SOME INTRODUCTORY NOTES ON THE HUBBARD MODEL

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Abstract. We give a short introduction to the most important model for correlated electron systems: the Hubbard model. Not much care is taken to rigor, but relevant references are given.

Contents

1. Introduction

The Hubbard model has a relatively long history. Very early (in the 1950s) it was used by Pariser, Pople and Parr for orbital calculations and to describe molecules in quantum chemistry (PPP-method, see e.g. [1] for some history of quantum chemistry). Variations were used subsequently by P. Anderson and others in different contexts.

The Hubbard model in its modern form was systematically introduced independently by Gutzwiller [2], Hubbard [3] and Kanamory [4] in the early 1960s. The aim was to study magnetism in transition metals. This early work initiated a burst of activity in the field lasting until today. However, despite its simplistic appearance, the Hubbard model is not fully understood yet.

The Hubbard model plays an extremely important role in the field of correlated lattice systems. We may call the Hubbard model (with some exaggeration) the Standard Model of solid state physics. The main reason of its popularity is the inclusion of electron correlation, its simplicity and the rich physics contained in the model.

We all remember (and use in our daily work) introductory solid state physics courses, when we were taught about the band structure of solids. In this approach, electrons are considered to move independently in a periodic background potential. The so-called Hartree-Fock approximation gives good quantitative and qualitative predictions for many solids, for example if they are metallic or insulating. However, the band model breaks down in a number if cases. We now know that electron-electron interaction is crucial to the understanding of important properties of some materials. In particular, high temperature (unconventional) superconductivity turns out to be impossible to understand in the Hartree-Fock approximation.

Let me just mention the well known example of Cobalt-Oxide(CoO) where the Hartree-Fock approximation brakes down. CoO has an odd number of electrons per unite cell and it should be metallic according to band theory. However, experimentally it turns out to be a very tough insulator.

Most of the information given here can be found in greater detail in standard solid state physics textbooks. For a good introduction to the Hubbard model and to correlated systems in general, see the book by P. Fazekas [5].

2. Tight binding picture of solids

In the tight binding approach, we start off from a very diluted solid with large lattice spacing. The atoms at each lattice site are supposed to be in their ground state with some hydrogen-like electronic configuration ($1s^1 1s^2 2s^1 2s^2 2p^4$ ...). First, we discard all inner structure of the atom: we forget about nucleus and the inner inert gas configuration. Then we allow electron tunneling from site to site. The steps in this approximation are cartooned in figure 1. In B) the electrons of the outer shells are in itinerant states, delocalized Bloch waves. The inner shells are well described in terms of localized states. However, these inner electrons may also tunnel to nearest sites and delocalize in this way. In C) we restrict ourselves to a single shell with hopping electrons. The last step D) consists in neglecting the whole inner structure of the atom and the orbital, and to consider the picture of localized electrons that hop from site to site.

