\sigma}\right) + \tilde{X} n_{i,-\sigma} n_{j,-\sigma}\right] c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{\langle ij\rangle} n_i n_j + \frac{W}{2} \sum_{\langle ij\rangle,\sigma,\sigma'} c^{\dagger}_{i,\sigma} c^{\dagger}_{j,\sigma'} c_{i,\sigma'} c_{j,\sigma}$$
$$+ Y \sum_{\langle ij\rangle} c^{\dagger}_{i,\uparrow} c^{\dagger}_{i,\downarrow} c_{j,\downarrow} c_{j,\uparrow} + P \sum_{\langle ij\rangle} n_{i,\uparrow} n_{i,\downarrow} n_j + \frac{Q}{2} \sum_{\langle ij\rangle} n_{i,\uparrow} n_{i,\downarrow} n_{j,\uparrow} n_{j,\downarrow} + \mu \sum_{i\sigma} n_{i,\sigma} \qquad (23)$$

This Extended Hubbard Hamiltonian contains 10 coefficients t, X, $\tilde{X}$, U, V, W, Y, P, Q, μ such that t is a hopping constant, U - on-site Coulomb interaction as in the ordinary Hubbard model, V is the neighboring site charge interaction, X the bond-charge interaction, W the exchange term, and Y the pair-hopping term. X correlates hopping with on-site occupation number, and P and Q describe three and four-electron interactions. And μ is the chemical potential. The choice of these parameters t, X, $\tilde{X}$ and others implies the Hamiltonian symmetry [28].

Gurin and Gulácsi analyzed an extended Hubbard model containing next-nearest-neighbor terms, the reader can refer to their paper in [29]. Delannoy *et al.* also presented an extended Hubbard model with next-nearest-neighbor (first, second and third neighbors) in the study of interaction strengths in cuprate superconductors and an effective spin-only description of La_2CuO_4 by the so-called low energy theory of the t-t'-t"-U Hubbard Model at half-filling [30]. The t-t'-t"-U Hubbard Hamiltonian is:

$$H_{exhub} = -t \sum_{\langle ij\rangle,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} - t' \sum_{\langle\langle ij\rangle\rangle,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} - t'' \sum_{\langle\langle\langle ij\rangle\rangle\rangle,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \quad U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} \qquad (24)$$

where t, t' and t" are energy scales which characterize direct hopping to first (⟨ij⟩), second ⟨⟨ij⟩⟩ and third ⟨⟨⟨ij⟩⟩⟩ nearest-neighbor respectively.

3. Metal – insulator transition (MIT) and Mott insulator

3.1- Metal – insulator transition

Although the metal-insulator transition (MIT) has certainly been one of the most studied phenomenon in condensed-matter physics, it is only in recent years that important progress has been achieved. This is mainly due to careful experimental and numerical studies but also to the improvement of the theoretical tools [31]. The insulating phase and its fluctuations in metals are indeed the most outstanding and prominent features of strongly correlated electrons [16]. The Mott transition is central to the problem of modeling strongly correlated electrons because it addresses directly the competition between the kinetic energy and correlation energy - that is the wavelike and the particle character of electrons in the solid [32]. In another words, D. Vollhardt [17] has observed that the Mott transition also called "Mott-Hubbard Metal-Insulator Transition" (MIT) is a delocalization-localization transition, demonstrating the particle-wave duality of electrons.

The two important parameters in the Hubbard model are the electron correlation strength U/t and the band filling n. In the case of a nondegenerate band, the n=0 and n=2 fillings correspond to the band insulator. For the half-filled case (n=1), it is believed that the change of U/t drives the insulator-to-metal transition (Mott transition) at a critical value of U/t except in the case of perfect nesting, where the critical value Uc is zero. This transition at a finite Uc is called a bandwidth control (BC)-MIT. The schematic metal-insulator phase diagram in terms of parameters U/t and n is shown in Fig.3. The shaded area in that figure is in principle metallic but under the strong influence of the metal-insulator transition, in which carriers are easily localized by extrinsic forces such as randomness and electron-lattice coupling. Two routes for the MIT (metal-insulator transition) are shown: the FC-MIT (filling-control MIT) and the BC-MIT (bandwidth-control MIT) [16].

