More is different - Emergence of collective properties in a Mott insulator

Francisco M. O. Brito
Final year student of the MSc in Engineering Physics at Instituto Superior Técnico, University of Lisbon
(Dated: Portuguese: October 2018, English translation: May 2024)

This article was originally published in the *Pulsar* magazine, published by the student union at Instituto Superior Técnico, University of Lisbon, Portugal. The original publication was aimed at undergraduate students and is written in the Portuguese language. It is available here (page 18).

There is a vast array of so called quantum phenomena that cannot be explained using classical physics. As might be expected, quantum theory differs from its classical counterpart — sometimes referred to as Newtonian mechanics — in many aspects. Let us focus on one such difference, which is particularly relevant for the physical system that shall be discussed in this article: the notion of indistinguishability. The classical description of a gas consists of a set of particles (here, the reader could picture billiard balls) in perpetual motion inside a container. Each particle has a given kinetic energy induced by thermal fluctuations. A given particle's velocity changes whenever it collides with another particle (or, more rarely, whenever the particle collides with the walls of the container). Assuming that the system is in thermal equilibrium, the distribution of the total kinetic energy among all particles is well defined and centred around an average value. It is this distribution that sets the temperature of the system. While the motion of the particles is deterministic, even a gas — for which this idea of independent particles colliding among themselves and bouncing on the walls of a container holds remarkably well— typically has such a large number of particles that the equations describing their motion simply can't be solved. Thus, these systems are usually approached probabilistically. Thermodynamic properties are obtained from statistical considerations (for example, via the average of a given quantity). At this point, more demanding readers are likely dissatisfied. Certainly, the average is not always a good statistical indicator even for day to day situations. Yet, in the case of thermodynamically large systems, the average is particularly useful because fluctuations around it are negligible when the number of particles is of the order of the Avogadro constant. The validity of a statistical analysis relying on the average relies on an assumption that is often taken for granted: the distinguishability of particles.

In quantum physics, the energy distribution of the particles in a system is the result of their intrinsic probabilistic nature. Unlike the more familiar case of classical particles, it is not possible to distinguish quantum particles of the same type. In fact, the very concept of individuality of such particles — dubbed identical — must be abandoned. The behaviour of a quantum system can only be described collectively and it is not possible to describe it by simply extrapolating the properties of its constituent particles. In 1927, Sommerfeld used the concept of identical particles to generalise the theory of the so called classical gas to quantum particles. This relatively simple free electron model turns out to be sophisticated enough to capture some of the properties of metals!

There is a rule of thumb that allows one to decide whether it suffices to treat a given system classically or if one must resort to quantum physics. One simply estimates the typical value of a quantity called action within the phenomenon at play. Quantum phenomena have a typical action of the order of the Planck constant $\hbar \sim 10^{-33}$ kg m^2/ s. The reader might now be wondering what is the order of magnitude of the typical action for particles, say within a solid. For instance, an electron with mass 10^{-30} kg and velocity 10^6 m/s, moving between atoms separated by distances of the order of the Angstrom ($1\,\mathring{A} = 10^{-10}$ m), has a typical action of 10^{-34} kg m^2/ s, putting electrons in a solid comfortably within the quantum regime!

In order to describe electrons in a solid, one considers a system of atoms on a periodic lattice. For concreteness, let us assume a square lattice. Electrons are much lighter than the nuclei of each atom, so the motion of the latter can be safely ignored. In an isolated atom, electrons can have energies belonging to a discrete set of energy levels. Analogously, electrons on a more complex system comprised of atoms in a solid can have energies in a set of energy bands, which may exclude some ranges of energies. Energy bands are occupied sequentially, starting from the lowest allowed energy. Each band may host a number of electrons equal to twice the number of atoms on the lattice (this factor of 2 is due to Pauli's exclusion principle, which allows two electrons with different quantum spin numbers —defining their intrinsic magnetism — to occupy the same energy band). Band theory classifies solids as: metals, if there are partially filled bands, or insulators, if the highest energy band (dubbed valence band) that is fully occupied is followed by a completely empty band called conduction band. The energy separation between the valence and conduction bands is called band gap. Figure 1 illustrates these two behaviours, with a third one, the semiconductor, usually highlighted due to its technological relevance, being no more than an insulator with a band gap of less than 4 eV. Band theory was enormously successful until a flaw was found in the classification of a type of materials that later became

known as Mott insulators, even though they were predicted to be metals within band theory.

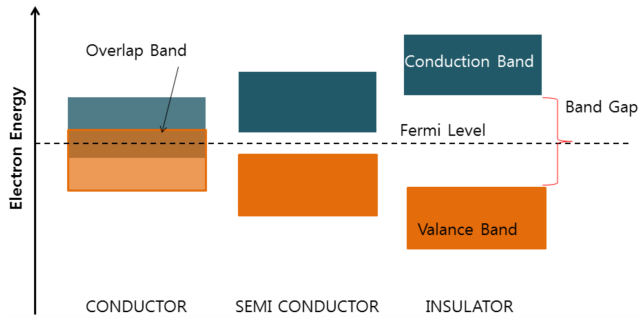

FIG. 1. Classification of materials according to band theory. Source: [1]

In fact, one of the assumptions of band theory is that electrons are not affected by the presence of other electrons in their vicinity (in other words, that electrons do not see other electrons). Effectively, this is equivalent to ignoring the Coulomb interaction between them. In reality, this assumption is actually valid as an approximation in some cases, but breaks down for some materials. The conjugation of the various types of interactions within a solid can lead to a variety of phenomena. Sometimes, their effects cancel out, whereas in other cases they can actually amplify each other. Even though, in some cases, the interaction between electrons may not be negligible, it can still get cancelled out by other effects. Still, in Mott insulators, the repulsive Coulomb interaction between electrons leads to insulating, rather than metallic behaviour. In this case, electronic correlations — quantifying their mutual interdependence —lead to the emergence of purely collective properties.

