I Introduction

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1 Emergent phenomena

The concept of emergence arose in arguments about the biological basis of consciousness that were sparked by Darwin's theory of evolution. It was formalized by the philosopher George Henry Lewes in his 1875 *Problems of Life and Mind* [1]. But John Stuart Mill, around whom a successful school of *British Emergentism* developed, had already noted in his 1843 *System of Logic* [2]

> *All organized bodies are composed of parts, similar to those composing inorganic nature, and which have even themselves existed in an inorganic state; but the phenomena of life, which result from the juxtaposition of those parts in a certain manner, bear no analogy to any of the effects which would be produced by the action of the component substances considered as mere physical agents. To whatever degree we might imagine our knowledge of the properties of the several ingredients of a living body to be extended and perfected, it is certain that no mere summing up of the separate actions of those elements will ever amount to the action of the living body itself.*

While it was hotly debated whether the constitutive principles of biology are reducible to those of physics and chemistry, the importance of emergence in physics was recognized only much later. From the inception of their science, physicists have been fascinated most with finding the ultimate laws of the universe. There is no doubt that our present understanding of the world owes a lot to this *reductionist* approach. That one and the same force, gravitation, explains how an apple falls and how the planets move around the sun is an astonishing discovery. Other ideas such as the existence of atoms, a finite number of particles from which all normal matter is made, revolutionized our worldview. The understanding of the differences between atoms, which led to the periodic table, opened the path to quantum mechanics and gave chemistry a microscopic basis. At the same time, the landscape grew more complex. It became clear that atoms are not at all the fundamental particles, but that they are composed of yet more elementary particles, electrons, neutrons, and protons. It was understood that a new force holds the nuclei together, which was later still understood to be the consequence of a more fundamental force, the strong force, between more elementary particles, the quarks. The stellar successes of the reductionist approach led a large part of the scientific community to think that the new grand challenge was to find the theory of everything, in which the ultimate elementary particles are identified and where all known forces are unified. From this point of view, everything will ultimately be explained in the same framework. Among the many successes of this approach, the most striking and perhaps least celebrated revelation is, however, that *every fundamental theory hides a more fundamental one* and that the target seems to elude us, today's elementary particles and fundamental forces becoming tomorrow's bound states and effective interactions. So the question is whether an ultimate fundamental theory of everything would solve all problems. A glimpse into the history of condensed-matter physics hints at the answer: not really. At the theory layer of chemistry and solid-state phenomena, the fundamental particles and interactions have actually been known since the first quarter of the 20th century. Most of solid-state physics and chemistry can indeed be described by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle \tag{1}$$

where the Hamiltonian for a set of atomic nuclei $\{\alpha\}$ with atomic numbers $\{Z_\alpha\}$ and masses $\{M_\alpha\}$ and their accompanying electrons $\{i\}$ is given, in atomic units, by

$$H = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_\alpha \frac{1}{2M_\alpha}\nabla_\alpha^2 - \sum_{\alpha,i}\frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2}\sum_{ii'}\frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} + \frac{1}{2}\sum_{\alpha\alpha'}\frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}\,.$$

As Laughlin and Pines pointed out [3], here we have the theory of (almost) everything (ToaE). Why then are we still working on condensed-matter physics? The history of 20th century condensed-matter physics is full of experimental discoveries showing genuinely novel behaviors that were not only unanticipated by theory, but took decades to fully clarify, even though, in principle, the equations, the ToaE, were well known. Examples are magnetism, superconductivity, the Kondo effect, or the quantum-Hall effect in its integer and fractional forms. Some of the mysteries discovered in the last century are still not or not fully clarified, such as high-temperature superconductivity and heavy-fermion behavior; new ones will certainly come to light in the years to come. The difficulties are not merely technical or computational, but fundamental. As P.W. Anderson pointed out in the now very famous article *More is Different* [4], when many particles interact, even if we know the type of interaction, and even if the interaction is as simple as a two-body term, totally surprising results can emerge: gold is made of gold atoms; but a single atom of gold is neither a metal nor does it appear in a golden color. Likewise, an Fe atom is not ferromagnetic, nor does a Pb atom superconduct at low temperatures. Perhaps it is easier to grasp the concept of emergence by going back to its origin. As Anderson writes [5]

