REVOLUTIONS IN SYSTEMS

What kinds of states arise when the interaction between particles becomes dominant over the quantum behavior of individual particles in the system?

When a crowd of experiences powerful political or religious emotions, it may result in instability, in the dominance of a particular element, or even in a spontaneous trend to arrange into an entirely new collective state. The same may happen to correlated quantum particles, such as electrons in the condensed state.

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When a crowd of individuals experiences powerful political or religious emotions, the behavior of individuals is driven by the crowd behavior. This can result in instability or dominance of a particular factor, or even in a spontaneous trend among a collection of individuals to arrange themselves into some new collective state. A physical system comprising a high number of strongly correlated objects or particles is in such a case said to have undergone a phase transition or a spontaneous breakdown of symmetry, giving rise to a new state of the entire system – a state not defined as just the sum of contributions of individual particles. In this instance, strong correlations generally transform normal states into highly collective states, with new properties distinct from those resulting from behaviors typical of the individual objects composing it.

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When the objects are electrons, for instance, the normal state may be metallic or semiconducting, whereas the collective state may be superconducting or magnetic. Normal states generally do not evolve into collective states slowly, for example by a gradual change of particle density – in fact, such changes are some of the most sudden processes found in nature. At a critical point during such a change there occur certain singularities, or jumps in the value of certain physical quantities, or even plain infinities. In such cases we are dealing with the *emergence* of condensed systems of objects, be they physical particles making up matter or human beings comprising a society. In the first instance the event could be the explosion of a ball of gas to form a star. In the latter, the catastrophic event could be a revolution. In both cases the transformation leads to a brand new kind of order (or disorder). Thousands of such instabilities are known to us in physics, in the form of phase transformations, although they only depend on certain features of the system. Here we are interested in changes that are typical of systems of strongly correlated quantum particles – electrons – whose collective state can change drastically.

Creation via a mutual repulsion

Practically all matter is made up of atoms, which in turn are made up of nuclei (frequently ions) and electrons. Systems comprising many electrons can be complex on the molecular level, in particular when these collections of atoms or molecules form functional systems such as DNA, crystalline bodies, or quantum liquids. The most regular (albeit not the simplest) arrangement is a crystal comprising a lattice of atoms. As Fig. 1 shows based on the example of a high-temperature superconductor, this can become a complex atomic architecture.

It turns out that depending on the distance between atoms in the system, electrons can continue behaving as though they still belong to their original atoms (this is not strictly correct, since such crystals are systems of many atoms interacting with one another). However, if external (valence) electrons still belong to individual atoms, the system is described as an *insulator* or atomic crystal. This is because electrons cannot move throughout the system (they do not conduct electricity), since they are still bound to their parent atoms. These systems are called *Mott-Hubbard* insulators, in which such atomic states are stabilized further by the repulsive Coulomb interaction between the valence electrons.

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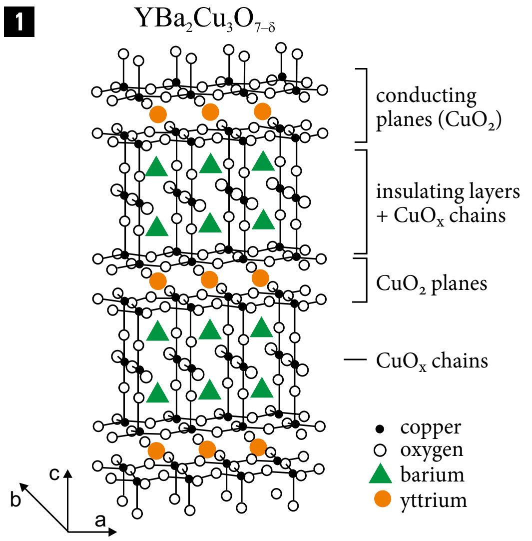

Fig. 1:
Superconducting copper-oxygen layers (CuO_2) are interspersed with non-metallic layers, hence their almost two-dimensional structure.

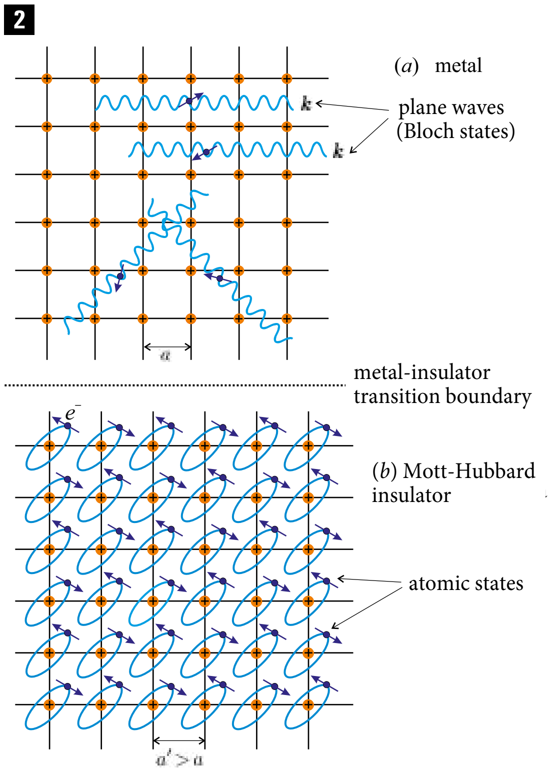

Fig. 2:
Schematic representation of a plane comprising a hydrogen atom lattice in a metallic state; above, Mott insulator (antiferromagnetic semiconductor); below, Mott-Hubbard transition.

