Strongly-correlated systems; the Hubbard model

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Given that the electron mass is $\sim 10,000$ times smaller than a typical atomic mass, electrons are subject to strong quantum fluctuations on the angstroem length scales. Therefore we do not see examples of the real-space orderings of electrons, the latter being objects that carry both charge and spin. The real space ordering of electrons usually accompanies other (lattice) degrees of freedom. We will see, however, that in the presence of strong electron-electron interaction we can get a magnetic (spin) ordering!

The band theory of solids is based on the independent-electron picture. The greatest achievement of this theory is that it successfully classified a huge number of crystalline solids into metals and insulators.

We call a material insulating if its static electrical conductivity approaches zero as the temperature is lowered:

$$\lim_{T\to 0} \sigma(T) = 0$$

If $\sigma(T)$ remains finite as $T \to 0$, then the system is metallic.

Alternately, we can say that the system is metallic if the density-of-states at the Fermi level is non-vanishing: $\rho(\epsilon_F) \neq 0$. The situation where $\rho(\epsilon_F) = 0$ arises if ϵ_F lies between the top of the uppermost filled band and the bottom of the first empty band, i.e., inside the gap between these two bands. Then the material must be an insulator.

This will be the case when the system contains an even number of electrons per unit cell!

According to the band theory, the systems with odd number of electrons per unit cell should then be metallic. This basic prediction, as it turns out, fails in many cases: for instance, an example is furnished by the transition-metal oxide CoO.
The outer shells of Co have the configuration $3d^7 4s^2$ and those of oxygen $2s^2 2p^4$ $\Rightarrow$ the number of electrons per unit cell is $9+6=15$, an odd number. And yet, CoO is not a metal, but in fact one of the toughest insulators known!

In the earlier parts of the course we have seen that Coulomb interaction between electrons in metals favors the Fermi liquid state. The picture changes drastically for electrons in orbitals strongly-localized to atomic cores, such as d-orbitals in transition metal oxides. The intratomic Coulomb energy corresponding to the repulsion of two electrons sharing the same orbital is given by ($e_0^2 \equiv e^2/(4\pi\varepsilon_0)$)

$$U = \int d\vec{r}_1 \int d\vec{r}_2 \, |\phi(\vec{r}_1)|^2 \frac{e_0^2}{|\vec{r}_1 - \vec{r}_2|} |\phi(\vec{r}_2)|^2 .$$

Since two electrons sharing the same orbital have a short mutual distance (~ 1 Å), Us can be very large — for d- and f-electrons U can be as large as 15-30 eV!

The other relevant energy is provided by the electron bandwidth W. [Remember that in tight-binding

models $W = 2zt$, where t is the hopping integral and z the coordination number (number of nearest-neighbors of a given atom).

While the kinetic energy (characterized by W) tends to delocalize the electrons into itinerant (Bloch) states (and thus favors metallic behavior), the on-site repulsive e-e interaction tends to localize electrons, thus driving a transition to an insulating state.

As long as $U \gg W$, the kinetic energy cannot overcome the interaction energy and the electrons are localized on the atoms. The resulting insulating state is called a 'Mott-Hubbard' (or only 'Mott') insulator. Such a state is usually characterized by a magnetic order.

To distinguish them from these interaction-induced insulators (Mott insulators), the more conventional insulators (those whose insulating behavior is due to completely filled bands) are referred to as band insulators.

Which materials would be typical Mott-Hubbard (magnetic) insulators?

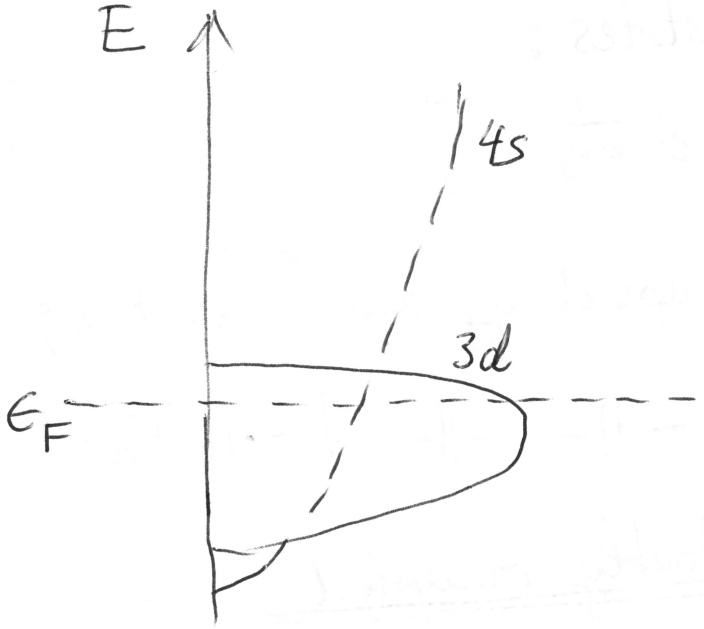
They are typically found in ionic substances such as oxides, fluorides, chlorides, etc.