In correlated systems, the 'motion' of a particle affects that of all other particles in the system. Perhaps this can be made clearer using an analogy. When a sound wave propagates, air molecules oscillate collectively. If that was not the case, i.e. if density fluctuations were random, we would not hear a sound. This phenomenon depends on collective behaviour, implying that molecules are correlated. So, in a correlated system, such as a system of interacting electrons, the same principle inherent to the sound wave example applies: there are phenomena that can't be explained solely by the properties of the molecules, instead requiring knowledge about the interactions between them. Collective behaviour is only possible because the various components of a system are sensitive to each other's presence, giving rise to the emergence of frequently counterintuitive properties. Another simple physical example is that of a magnet. Its microscopic description consists of imagining each atom as being a compass, or, in the physical jargon, a magnetic moment. Picture a set of compasses very far away from Earth's magnetic field, so that they don't all tend to align in the same direction. Now, let us introduce a rule. Rather than being influenced by an external entity, each compass affects how the nearest neighbouring compasses align, for example, by making it more energetically efficient for all neighbouring compasses to align. Then, a situation in which all compasses align in the same direction is an example of emergent behaviour, leading to inherent magnetism of the system of compasses. This emergent phenomenon does not occur spontaneously for a single isolated compass, or magnetic moment. It is collective in nature and occurs due to the high number of atoms in a solid, each behaving like a compass.

Now, let us go back to the case of the Mott insulator. In certain materials (namely transition metal oxides), when pressure is high, electrons are more likely to be shared by the atoms of the lattice, constantly hopping from atom to atom. In terms of their energy, this translates into a high kinetic energy, favouring the establishment of an electrical current. The material then becomes metallic. At high pressure, despite other interactions, such as that between electrons, affecting the overall energy of the system, they remain small compared to the kinetic energy. However, as pressure is reduced, the ratio between the kinetic energy and electronic interactions decreases and, eventually, there is a critical pressure at which they balance out and the electrical current is inhibited.

The Hubbard model is the simplest model that is able to capture the essence of the Mott transition. On the one hand, it considers that valence electrons hop between the orbitals of different atoms. This favours the onset of an electrical current. On the other hand, the situation mentioned above, where two electrons with different quantum spin number occupy the same orbital (Pauli's exclusion principle) is energetically penalised due to the Coulomb repulsion that becomes more and more relevant as electrons are brought closer together, and, dramatically so, when they occupy the same orbital of a given atom. In Mott insulators, an insulating phase, where each orbital is occupied by a single electron — avoiding double occupation — is favoured energetically. The movement of electrons (hopping between orbitals of different atoms) requires double occupation. This implies a strong energy penalty. Therefore, the system becomes an insulator because the onset of a current is not favourable. Electrons tend to get stuck to the atomic orbitals that they are already occupying. This is to be contrasted with the picture obtained from band theory, where a system with one electron per atom is a metal because it will have at least one partially occupied band.

Mott insulators can be used to fabricate memory devices with remarkably fast writing speeds (10^{-100} ns). In these devices, the control over the occupation of atomic orbitals is key. Structural and electronic phase transitions within correlated electron systems originate peculiar properties. The transition between collective states

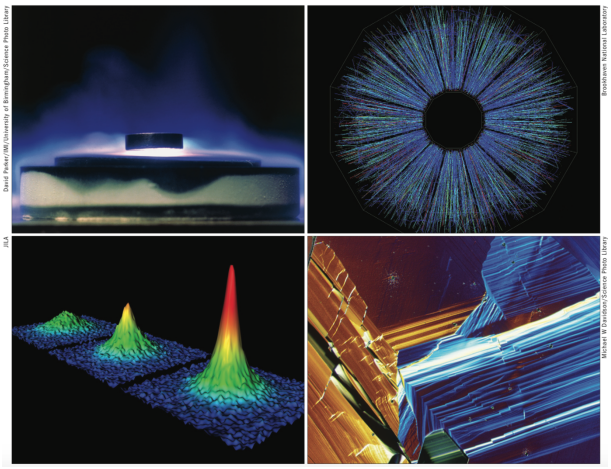

FIG. 2. Strong correlations between particles comprising a system are the common thread connecting various fascinating physical phenomena, such as (clockwise, from the top left panel): high-temperature superconductors, quark-gluon plasmas, organic superconductors and - under certain conditions — ultracold atoms. Source: [2].

under external stimuli allows one to encode, store and process information. Mott insulators could also be crucial in the fabrication of memristors, neuromorphic components used to replicate the neurobiological architecture of the system in an electrical circuit (as their name implies). In a memristor, electrical resistance depends on the current that circulated through the system in the past. The history of the system affects its properties: the device remembers its past. This property is called nonvolatility. In the brain, neurons adapt over the course of the learning process, storing a "memory" of their history and synapses acquire an adaptive property called plasticity. In the future, this effect could be mimicked by memristors.

[1] N. Mahato, M. O. Ansari, and M. H. Cho, Production of utilizable energy from renewable resources: Mechanism, machinery and effect on environment, Advanced Materials Research **1116**, 1 (2015).

[2] J. Quintanilla and C. Hooley, The strong-correlations puzzle, Physics World **22**, 32 (2009).