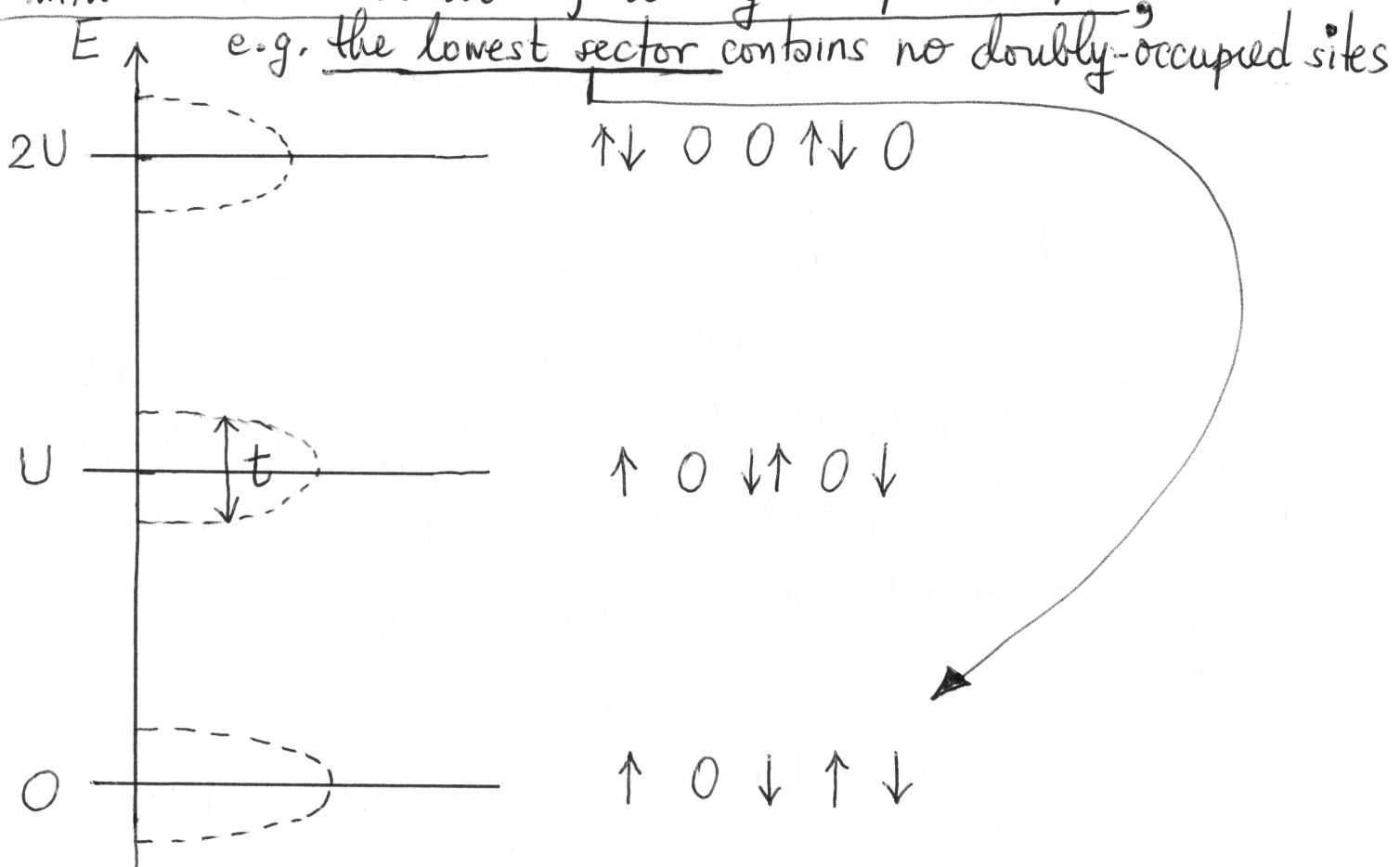


The Hubbard model at half-filling and the Mott-Hubbard insulators

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We have already introduced the Hubbard model and its basic properties and symmetries. Now we'll discuss the strong-coupling limit of this model ($\frac{U}{t} \rightarrow \infty$) with particular emphasis on the half-filling case. We will show that only the spin degree of freedom of electrons will be relevant for the low-energy behavior. The procedure we will utilize to show this is sometimes referred to as projective renormalization.