According to Kotliar and Vollhardt [32] the parameters that determine the properties described by the Hubbard model are the ratio of the Coulomb interaction U and the bandwidth W, the temperature *T*, and the doping or number of electrons. The computation of the DOS (density of state) as a function of U/W in the framework of DMFT (Dynamic Mean Field Theory), a numerical approach to solve HH, has shown the opening of a gap (E_g=U-W) with the increasing of U [32][33].

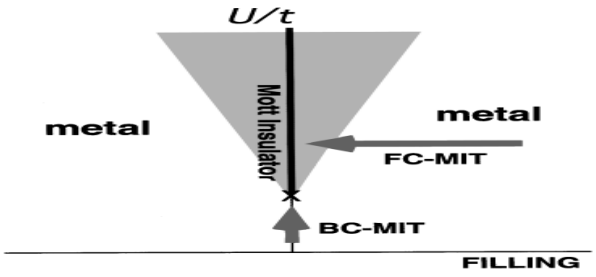

Fig.3 Metal-insulator phase diagram based on the Hubbard model in the plane of U/t and filling n [16].

3.2- Mott insulator

Mott insulator is defined by Imada *et al.* as an insulator caused by intrasite Coulomb repulsion, as in the Hubbard model [16]. Unlike conventional band insulators (which are shown in Fig.4) and semiconductors, Mott insulators contain unpaired electrons in their ground state [34].

According to the band theory of metals (Bloch theorem), a half-filled band (valence band) leads to a metallic conductivity. A fully filled band (valence band) leads to an insulator. There is an energy gap between the valence band and the conduction band. There is no electrical conduction. In this band theory no interaction between electrons is taken

into account and depending on the number of electrons, the system becomes metallic for the odd number and insulator for the even number [36]. Considering the same band theory (the independent-electron description of crystals), according to P. Fazekas [37], a material predicted to be metallic if the density of states at the Fermi level in non-vanishing ($\rho(E_F)\neq 0$) and the material must be insulator (or semi-conductor, etc) if ($\rho(E_F)=0$).

The failure of the band theory was recorded in1937, when de Boer and Verwey [38] reported that many transition metal oxides such as NiO and CoO are insulator, but not a metal in spite of the fact that the *d*-band of these systems is partially filled by electrons. Peierls pointed out that such a behavior may be caused by the electron correlation. In 1949, Mott [39] proposed a model for NiO as insulator with the bandgap energy E_g. The latter can be understood as the competition between the Coulomb potential U between *3d*- electrons and the transfer integral *t* between *3d*- electrons of neighboring atoms. Let's remind that E_g=U-W with W≈2zt, where z is the number of the nearest-neighbor atoms.

In general, Mott insulators occur when the repulsive Coulomb potential U is large enough to create an energy gap. In that conditions, where U exceeds the bandwidth *W*, the half- filled band splits into two sub-bands, the lower (LHB) and the upper (UHB) Hubbard bands [34] (see Fig.5). Frésard and Kotliar expressed in thy paper titled " Interplay of Mott transition and ferromagnetism in the orbitally degenerate Hubbard model" the (LHB) and (UHB) bandwidths by $W_{LHB}=\langle\{c_{L\alpha},c^{\dagger}_{L\alpha}\}\rangle$ and $W_{UHB}=\langle\{c_{U\alpha},c^{\dagger}_{U\alpha}\}\rangle$ respectively. And $c^{\dagger}_{L\alpha}$ ($c^{\dagger}_{U\alpha}$) is the contribution to $c^{\dagger}_{\alpha}$ (see more in [40]).

In their insulating phase, transition-metal oxides can present two types of insulators: the Mott-Hubbard insulator and the charge transfer insulator (CT) [16] [35] [41]. These compounds made of *3d*-orbital and *p*-orbital have characterized by two parameters: $\Delta=|\varepsilon_d-\varepsilon_p|$ (charge transfer energy) and U. When the oxygen p_σ level, ε_p , is much lower than ε_d , the oxygen *p*-orbital contributes only through virtual processes and $|\varepsilon_d-\varepsilon_p|>U_{dd}$; this type of transition-metal oxide is called a Mott-Hubbard-type compound. In contrast, if $|\varepsilon_d-\varepsilon_p|<U_{dd}$, in this case, the type of transition-metal oxide is called charge-transfer-type compound. The difference between the two cases is schematically illustrated in Fig.6.