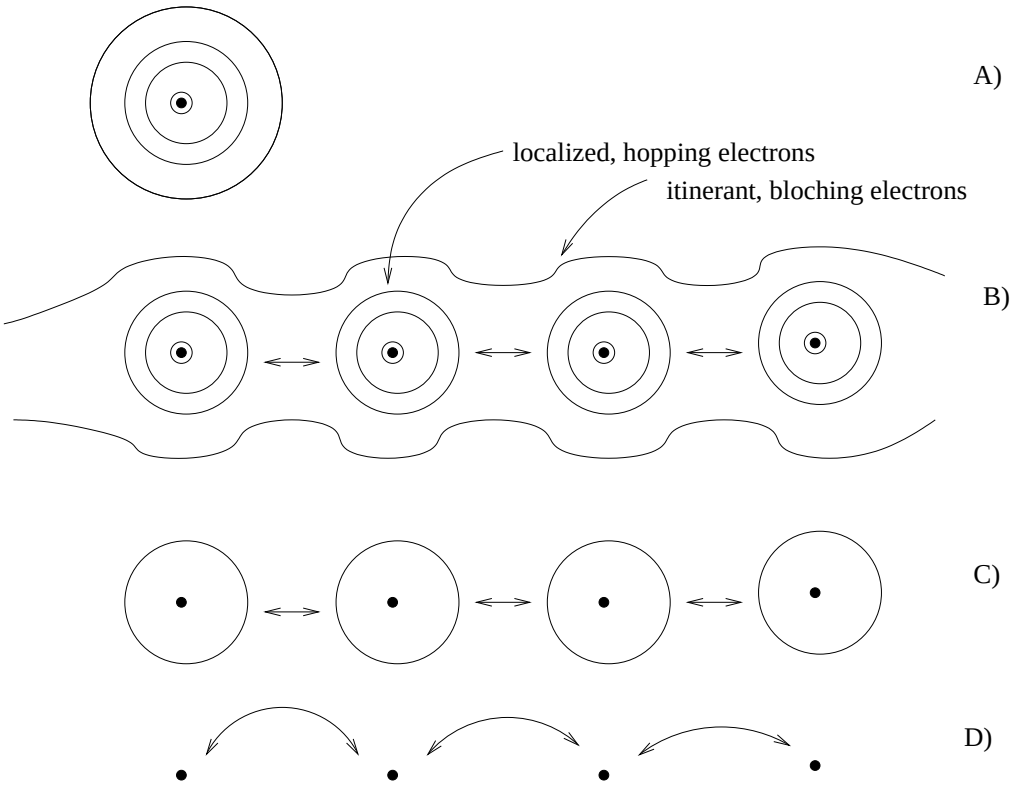

Figure 1. Tight binding approximation: The internal structure of the atoms is neglected and localized electrons tunnel from site to site.

In order to bring this tight binding picture in a mathematical form, we have to go to the usual second quantized picture of many particle physics. See appendix A for some remainders on second quantization.

First, we define the electron *creation* and *annihilation* operators of electrons in localized, so called *Wannier* states:

Be $\phi(\vec{r}-\vec{R}_i)$ the wave function of the electron bound to site i, then $c^\dagger_{i\sigma}$ is the *creation* operator of such a state:

$$\phi(\vec{r}-\vec{R}_i)\chi(\sigma) = c^\dagger_{i\sigma}\,|0\rangle \tag{1}$$

$\sigma \in \{\uparrow,\downarrow\}$ is the spin of the electron on site i. The vacuum state $|0\rangle$ is defined as the state with no electrons, i.e. it vanishes by the action of the destruction operator: $c_{i\sigma}\,|0\rangle = 0$. Because of the Pauli exclusion principle and by anti-symmetricity of the wave functions, we have:

$$\begin{aligned} &\{c_{i\sigma}, c_{j\sigma'}\} = 0 \\ &\{c_{i\sigma}, c^\dagger_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'} \qquad\qquad \forall i,j,\sigma,\sigma' \end{aligned} \tag{2}$$

2.1. **Vagabonding electrons.** Now, what could be the hamiltonian for the hopping process? The reason for the electron hopping is their overlapping bound state wave functions. The matrix element of such a tunneling process from one site to another is:

$$t_{ij} \propto \langle i|j\rangle = \int d^3r\, \phi(\vec{r}-\vec{R}_i)^*\phi(\vec{r}-\vec{R}_j) \tag{3}$$

t_{ij} in (3) is the probability of an electron on site i to tunnel to site j. Of course this process occurs also the other way round, and for any site to any other site of the lattice. We suppose here that no spin flip can occur during a hopping. The full operator of all these processes is conveniently written in terms of Wannier operators:

$$H_t = -\sum_{ij\sigma} t_{ij}\; c^\dagger_{i\sigma}c_{j\sigma}, \quad t_{ii} = 0\,, t_{ij} = t_{ji} \tag{4}$$

The *hopping hamiltonian* is the sum over all hopping processes: $c_{j\sigma}$ destroys an electron on lattice site j with spin σ and $c^\dagger_{i\sigma}$ recreates the electron on an other site i.

You might wonder about the negative sign we gave to the hopping hamiltonian (4). However, this sign is just chosen for convenience. In this model there is the symmetry $t \to -t$.

It is clear that we can neglect hopping between more distant sites in a first approach. This is because the hydrogen electron wave function has an exponential tail far from the center, so we can expect the hopping integral (3) to be small for all sites more than one lattice spacing distant. However, this need not be the case! Consider for example the

electron not in a spherical s-shell, but in a p- or d-shell. Due to the anisotropy of these shells, it can even happen that next nearest hoping is more important than nearest, as figure 2.1 illustrates. In practice it is often a very good approximation to restrict to nearest neighbor t and next-nearest t' or perhaps t'' hopping.