The analysis of the Hubbard model is easier to carry out if we think of the electronic Hilbert space as being organized in sectors, where each sector contains electronic configurations with the same number of doubly occupied sites;



The total Hamiltonian can be written as the sum of the zeroth-order term (describing the intrasector physics) and a fluctuation

$$H = H_0 + H_1, \text{ where}$$

describing fluctuations between different sectors

$$H_0 = V + T_0, \text{ with } V = U \sum_i n_{i\uparrow} n_{i\downarrow} \text{ and}$$

$$T_0 = -t \sum_{i, \delta, \bar{\sigma}} \left\{ (1 - n_{i\bar{\sigma}}) c_{i\bar{\sigma}}^+ c_{i+\delta, \bar{\sigma}} (1 - n_{i+\delta, \bar{\sigma}}) + n_{i\bar{\sigma}} c_{i\bar{\sigma}}^+ c_{i+\delta, \bar{\sigma}} n_{i+\delta, \bar{\sigma}} \right\};$$

(here $\bar{\sigma} = \downarrow$ if $\sigma = \uparrow$, and vice versa)

$$H_1 = T_+ + T_-, \text{ with}$$

$$T_+ = -t \sum_{i, \delta, \bar{\sigma}} n_{i\bar{\sigma}} c_{i\bar{\sigma}}^+ c_{i+\delta, \bar{\sigma}} (1 - n_{i+\delta, \bar{\sigma}})$$

$$T_- = -t \sum_{i, \delta, \bar{\sigma}} (1 - n_{i\bar{\sigma}}) c_{i\bar{\sigma}}^+ c_{i+\delta, \bar{\sigma}} n_{i+\delta, \bar{\sigma}}$$

The term $H_0 = V + T_0$ describes the physics within a Hubbard sector (in particular, T_0 includes all possible hopping events within a sector), while H_1 includes the hoppings that change the number of doubly-occupied sites, hence change the Hubbard sector!

What is the interpretation for the form of T_0 and T_+, T_- ?

For instance, $C_{i+\delta, \sigma} (1 - n_{i+\delta, \bar{\sigma}})$ means that an electron with spin σ can only be annihilated on site $i+\delta$ if there is no electron with spin $\bar{\sigma}$ on that site. Otherwise, a doubly occupied site would be annihilated \Rightarrow but this means that we would leave the desired Hubbard sector!

The first term in T_0 describes the exchange between empty and singly-occupied sites, while the second term describes the exchange between singly- and doubly-occupied sites!

The meaning of T_+ and T_- is the following:

T_+ adds a doubly-occupied site, while T_- removes a doubly-occupied site.

We introduce the following canonical transformation:

$$(\#) \quad H_{\text{eff}} = e^S H e^{-S} \equiv H + [S, H] + \frac{1}{2} [S, [S, H]] + \dots$$

We will combine this canonical transformation (with as yet undefined S !) with a perturbation theory using t/U as a small parameter.

Assume that $S^{(1)}$ is a contribution of S , which is of first order in t/U . \Rightarrow

up to first order in t/U , H_{eff} is given by

$$H_{\text{eff}}^{(1)} = H_0 + T_+ + T_- + [S^{(1)}, H] + o(S^2)$$

We demand that up to linear (first) order in t/U , $H_{\text{eff}}^{(1)} = H_0 \Rightarrow$

$$T_+ + T_- = -[S^{(1)}, H]$$

since with one hopping event only, we are leaving the Hubbard sector under consideration!

Since $T_+ + T_- \propto t$ and $S^{(1)} \propto t/U$, it must hold that

$$[S^{(1)}, H] = [S^{(1)}, V] \quad \left(\begin{array}{l} \text{or, in other words,} \\ [S^{(1)}, T_0] = 0 \end{array} \right)$$

$$\Rightarrow T_+ + T_- = -[S^{(1)}, V]$$

\Rightarrow this equation implies that $S^{(1)} = \frac{1}{U}(T_+ - T_-)$.

Let us now determine the second-order (in t/U) contribution to S : (denote this contribution with S')

\Rightarrow up to second-order $S^{(2)} = S^{(1)} + S'$,

and, accordingly,

$$H_{\text{eff}}^{(2)} = H_0 + H'_{\text{eff}} + O(t^3/U^2), \text{ with}$$

$$H'_{\text{eff}} = [S^{(1)}, T_+ + T_-] + [S^{(1)}, T_0] + \frac{1}{2} [S^{(1)}, [S^{(1)}, V]] + [S', V] \quad (*)$$

containing the contributions $\propto t^2/U$.

In the last equation, we made use of the fact that

$$[S', H] \text{ must be equal to } [S', V]$$

for this term to be of the order of t^2/U

(since, by assumption $S' \propto \frac{t^2}{U^2}$!)

Eq. (*) simplifies to

$$H'_{\text{eff}} = \frac{1}{U} [T_+, T_-] + [S^{(1)}, T_0] + [S', V]$$

$H_{\text{eff}}^{(2)}$ should not contain terms that lead to leaving the considered Hubbard sector;

note that term $[T_+, T_-]$ is allowed since it

describes processes after which the system ends up in the same Hubbard sector.