For instance, consider the 3d oxides (CaO, NiO, Fe_2O_3, ...) and take ZnO as a reference: this material is a band insulator since it has completely filled 3d band, separated by a large bandgap (~ 10 eV) from an empty 4s conduction band. In CaO there is one more hole on the metal ion $\Rightarrow$ this hole then makes the 3d band only partially filled; but because of the strong effective interactions these holes are localized.
Going further to the left in the 3d series, the d-band becomes gradually emptied until one arrives at CaO which is again a band insulator. All monoxides involving transition-metal ions are Mott-Hubbard insulators.

It should be emphasized that there are materials, like V_2O_3, which at ambient pressure are Mott-Hubbard insulators, but undergo a transition into a metallic state under pressure; pressure decreases the lattice constant, resulting in increased W; when $W \approx U$, a transition to a metallic state takes place.

Non-integer filling (arising from doping) or the overlapping of bands stabilize the metallic state even at very high interaction strengths.

The tightly-bound d and f electrons typically satisfy the criterion of large U and small W, while the s/p electrons are in the small U/W limit. Because s- and p-bands have large bandwidths it often happens that both f/d and s/p bands are partially filled, causing a non-integer occupancy of d/f bands. An example is provided by a metal like <u>Ni</u>. Its electronic configuration is $3d^9 4s^1$. The s-band crosses ϵ_F in Ni, and the local electron distribution is $3d^{9.4} 4s^{0.6}$.



The d-electrons can easily delocalize and the system is not a Mott-Hubbard insulator.

The <u>Hubbard model</u> is the most studied lattice fermion model. At the same time it is the simplest model that can describe the aforementioned competition between the kinetic-energy and interaction effects.

The <u>single-band</u> Hubbard Hamiltonian reads

$$H = -t \sum_{i,\delta,\sigma} c^{\dagger}_{i\sigma} c_{i+\delta,\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow},$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) an electron with spin σ ($\sigma = \uparrow, \downarrow$) on a lattice site i; here $n_{i\sigma} \equiv c^{\dagger}_{i\sigma} c_{i\sigma}$. The interaction strength U is the intratomic Coulomb interaction energy and is usually referred to as the 'Hubbard U'. [The atomic level about which the tight-binding band is centered is usually chosen at $\varepsilon = 0$.]

The Hubbard model is a four-state model, in the sense that each lattice site can be found in any of the four local basis states:

$|0\rangle_i$ → site i is empty;

$|\uparrow\rangle_i$ → site i is occupied by an $\uparrow$-electron;

$|\downarrow\rangle_i$ → -||- -||- -||- -||- $\downarrow$-electron;

$|\uparrow\downarrow\rangle_i$ → site i is doubly occupied

The $T = 0$ behavior of the Hubbard model is governed by two parameters:

the relative interaction strength $\frac{U}{t}$ and the electron density $n = \frac{N_e}{N}$ (N → number of sites; N_e -||- of electrons)

We will be most interested in the situation with $n = 1$ (one particle per site), usually referred to as HALF-FILLING.

We will study the strongly-interacting limit $\frac{U}{t} \gg 1$ of this model, most prominently at half-filling.

But first we can remind ourselves of the toy version of the Hubbard model – <u>two sites</u> with <u>2 electrons</u>.

$$H = -t \sum_{\sigma} (c_{1\sigma}^{+} c_{2\sigma} + c_{2\sigma}^{+} c_{1\sigma}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow})$$

For $U = 0$ the ground state for an electron with spin σ (the <u>bonding</u> state) is $b_{\sigma}^{+} |0\rangle_e = \frac{1}{\sqrt{2}} (c_{1\sigma}^{+} + c_{2\sigma}^{+}) |0\rangle$, and for 2 electrons it is given by

$$b_{\uparrow}^{+} b_{\downarrow}^{+} |0\rangle_e = \frac{1}{2} (c_{1\uparrow}^{+} c_{1\downarrow}^{+} + c_{2\uparrow}^{+} c_{2\downarrow}^{+} + c_{1\uparrow}^{+} c_{2\downarrow}^{+} + c_{2\uparrow}^{+} c_{1\downarrow}^{+}) |0\rangle_e$$

the 'singly occupied' configurations have for $U = 0$ exactly the same weight as doubly occupied ones $c_{i\uparrow}^{+} c_{i\downarrow}^{+} |0\rangle_e$ $(i = \overline{1,2})$.

However, for large $\frac{U}{t}$ the ground state is

$$\frac{1}{\sqrt{2(1+4t^2/U^2)}}\left[(c^+_{1\uparrow}c^+_{2\downarrow}-c^+_{1\downarrow}c^+_{2\uparrow})+\frac{2t}{U}(c^+_{1\uparrow}c^+_{1\downarrow}+c^+_{2\uparrow}c^+_{2\downarrow})\right],$$

$$\times|0\rangle_e$$

meaning that the admixture of doubly-occupied states becomes very small for $\frac{U}{t}\gg 1$!

The two electrons tend to stay away from each other!

The size of the electronic Hilbert space grows rapidly if we increase the number of sites. The system with, say, 20 sites and 20 electrons is not an easy task for modern supercomputers!

But we will show that at half-filling the effective model becomes an antiferromagnetic Heisenberg model.