> *The idea of emergence began in biology, where it was realized that the course of evolution is one long story of novel properties emerging out of the synergy of large collections of simpler systems: cells from biomolecules, organisms from cells, societies from organisms. But that emergence could occur in physics was a novel idea. Perhaps not totally novel: I heard the great evolutionist Ernst Mayr claiming that 30 or 40 years ago, when he described emergence to Niels Bohr, Bohr said; "but we have that in physics as well! – physics is all emergent", but at the time, as usual, only Bohr knew what he meant.*

Thus the challenge in condensed-matter physics is to understand the *behavior of complex systems*, starting from the apparently *simple underlying theory*, the Schrödinger equation. This is what Anderson defines the *Complex Way*, in contrast to the *Glamor Way* travelled by high-energy physics in the search of the ultimate theory. Complexity is tamed by *universality*: it is rather the consequence of many-body correlations – one particle influenced by all the others – than of the specific type of interaction. New complex entities can then form under well defined conditions, such as high pressure, low temperature, or in the presence of magnetic fields, often in radically different systems. These entities are stable in a certain regime, in which they represent the fundamental "particles" – but actually are effective- or quasi-particles. They feel effective interactions among themselves, yielding on a higher level yet other states of matter. Can we predict such states without experimental facts, just from the equations? As Anderson writes [5]

> *The structure of Nature is so completely hierarchical, built up from emergence upon emergence, that the very concepts and categories on which the next stage can take place are themselves arbitrary.*

Remarkably, modern molecular biology has made enormous progress by identifying genes as fundamental entities. Still, the evolutionary biologist Ernst Mayr rejects the reductionist approach that evolutionary pressure acts on single genes, arguing that it instead acts on organisms, that genes influence each other, and that accounting for this influence is essential. Even if we take genes as the fundamental entities, their definition might appear to the outsider as airy as that of quasiparticles in physics or what we before called complex entities. It is clear that, whatever they are, they are composite rather than fundamental objects; but it is also clear that they are a better starting point than their more fundamental components. It would, e.g., not be of much help for molecular biology to start from the Schrödinger equation. Returning to the layer of electrons and nuclei, the message is that at a given energy scale new intermediate layers can form at which novel emergent behavior occurs. But, when dealing with systems made of $N \sim 10^{23}$ particles, to predict novel emergent behavior is hardly possible. Again, quoting Anderson [5]

> *How can you predict the result when you can't predict what you will be measuring?*

The classical path to discoveries of new states of matter is, with few precious exceptions, led by experiment. It is the recognition of a paradox, an experimental result apparently contradicting our well established theories, which leads to the identification of new phenomena; Nature has to provide us some strong hint. And it is hardly the *ab-initio* path, from the ToaE to the real world, that leads us to understanding the physics of the new phenomenon. It is rather the identification of mechanisms, which often is based on simple models, apparently wild ideas, and a good measure of approximation.

It is natural to ask ourselves how emergent phenomena arise. The formation of layers of physical theory is best understood in terms of the idea of *renormalization*. The exact solution of the Schrödinger equation involves phenomena at many energy scales. However, at low energy – meaning the energy window on which we are focusing – high-energy states play a small role. They can only be reached via virtual excitations, which have a time-scale proportional to $\hbar/\Delta E$, where ΔE is the excitation energy. Thus it is not necessary to account for them in full detail. It is more meaningful to downfold them and work in the subspace in which only low-energy states and, if sizable, the low-energy effects of these virtual excitations are taken into account. Between different branches of physics, this separation is quite clear-cut: in condensed-matter physics, we do not need quarks to describe atoms, not even neutrons and protons. Instead we can simply talk about their bound states, the nuclei as immutable objects. In these cases, the high-energy states are so far away that the only effect of the downfolding is the emergent object, e.g., the atomic nucleus. For intermediate energy scales the scenario can become much more complicated; the effect of the downfolding is to generate *effective Hamiltonians*, the new effective theory in that energy window. The effective Hamiltonian is typically made of the original Hamiltonian, however restricted to the low-energy Hilbert space and with renormalized parameters, plus new interactions; in the smaller Hilbert space some degrees of freedom are frozen, and the effective Hamiltonian typically can be rewritten in term of new entities, stable in that subspace; examples are quasiparticles, Cooper pairs, or local spins. The major difficulty in condensed-matter is that there is always a chance of crossing the boundaries between effective theories, e.g., in a phase transition to a new state of matter. Still it is possible to identify truly emergent regimes from their robustness or universality. Often the cooperative behavior of a many-particle system is surprisingly independent of the details of their realization – their substrate. The Kondo effect, for example, was initially found in diluted magnetic alloys and ascribed to the antiferromagnetic exchange interaction of the localized impurity-spins with the spin-density of the conduction electrons at the impurity site. But is has been realized in a number of systems in which there are no local magnetic moments, such as in quantum dots or in carbon nanotubes. Recently it has even been shown to be intimately related to the metal-insulator transition of the Mott type, a connection that is at the core of the dynamical mean-field theory approach (DMFT) [6, 7]. Another striking example is conventional superconductivity, explained via the BCS theory. First observed in simple metals at very low temperatures, the same kind of phenomena has been found in liquid ^{3}He, which becomes superfluid below a certain critical temperature and even in systems as exotic as neutron stars [8]. Returning to less massive systems, the mechanism of the metal-insulator transition in transition-metal oxides is typically described via the Hubbard model, which in recent years has also been employed to model the behavior of very different systems: ultra-cold atoms in optical lattices.