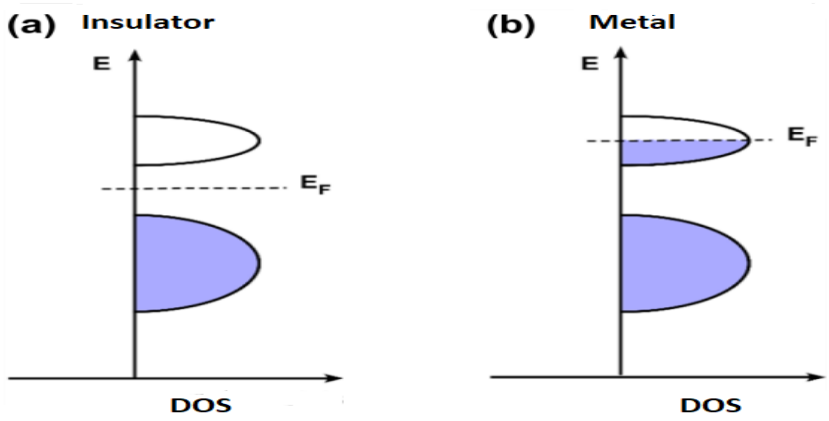

Fig.4 : Conventional band insulator (a) and metal (b) in band theory [35].

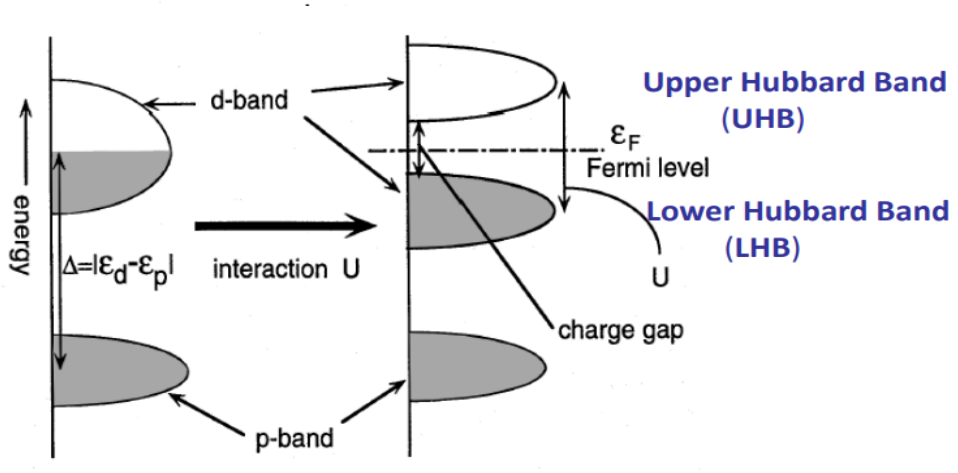

Fig.5 : Splitting of the *d*-band into two sub-bands (UHB) and (LHB) [41].