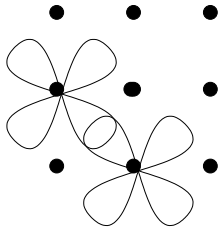

FIGURE 2. The hopping integral might be bigger on next nearest neighbors than on nearest neighbors, if the wave function of the bound electron is anisotropic.

2.2. **Interacting electrons.** A very important aspect of the Hubbard model is the explicit inclusion of electron-electron interaction. The most important interaction is of course between two electrons on the same site. Because of the Pauli exclusion principle, there can maximally be two electrons per site, one with up, the other with down spin. The electrostatic energy of two intra-site electrons is given by:

$$U = \int d^3r_1 \, d^3r_2 \, |\phi(\vec{r_1})|^2 \frac{e^2}{|\vec{r_1} - \vec{r_2}|} \, |\phi(\vec{r_2})|^2 \tag{5}$$

Since coulomb interaction is long range, (5) may diverge if we naively take the non-interacting electron orbital for $\phi(\vec{r})$. Some care must be taken to normalize this integral properly. (5) is the energy of a doubly occupied site. So the intra-site interaction hamiltonian is just the sum over all doubly-occupied sites:

$$H_U = U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{6}$$

where $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the electron number operator for spin σ on site i.

For more realistic models, we should also include nearest and next nearest coulomb interaction. These are neglected in the Hubbard model. This in not justified a priori, since coulomb interaction is long

ranged. However, we may think of the long range interaction being screened by the electrons.[1]

Finally, the Hubbard hamiltonian is a sum of the two terms:

$$H = H_t + H_U = -\sum_{<i,j>\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{7}$$

Despite the simple appearance, the Hubbard model is notoriously difficult to solve. And surprisingly rich physics is contained in the model.

To gain some qualitative insight, let us have a look at the two terms separately. The hopping (itinerant) part is responsible for the band structure and it is diagonalized by Block-waves. Let us define the Fourrier transform of the Wannier operators:

$$c_{\vec{k}} = \frac{1}{\sqrt{L}} \sum_i c_i \; e^{-i\vec{r}_i \cdot \vec{k}} \tag{8}$$

where L is the total number of lattice sites. The wave vector $\vec{k}$ lies in the first Brillouin zone (BZ) of the lattice.

With the help of (8) we can write the hopping hamiltonian (4) in a diagonal form:

$$H_t = \sum_{\vec{k} \in BZ, \sigma} \epsilon(\vec{k}) \; c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} \tag{9}$$

In the case of a square lattice and nearest neighbor hopping t only, the dispersion relation ϵ is given by

$$\epsilon(\vec{k}) = -t(\cos k_x + \cos k_y + \ldots) \tag{10}$$

Because of this simple relation, the model is sometimes called the *single band Hubbard model*. If we take next nearest hopping into account, then the dispersion will be more complicated. We may also forget about the real space representation of the hopping term and simply postulate a particular band structure $\epsilon_n(\vec{k})$.

The eigenstates of the hamiltonian (9) are Bloch waves:

$$|\vec{k}, \sigma\rangle = c^\dagger_{\vec{k}\sigma} \, |0\rangle \tag{11}$$

[1]Screening itself is an effect of electron correlation, so this point needs some careful justification.

with energy $\epsilon(\vec{k})$. The ground state[2] is the Fermi sea $|FS\rangle$, where up and down spins are filled up in $\vec{k}$ space up to the fermi energy:

$$|FS\rangle = \prod_{\epsilon(\vec{k})<\epsilon_f} c^\dagger_{\vec{k}\uparrow} c^\dagger_{\vec{k}\downarrow} \, |0\rangle \tag{12}$$

It is clear that this Fermi sea is completely uncorrelated. The electrons do not feel each other and the state has a lot of charge fluctuations, it is conducting.

Let us now have a look at the interaction part (6) of the hamiltonian. This part is diagonal in the local basis. If we restrict us to a single electron per site (half-filled case), then the ground state is given by

$$|GS\rangle = \prod_i c^\dagger_{i\sigma_i} |0\rangle \tag{13}$$

where $\{\sigma_i\}$ is a spin configuration. Doubly occupied sites must be excluded from the ground state, because they lead to higher energy. Note that this groundstate is highly degenerate (2^L times): there are many spin configurations with the same energy.