Fig. 3:
Structure of La_2CuO_4 – a starting material for the high-temperature superconductor $La_{2-x}Sr_xCuO_4$. The antiferromagnetic structure of the electron spins belonging to the Cu^{2+} ions is shown as horizontal arrows. The temperature of the transition into this magnetic state (Néel) is ≈240 K. Note the layer structure of the compound: the distances between layers (5 Å) are significantly greater than the distances between Cu atoms within the plane (on the order of 2 Å); this means that remaining atoms in this structure play a passive role.

What happens when the distance between atoms is reduced, for example by applying external pressure? For high enough pressure, we will be pressing the electron shells against each other! We say that their electron states increasingly overlap, and there comes a point where the distance between neighboring atoms becomes so small that the electrons lose their original affiliation, since neighboring atoms attract them just as powerfully. This is the critical point we have discussed earlier, where electrons break away from their parent atoms and in spite of their mutual repulsion, they form a metallic (delocalization) state. This state can be described as that of a quantum electron liquid, filling the container made of a scaffold of bare ions which remain in the positions originally held by the neutral atoms.

At absolute zero, this involves a change of resistivity from an infinite value for insulators to zero for metallic state – an infinite change of electrical conductivity. Additionally, suppose each atom possesses a single electron in the valence shell. In Mott insulators, their spins are arranged in an anti-parallel pattern; this means they are in an *antiferromagnetic* state due to powerful exchange (magnetic) interactions. Such a magnetic state, typical of simple Mott insulators, is also found in the original atomic material for high-temperature superconductors such as La_2CuO_4.

What happens to spins in the metallic state? Electrons with opposite spins avoid one another as they move through the crystal. Fig. 2 shows the situation during the transition to metallic state. However, what happens to correlations between the opposite spins in the metallic state when the exchange interactions also take place in the collective state? It turns out those correlations survive. They lead to the formation of moving pairs with opposite spins (known as *Cooper pairs*), which in turn are responsible for superconductivity, i.e. conductivity of an electrical current with zero electrical resistance at temperatures up to about 100 K. We hope that one day it will be possible to achieve superconductivity at room temperature. The connection of these antiferromagnetic interactions with pairings in metallic states was first proposed in 1986 by P.W. Anderson of Princeton University and a year later applied to the theoretical t-J model, which I originally proposed in the 1970s.

New collectivity

As a decent approximation, high-temperature superconductors can be modeled by a single copper-oxygen plane (compare Figures 3 and 4). Usually we ignore the oxygen atoms as well, leaving only Cu ions. The individual minima shown in Fig. 4 depict the potential energy of the electron corresponding to the Cu^{2+} ion – the $3d^9$ configuration. It is only the ninth electron which is regarded as the valence electron, whereas the remaining eight are bound strongly within the atom and form part of the non-spin ion core Cu^{3+} ion. Among those "ninth" electrons, the key role is played by the following parameters: J_{ij} (antiferromagnetic exchange) of the extremely high value of about 0.1 eV, and U on the order of 8÷10 eV (repulsive interaction between electrons when they find themselves on the same atom, known as the *Hubbard interaction*).

Let us consider electron states in a two-dimensional space, for which the kinetic energy, proportional to the amplitude of their jumps $i \to j$ (with $t_{ij} \approx 0.35$ eV)

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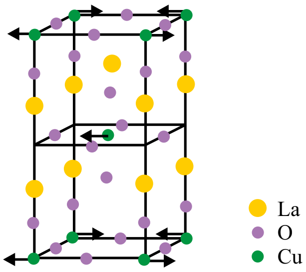

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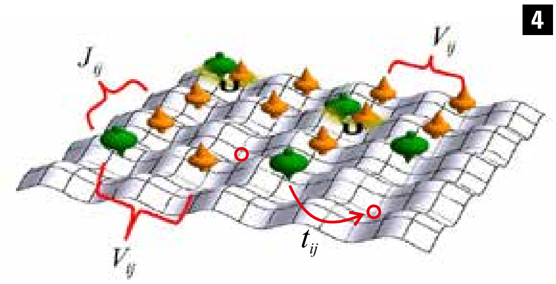