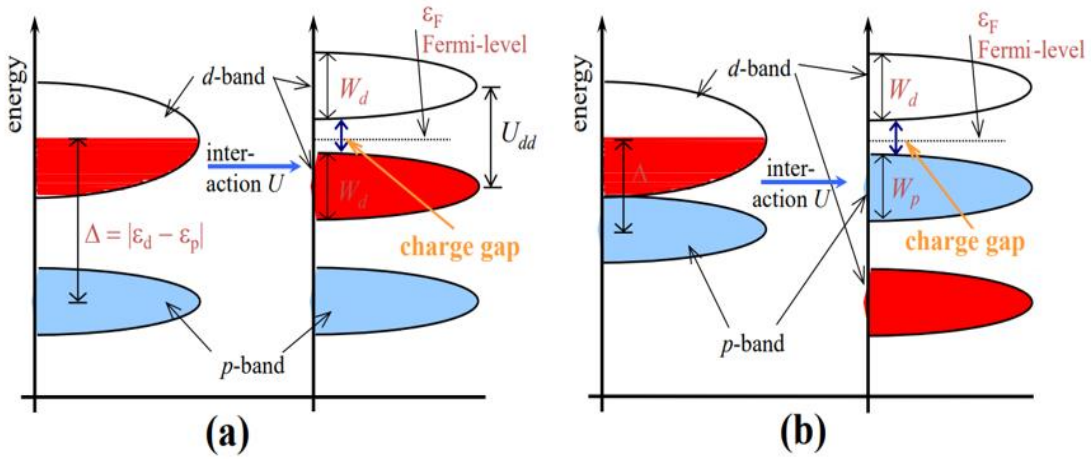

Fig.6 : Two types of Mott insulators: a) Mott-Hubbard insulator, b) Charge-transfer insulator (CT) [41].

La*M*O_3 compounds are Mott-Hubbard-type with *M* corresponding to Co and Fe, and CT-type if *M* is Ti or V [41]. Moreover, the most prominent examples of strongly correlated systems, known as Mott insulators, are $(V_{1-x}Cr_x)_2O_3$, $NiS_{2-x}Se_x$ and AM_4Q_8 [34]. The so-called the narrow gap Mott insulator AM_4Q_8 (A = Ga, Ge; M = V, Nb, Ta; Q = S, Se) exhibit very interesting electronic properties such as a very small Mott-Hubbard gap (0.2 ± 0.1 eV). And the direct consequence of this low gap value is the high sensitivity of this compounds to external perturbations. AM4Q8 materials belong to a new class of Mott-memories for which Joule heating, thermochemical or electrochemical effects are not involved [42].

4. Conclusion

Problems of strongly interacting electrons can be greatly simplified by reducing them to effective quantum spin models, such as the Hubbard model. As that has been observed, the literature of Hubbard model is vast. This paper has provided an overview of different approaches to the Hubbard model such as: the basic approach (the one-band approximation) and others versions which are the multi-band and the extended Hubbard model. Although various symmetries that the Hubbard model exhibits have not been discussed, little attention has been paid to the so-called

Particle-Hole Symmetry (PHS), due to the crucial role it plays in QMC simulations. Mott insulator and Metal-Insulator Transition (MIT) have actually been analyzed. The MIT is a delocalization-localization transition, demonstrating the particle-wave duality of electrons. Some compounds which are Mott-Hubbard type have also been presented. It is finally necessary to underline that analytical solutions of HH are not possible in all dimensions.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

[1] Ashcroft, N. W., & Mermin, N. D. (1976). Solid State Physics. ISBN 0-03-083993-9.

[2] Drude, P. (1900). Annalen der Physik. 306 (3) 566-613.

[3] Drude, P. (1900). Annalen der Physik .308 (11) 369-402.

[4] Sukuzi, M. (2020). "Electrical conductivity in the metal" in *Lecture notes of solid state physics*. https://bingweb.binghamton.edu.

[5] Gariglio, S. (2003). Transport properties $LaTiO_{3+\delta}$ and $REBa_2Cu_3O_{7-\delta}$ Thin Films: a Study of Correlation Effects. PhD-thesis. University of Geneva. Switzerland.

[6] Pavarini, E., Koch, E., Vollhardt, D., & Lichtenstein, A. (2011). The LDA+DMFT approach to strongly correlated materials. Modelling and Simulation Vol. 1 Forschungszentrum Jülich, ISBN 978-3-89336-734-4. http://www.cond-mat.de/events/correl11.

[7] Arovas, D. P., Baerg, E., Kivelson, S. A., & Raghu, S. (2020). The Hubbard Model. *Annual Review of Condensed Matter Physics*. https://doi.org/10.1146/annurev-conmatphys-031620-102024.

[8] Pavarini, E., Koch, E., van den Brink, J., Sawatzky, G. (2016). Quantum Materials: Experiments and Theory Modeling and Simulation Vol. 6 Forschungszentrum Jülich, ISBN 978-3-95806-159-0. http://www.cond-mat.de/events/correl16.