On the other hand, $[S^{(1)}, T_0]$ causes transitions to the other sectors (which are not allowed in $H_{\text{eff}}^{(2)}$!) and therefore S' should be chosen in such a way as to cancel $[S^{(1)}, T_0]$:

$$\Rightarrow [S^{(1)}, T_0] + [S', V] = 0$$

Note that we do not have to find the explicit form of S' to find $H_{\text{eff}}^{(2)}$:

$$H_{\text{eff}}^{(2)} = T_0 + V + \frac{1}{U} [T_+, T_-] + O\left(\frac{t^3}{U^2}\right)$$

The last effective Hamiltonian describes the intra-Hubbard sector physics of all sectors!!

Our primary interest, however, is the lowest Hubbard sector — the one that contains no doubly-occupied sites! (since we are interested in the low-energy properties of the system!)

Clearly, the term $T_+ T_-$ yields 0 when acting on any configuration (state) in the lowest Hubbard sector!

Thus in the lowest sector $H_{\text{eff}}^{(2)}$ simplifies to

$$H_{\text{eff}}^{(2)} = T_0 + V - \frac{1}{U} T_- T_+ \quad , \text{ or, more specifically,}$$

$$H_{\text{eff}}^{(2)} = -t \sum_{i, \delta, \bar{\delta}} (1 - n_{i, \bar{\delta}}) c_{i\bar{\delta}}^{\dagger} c_{i+\delta, \bar{\delta}} (1 - n_{i+\delta, \bar{\delta}}) \\ - \frac{J}{2} \sum_{\substack{i, \delta, \delta', \\ \bar{\delta}, \bar{\delta}'}} (1 - n_{i+\delta, \bar{\delta}'}) c_{i+\delta, \bar{\delta}'}^{\dagger} c_{i\bar{\delta}'} \times \\ \times n_{i\bar{\delta}'} n_{i\bar{\delta}} c_{i\bar{\delta}}^{\dagger} c_{i+\delta, \bar{\delta}} (1 - n_{i+\delta, \bar{\delta}})$$

Here $J \equiv \frac{2t^2}{U}$ is the energy scale corresponding to the virtual hopping fluctuations between Hubbard sectors — the "superexchange interaction". The last Hamiltonian is usually called the '(extended) t-J model'.

Let us now consider the special case of half-filling (one particle per site, i.e., $N_e = N$):

in this case the hopping term ($\propto t$) in $H_{\text{eff}}^{(2)}$ obtained above has to vanish, since every hop would cause a doubly-occupied site (and, by assumption, we want to be in the lowest sector!).

For the same reason, in the term proportional to J we have to take $\delta = \delta'$ (an electron has to return to the original site in order to avoid creation of doubly-occupied sites!). Finally, in the lowest sector the "projections" $\propto 1 - n_{i+\delta, \bar{\delta}}$ are satisfied automatically \Rightarrow at half-filling $H_{\text{eff}}^{(2)}$ reduces to

$$H_{\text{eff}}^{(2)} = -\frac{J}{2} \sum_{i, \delta, \delta'} C_{i+\delta, \delta'}^{\dagger} C_{i\delta}^{\dagger} n_{i\bar{\delta}} n_{i\bar{\delta}} C_{i\delta} C_{i+\delta, \delta}$$

Note that the creation and annihilation operators in the last expression appear in pairs!

What is the physical meaning of this?

The meaning is that the electrons are localized and charge transport is not possible!

(the Mott-Hubbard insulating state!)

Recalling that spin- $\frac{1}{2}$ operators can be expressed in terms of fermion operators as

$$S_i^z = \frac{1}{2} (C_{i\uparrow}^{\dagger} C_{i\uparrow} - C_{i\downarrow}^{\dagger} C_{i\downarrow}); \quad S_i^+ = C_{i\uparrow}^{\dagger} C_{i\downarrow}; \quad S_i^- = C_{i\downarrow}^{\dagger} C_{i\uparrow}$$

the last Hamiltonian can be rewritten (see Problem 2)
(Blatt 11)

as the spin-only Hamiltonian of Heisenberg type:

$$H_{\text{eff}}^{(2)} = J \sum_{i,\delta} \left(\vec{S}_i \cdot \vec{S}_{i+\delta} - \frac{1}{4} \right)$$

Since $J \equiv \frac{2t^2}{U} > 0$ the last Hamiltonian is antiferromagnetic!

So we have shown that at half-filling only the spins of the electrons matter! The projections involved in the derivation of this spin-only effective Hamiltonian have drastically reduced the effective electronic Hilbert space.

The effective antiferromagnetic Heisenberg interaction are, once again, a result of the virtual hopping fluctuations ('virtual' because a particle hops back to its original site in two steps). and is often called 'kinetic exchange'. This is to be contrasted with the 'Hunds rule' exchange mechanism (of ^{e.g.} atomic physics) which applies to strongly overlapping electrons; such electrons tend to stay further apart to minimize the (repulsive) Coulomb interaction. Such exchange interaction favours ferromagnetism. An example is provided by all metallic magnets