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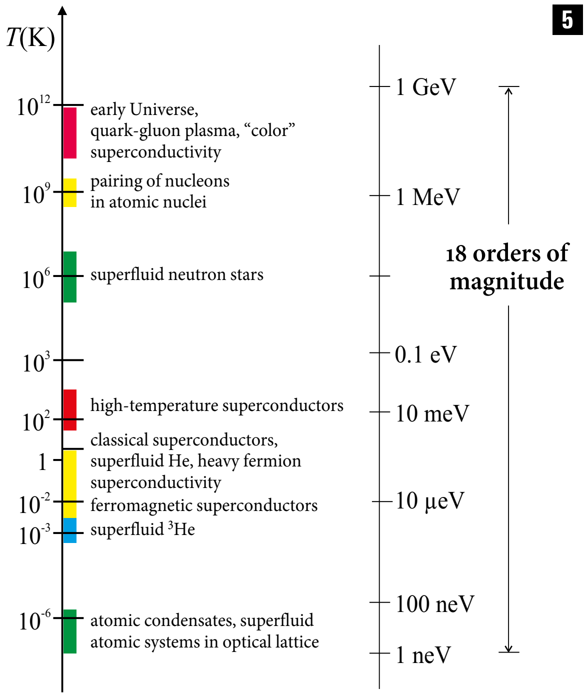

and denoted by a red arrow, is dominated by the interaction *U*. The name of the *t-J model* describing such a correlated-electron state derives from the fact that those two factors are seen as being dominant; however, I now believe that it would be more accurate to describe it as the so called *t-J-U model* or even expand the starting model even further.

The resultant situation is as follows: for a stoichiometric system $La_2CuO_4 = La_2^{3+}Cu^{2+}O_4^{2-}$, each Cu atom contains a "ninth" electron and the system is a *Mott-Hubbard insulator* (see Fig. 3). Simply put, the repulsion U is sufficiently powerful ($U >> |t_{ij}|$) to hold the electrons on their original atoms. At temperatures $T > O$ such systems are (*antiferro*)*magnetic semiconductors*. J.G. Bednorz and K.A. Müller had the idea in 1986 to create a non-stoichiometric system $La_{2-x}Sr_xCuO_4$, in which certain La^{3+} ions were replaced by Sr^{2+} ions, supplying the system with two valence electrons instead of the three supplied by La^{3+}. Such an electron deficit results in creation of "*electron holes*," allowing other electrons to move freely throughout the system while avoiding double-occupied states; the latter bear extremely high energy costs on the system, which means they do not occur in practice. The biggest surprise here is that electrons moving through the hole states form pairs at close interatomic distances due to exchange interactions, and thus create a superconducting state with high transition temperature (the current record is 165 K in cuprate samples under high pressures). Note that our description of superconductivity uses terminology describing pair formation in real space rather than in momentum space, as was described by the groundbreaking Bardeen, Cooper, and Schrieffer (BCS) theory formulated in 1957 as description of the first superconductors. This is one of the fascinating features of these new superconductors. The most distinctive attribute, however, is the fact that the superconducting state evolves from doping the Mott insulator (semiconductor) resulting in the formation of a metallic state which immediately becomes a strong superconductor. It was this unconventional idea that earned Bednorz and Müller their Nobel prize.

What's next?

The description of high-temperature superconductivity and, in general, of highly correlated condensed systems poses the fundamental challenge at present and is at the forefront of contemporary physics. In fact, superconductivity and superfluidity appear at all scales of available energy (comprising18 orders of magnitude), so they can be described as a universal phenomenon (cf. Fig. 5).

It seems that a clear version of the theories of those systems are beginning to emerge, including our own contribution. Our theory complements an earlier quantum theory of multiparticle systems based on an effective single-particle description. Systems of strongly correlated particles also have many other unique properties, such as *spin-dependent* effective masses of quasi-particles and *quantum phase transitions* with accompanying them critical phenomena. Is it thus a high time to step beyond the traditional solid state physics, semiconductor physics or magnetism, as practiced successfully in Poland in past research?

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Fig. 4:
Individual copper-oxygen plane depicted as a lattice of copper ions, located at the energy minima on the plane of potential energy for individual electrons. Individual interactions between neighbors at nodes i and j of the lattice are discussed in the text. Electron spins are depicted as bold arrows.

Fig. 5:
Temperature value below which superconductivity is observed in physical and astrophysical systems. The hierarchy of superconducting/superfluid condensed systems occurring in nature according to particle interaction energy (temperature) scales (energy scale is shown on the right). This is the state found at all existing energy scales, making it universal (from J. Spałek, D. Goc-Jagło, *Phys. Scr.* 86, 048301, 2012).

Acknowledgements

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Further reading:

Honig, J. M. & Spalek, J. (2016). *A Primer to the Theory of Critical Phenomena*. Elsevier.