[9] Essler, F. H. L., Frahm, H., Göhmann, F., Klumper, A., & Korepin, V. E. (2005). *The one-dimensional Hubbard model.* Cambridge, Cambridge University, 1st Edition February 7, 2005.

[10] Gutzwiller, M.C. (1963). *Phys. Rev. Lett.* 10, 159.

[11] Kanamori, J. (1963). *Prog. Theor. Phys*. 30, 275.

[12] Hubbard, J. (1963). *Proc. R. Soc*. A 276, 237.

[13] Hubbard, J. (1964). *Proc. R. Soc*. A 281, 401.

[14] Pavarini, E., Koch, E., Anders, F., & Jarrell, M. (2012). Correlated Electrons: From Models to Materials. Modeling and Simulation Vol. 2 Forschungszentrum Jülich, ISBN 978-3-89336-796-2. http://www.cond-mat.de/events/correl12.

[15] Bai, Z., Chen, W., Scalettar, R., & Yamazaki, I. (2013). Numerical Methods for Quantum Monte Carlo Simulations of the Hubbard Model. DOI:10.1142/9789814273268_0001

[16] Imada, M., Fujimori, A., & Tokura, Y. (1998). Metal-insulator transitions. *Reviews of Modern Physics*. 70 (1039). https://doi.org/10.1103/PhysRevB.49.10869.

[17] Vollhardt, D. (2011). "Dynamical Mean-Field Approach for Strongly Correlated Materials" in *The LDA+DMFT approach to strongly correlated materials*. Modelling and Simulation Vol. 1 Forschungs-zentrum Jülich, ISBN 978-3-89336-734-4. pp. 1-29. hhtp://www.cond-mat.de/events/correl11.

[18] Scalettar, R.T. (2007) . Numerical Studies of Disordered Tight-Binding Hamiltonians. https://doi.org/ 10.1063/1.2751991.

[19] Claveau, Y., Arnaud, B., & Di Matteo, S. (2014). Mean-field solution of the Hubbard model: the magnetic phase diagram. http://dx.doi.org/10.1088/0143-0807/35/3/035023.

[20] Lechermann, F. (2011). "Model Hamiltonians and Basic Techniques" in *The LDA+DMFT approach to strongly correlated materials*. Modelling and Simulation Vol. 1 Forschungszentrum Jülich, ISBN 978-3-89336-734-4. pp.1-29. http://www.cond-mat.de/events/correl11.

[21] Pavarini, E. (2011). "The LDA+U Approach: A Simple Hubbard Correction for Correlated Ground States," in *The LDA+DMFT approach to strongly correlated materials.* Modelling and Simulation Vol. 1 Forschungszentrum Jülich, ISBN 978-3-89336-734-4. pp. 6.1-6.38. http://www.cond-mat.de/events/correl11.

[22] Lechermann, F., Georges, A., Kotliar, G., & Parcollet, O. (2007). Rotationally invariant slave-boson formalism and momentum dependence of the quasiparticle weigh. *Physical Review B 76, 155102. 2007*.

[23] Himmetoglu, B., Floris, A., Gironcoli, S., & Cococcioni, M. (2014). Hubbard-corrected DFT energy functionals: the LDA+U description of correlated systems. *Int. J. Quantum Chem.* 114 14–49 https://doi.org/10.1002/qua.24521.

[24] Schüler, M., van Loon, E. G. C. P., Katsnelson, M. I., & Wehling, T. O. (2018). First-order metal-insulator transitions in the extended Hubbard model due to self-consistent screening of the effective interaction. DOI: 10.1103/PhysRevB.97.165135.

[25] Cococcioni, M. (2012). "The LDA+U Approach: A Simple Hubbard Correction for Correlated Ground States," in *Correlated Electrons: From Models to Materials.* Modeling and Simulation Vol. 2 Forschungszentrum Julich, ISBN 978-3-89336-796-2. pp 4.1-4.40. http://www.cond-mat.de/events/correl12.