3. Mott transition

We see from the above discussion that each term of the Hubbard hamiltonian (7) is very simple: The hopping part has an itinerant electron ground state and the interaction part has a localized ground state. However, the sum of these very simple parts is highly non-trivial and very difficult to understand quantitatively. But we can be sure that the two effects (localize, delocalize) will compete with each other.

3.1. **Energies of the competing ground states.**

Let us calculate the energies of the two competing groundstates found earlier:

Suppose that we are in the half filled case, i.e. same number of electrons as sites. Let us further suppose for simplicity that the ground state is non-magnetic, i.e. that there are the same number of up and down electrons.

[2]Remember that we are mainly interested in ground state properties since superconductivity is exclusively observed at low temperatures.

3.1.1. *Fermi sea.* The hopping energy of the Fermi sea is easy to guess: Since the Fermi sea is a superposition of Bloch waves, we can sum over their energy to get the total Energy:

$$E_t = \langle FS| H_t |FS\rangle = 2 \sum_{\epsilon(\vec{k})<\epsilon_f} \epsilon(\vec{k}) \tag{14}$$

In case of nearest hopping only on a square lattice, $E_t = -\alpha t$. The numerical factor α being roughly unity.

To find the interaction energy of the Fermi sea, we first have to find the fraction of doubly occupies sites, since only they contribute. The Fermi sea is uncorrelated: the probability to find an up spin on a site is completely independent of the probability to find a down spin. So let us forget about down spins for a moment, suppose that we have only up spins in the system. Now, half of the sites are empty and the other half contain a single up spin (Pauli principle). Since we are interested in the thermodynamic limit (macroscopic crystal), the fraction of up spins per site is equal to the probability to find an up spin on a given site.[3] Thus, the probability to find an up spin is 1/2. The same argument applies to the down spins. The probability to find a doubly occupied site is given by the product of the probability to find down and up spins: $p_{doubly} = 1/2 \cdot 1/2 = 1/4$. Again by the central limit theorem, this corresponds to the fraction of doubly occupied sites. Finally, the interaction energy per site is given by: $E_U = \langle FS| H_U |FS\rangle = \frac{U}{4}$. The total Fermi sea energy per site is:

$$E_{FS} = -\alpha t + \frac{U}{4} \tag{15}$$

3.1.2. *Localized groundstate.* Let us now calculate the energy of the localized state. The hopping term vanishes in the half filled case, because hopping would necessarily produce a doubly occupied site. But such a state is orthogonal to the ground state, thus it vanishes.

$|GS\rangle$ is the ground state of the interaction part with no doubly occupied sites. Its energy vanishes:

$$E_{GS} = \langle GS| H_t |GS\rangle + \langle GS| H_U |GS\rangle = 0 \tag{16}$$

Suppose we vary the parameters U and t of the Hubbard model. Experimentally, it is probably difficult to vary U, but the hopping integral t varies steeply with the lattice spacing, so we may change it by squeezing the crystal. What is important is varying U/t.

The energies of the two competing ground states are plotted in figure 3 as a function of U. The true ground state at intermediate U is of

[3]This is called the *central limit theorem* in mathematics

course much more complicated. The true ground state is not known rigorously, some indications come from exact or approximate calculations on small lattice clusters.[4] See [6] for more details.

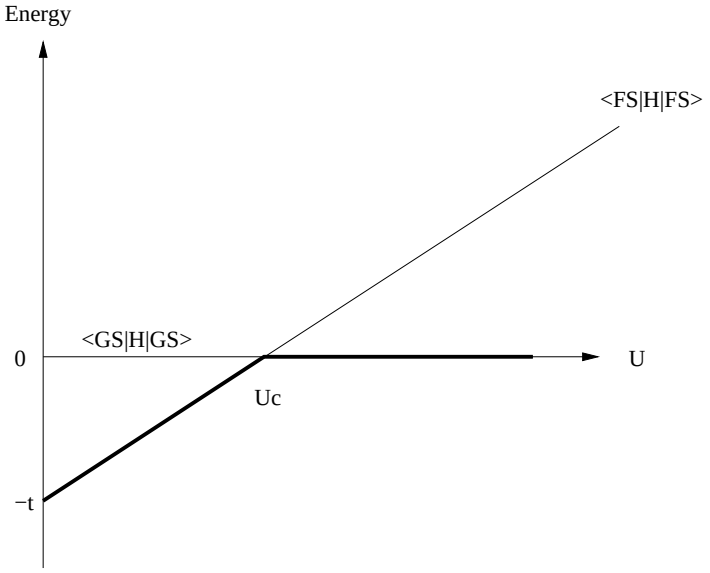

FIGURE 3. Energy of the Hubbard model in the two competing ground states as a function of U. At small U, the conducting Fermi sea is preferred, large U prefers a localized and insulating ground state (Mott insulator).

Figure 3 gives a qualitative indication that there must be a phase transition at intermediate $U \simeq U_c = 4t\alpha$. The predominant Fermi sea character changes to a more localized state. This must also be a metal-insulator transition and it is called a *Mott transition*.[5]

[4]The commonly used techniques are exact diagonalization (up to 4×4 sites) and quantum monte carlo methods (up to 16×16 sites).

[5]This discovery is due to Sir Nevil Francis Mott, who won the Nobel price for his work on strongly correlated electron systems in 1977, together with P.W. Anderson and J. van Fleck.

4. Outlook

In the previous sections we have seen that introducing explicit correlation even in a very simple model leads to interesting new phenomena like Mott transition. It is believed that these correlations are very important to other phenomena, like high temperature superconductivity. For example, the Hubbard model on a square lattice is believed to contain the main physics of cuprate plains in La_2CuO_4. However, to see high temperature superconductivity in Hubbard-like models, one has to go away from half-filling. This field is currently subject to intensive research in theoretical solid state physics.

Appendix A. Some second quantization reminders

In section 2 the tight binding model of solids was introduced. I would like to give here some basic reminders of second quantization formalism. I want to show you, why anti-commuting operators should be taken as the creation operators for electrons.

The first step is to write down the definition of the creation operator. Def.:

$$
\begin{aligned}
&(17a) && |i,\sigma\rangle && \equiv c^\dagger_{i\sigma}\,|0\rangle && \text{Creation operator}\\
&(17b) && c_{i\sigma} && \equiv (c^\dagger_{i\sigma})^\dagger && \text{Annihilation operator}\\
&(17c) && c_{i\sigma}\,|0\rangle && \equiv 0 && \text{Electron vacuum}
\end{aligned}
$$

We use now the following two famous experimental results:

(1) Pauli exclusion principle: two electrons cannot sit in the same quantum state.
(2) Anti-symmetricity of the electronic wave function: $|i,\sigma;j,\sigma'\rangle = -\,|j,\sigma';i,\sigma\rangle$

From (1) and (2) we can infer the following relations:

$$
\begin{aligned}
(18)\qquad 0 = |i,\sigma;i,\sigma;\phi\rangle &= (c^\dagger_{i\sigma})^2\,|\phi\rangle && \forall\,|\phi\rangle\\
&\Rightarrow (c^\dagger_{i\sigma})^2 = 0
\end{aligned}
$$

$$
\begin{aligned}
(19)\qquad c^\dagger_{i\sigma}c^\dagger_{j\sigma'}\,|\phi\rangle = |i,\sigma;j,\sigma';\phi\rangle &= -\,|j,\sigma';i,\sigma;\phi\rangle = -c^\dagger_{j\sigma'}c^\dagger_{i\sigma}\,|\phi\rangle && \forall\,|\phi\rangle\\
&\Rightarrow c^\dagger_{i\sigma}c^\dagger_{j\sigma'} + c^\dagger_{j\sigma'}c^\dagger_{i\sigma} = \{c^\dagger_{i\sigma}, c^\dagger_{j\sigma'}\} = 0\\
&\Rightarrow \{c_{i\sigma}, c_{j\sigma'}\} = 0 && \forall i,j,\sigma,\sigma'
\end{aligned}
$$

Of course, the wave function must also be anti-symmetric under the exchange of electron and holes:

$$
\begin{aligned}
(20)\quad c^\dagger_{i\sigma}c_{j\sigma'}\left|\phi\right\rangle &= c^\dagger_{i\sigma}\left|h_{j\sigma'};\phi\right\rangle = \left|e_{i\sigma};h_{j\sigma'};\phi\right\rangle && \forall i\neq j,\sigma\neq\sigma',\left|\phi\right\rangle\\
&= -\left|h_{j\sigma'};e_{i\sigma};\phi\right\rangle = -c_{j\sigma'}c^\dagger_{i\sigma}\left|\phi\right\rangle &&\\
&\Rightarrow \{c^\dagger_{i\sigma},c_{j\sigma'}\}=0 && \forall i\neq j,\sigma\neq\sigma'
\end{aligned}
$$

where $\left|h_{i\sigma}\right\rangle$, $\left|e_{i\sigma}\right\rangle$ means a hole respectively an electron on site i with spin σ.