[26] Campo Jr, V. L., & Cococcioni, M. (2010). Extended DFT + U + V method with on-site and inter-site electronic interactions. http://dx.doi.org/10.1088/0953-8984/22/5/055602.

[27] Dolcini, F. & Montorsi, A. (2000). Integrable Extended Hubbard Hamiltonians from Symmetric Group Equations. *International Journal of Modern Physics* B 14(17):1719-1728. DOI: 10.1142/S0217979200001540.

[28] Fomin, V. (2010). Modèles de Hubbard unidimensionnels généralisés. Mathematical Physics [math-ph]. PhD-Thesis. Université de Savoie, 2010. English. tel-00608340.

[29] Gurin, P., & Gulácsi, Z. (1997). " Hubbard model with next-nearest neighbor interaction terms in higher dimensions: New, exactly solvable cases, " *Philosophical Magazine Part B*, 76:5, 827-831, DOI: 10.1080/01418639708241146.

[30] Delannoy, J. -Y., Gingras, M. J. P., Holdsworth, Peter., & Tremblay, A. -M. S. (2008). Low energy theory of the t-t'-t"-U Hubbard Model at half-filling: interaction strengths in cuprate superconductors and an effective spin-only description of La2CuO4. 2008. DOI: 10.1103/PhysRevB.79.235130.

[31] Assaraf, R., Azaria, P., Caffarel, M., & Lecheminant, P. (1999). Metal-insulator transition in the one-dimensional $SU(N)$ Hubbard model. http://dx.doi.org/10.1103/PhysRevB.60.2299.

[32] Kotliar, G., & Vollhardt, D. (2004) . Strongly correlated materials: Insights from dynamical mean- field theory. *Physics Today, 57(3) :53–60*. https:// doi.org/ 10.1063/1.1712502.

[33] Georges, A., Kotliar, G., Krauth, W., & Rozenberg, M. J. (1996). Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions. *Reviews of Modern Physics, 68(1) :13, 1996*.

[34] Janod, E., Tranchant, J., Corraze, B., Querré, M., Stoliar, P., Rozenberg, M., Cren, T., Roditchev, D., Ta Phuoc, V., Besland, M. -P., & Cario, L. (2015). Resistive Switching in Mott Insulators and Correlated Systems. https://doi.org/10.1002/adfm.201500823

[35] Émond, N. (2017). Synthèse et caractérisation de couches minces de VO_2 et de $W_xV_{1-x}O_2$ pour des applications dans les domaines infrarouge et térahertz . Université du Québec. Ph. D-thesis.

[36] Sukuzi, M. (2019). "Mott insulator and Hubbard model" in *Lecture notes of solid state physics*. https://bingweb.binghamton.edu.

[37] Fazekas, P. (1999). Lecture Notes on Electron Correlation and Magnetism. Physics: Vol. 5. ISBN: 978-981-4499-62-0/ ISBN: 978-981-02-2474-5. (pages 796, Budapest). https://doi.org/10.1142/2945.

[38] de Boer, J. H., & Verwey, E. J. W. (1937). Semi-conductors with partially and with completely filled *3d*-lattice bands. *Proceedings of the Physical Society*. 49 (4S): 59.

[39] Mott, N.F. (1949). The basis of the electron theory of metals, with special reference to the transition metals. *Proceedings of the Physical Society*. Series A. 62 (7): 416.

[40] Frésard, R. & Kotliar, G. (1997). Interplay of Mott transition and ferromagnetism in the orbitally degenerate Hubbard model. *Physical Review B* Vol. 5(20). https://doi.org/10.1103/PhysRevB.56.12909.

[41] Abd-Elmeguid, M.M. (2022). Introduction to Strongly Correlated Electron System (Lecture notes). https://ph2.uni-koeln.de.

[42] Cario, L., Janod, E., Tranchant, J., Stoliar, P., Rozenberg, M., Besland, M.-P., & Corraze, B. (2013). Mott-memories Based on the Narrow Gap Mott Insulators AM4Q8 (A=Ga, Ge ; M = V, Nb, Ta ; Q = S, Se). *Mater. Res. Soc. Symp. Proc.* Vol. 1562. http://dx.doi.org/10.1557/opl.2013.581