In case of $i=j,\sigma=\sigma'$, (20) should be the identity operator:

$$
\begin{aligned}
(21)\qquad c^\dagger_{i\sigma}c_{i\sigma}\left|i,\sigma;\phi\right\rangle &= c^\dagger_{i\sigma}\left|\phi\right\rangle = \left|i,\sigma;\phi\right\rangle &&\\
c_{i\sigma}c^\dagger_{i,\sigma}\left|\phi\right\rangle &= c_{i,\sigma}\left|i,\sigma;\phi\right\rangle = \left|\phi\right\rangle && \forall\left|\phi\right\rangle\\
&\Rightarrow \{c^\dagger_{i,\sigma},c_{i,\sigma}\}=1 && \forall i,\sigma
\end{aligned}
$$

This shows indeed that we should use the familiar commutation relation for fermion operators:

$$
\begin{aligned}
(22)\qquad &\{c_{i\sigma},c_{j\sigma'}\}=0 &&\\
&\{c_{i,\sigma},c^\dagger_{j,\sigma'}\}=\delta_{ij}\delta_{\sigma\sigma'} && \forall i,j,\sigma,\sigma'
\end{aligned}
$$

Appendix B. Remarks on the low energy effective t-J model

As we have seen earlier, the one band Hubbard model is written as

$$H = -t \sum_{<i,j>,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{23}$$

Now in real solids, the on-site repulsion U is normally quite large with respect to the hopping integral t. The limit $U \gg t$ means that it costs a lot of energy to have doubly occupied sites on the lattice and, as a result, we expect them to be highly suppressed in the ground state. It is possible to (canonically) transform (23) to a low energy effective hamiltonian which acts in the sub-space of no doubly occupied sites, and to neglect terms of high order in t/U.

The so-called t-J model, written as

$$H = -t \sum_{<i,j>,\sigma} P_d \, c^{\dagger}_{i\sigma} c_{j\sigma} P_d + J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j \tag{24}$$

is sometimes referred to as a low energy effective model derived from the Hubbard model. However, this is rigorously not true, for the following reasons:

- t-J is not a systematic expansion in t/U of the Hubbard model: some terms to order t/U are kept while others of the same order are neglected. (The so-called *3-site hopping term* is dropped. There is a priori no reason why this term should be less important than others.)
- The mean values of operators in the t-J model are calculated with respect to the bare eigenstates. This is not consistent, since the canonically transformed eigenstates should be taken.

For this reason, the t-J model should rather be understood as an independent model from the Hubbard model. For more details see [7].

References

[1] http://www.quantum-chemistry-history.com/Pari_Dat/Pariser2.htm
[2] M. C. Gutzwiller:
Effect of correlation on the ferromagnetism of transition metals.
Phys. Rev. Lett. 10, 159 (1962)
Phys Rev. 134, A923 (1963)
[3] J. Hubbard: *Electron correlations in narrow energy bands*
Proc R. Soc. A, Vol. 276 No. 1365 (1963) 238-257
Proc R. Soc. A, Vol. 277 No. 1369 (1964) 237-259
Proc R. Soc. A, Vol. 281 No. 1386 (1964) 401-419
[4] J. Kanamory, Prog. Theor. Phys. 30, (1963) 275
[5] P. Fazekas, *Lecture Notes on Electron Correlations and Magnetism*,
World Scientic Publishing, Singapore, 1999.
[6] E. Dagotto, D. Poilblanc et al.:
Static and dynamic properties of doped Hubbard clusters
Phys. Rev. B 45, 10741 (1992)
E. Dagotto et al.: *Density of states of Doped Hubbard Clusters*
Phys. Rev. Lett. 67, 1918 (1991)
A. Moreo, D. J. Scalapino:*Correlations in the 2D Hubbard model*
Phys. rev. B 43, 8211 (1991)
[7] J.-Y. P. Delannoy et al.
Spin operators beyond the Heisenberg limit of the half-filled Hubbard model
http://arxiv.org/abs/cond-mat/0412033