But how do we go from the Schrödinger equation to emergent properties? It is certainly tempting to start from the exact many-body wave function, as we know a straightforward prescription for calculating observables from it. But for what system should we calculate that exact wave function? We are certainly not interested in the properties of just one particular sample with its unique arrangement of atoms. What we are interested in are the properties of a *material*, i.e., a class of samples that can be reproducibly manufactured. Any single one of these samples will be quite different from the others in terms of its microscopic details. So, even if we could calculate them, the exact ground state wave functions for two such samples would, for all practical purposes, be orthogonal. Chipping off an atom from a bulk of gold does not change its characteristics. Thus, we are not really interested in the exact solution for some particular situation, but in general properties. Emergent properties abstract from the idiosyncrasies of a particular realization. A typical idealization is the *thermodynamic limit*, where we assume that the number of particles $N \to \infty$, even though any real sample can only be made of a finite number of atoms. This lets us exploit the advantages of the continuum over discrete sets. Only in the thermodynamic limit can we define a phase transition where every actual sample shows a mere crossover. Only in an infinite system can we speak of a continuum of excited states where for every actual sample there is only a finite number of excitations with a distribution that depends critically on its size. Another important idealization is the perfect-crystal approximation, in which we assume that defects are of minor importance for the physical properties of interest and where, in particular, we abstract from surface effects by introducing periodic boundary conditions. It is of course crucial to keep in mind that these idealizations only make sense for properties that can be transfered from the idealization to the real materials. Experimentally we can, for all practical purposes, distinguish metals and insulator and observe phase transitions in crystals. Thus the thermodynamic limit is a good starting point. Conversely, trying to describe a bulk system with a finite number of atoms, we eventually get lost in irrelevant details. The importance of getting rid of irrelevant details has been succinctly expressed by Lipkin [9]

> *On the other hand, the exact solution of a many-body problem is really irrelevant since it includes a large mass of information about the system which although measurable in principle is never measured in practice. In this respect, the quantum-mechanical many-body problem resembles the corresponding problem in classical statistical mechanics. Although it is possible in principle to solve Newton's equations of motion and obtain the classical trajectories of all the particles in the system for all times, only a small part of this information is relevant to anything that is measurable in practice. Classical statistical mechanics uses a statistical description in which measurable macroscopic quantities such as temperature, pressure and entropy play an important role. An incomplete description of the system is considered to be sufficient if these measurable quantities and their behavior are described correctly.*

Thus, approximate methods that grasp the essential details are bound to be more successful than exact methods – if available [10] – since they shield us from all the irrelevant information. So it is not the "Great Solid State Physics Dream Machine" [5] that we should be after, or in the words of Wigner and Seitz [11]

> *If one had a great calculating machine, one might apply it to the problem of solving the Schrödinger equation for each metal and obtain thereby the interesting physical quantities, such as the cohesive energy, the lattice constant, and similar parameters. It is not clear, however, that a great deal would be gained by this. Presumably the results would agree with the experimentally determined quantities and nothing vastly new would be learned from the calculation. It would be preferable instead to have a vivid picture of the behavior of the wave functions, a simple description of the essence of the factors which determine cohesion and an understanding of the origins of variation in properties [. . .].*

Lipkin concludes that it is actually misleading to think that our job is to find approximations to the exact solution of the Schrödinger equation [9]

> *In fact, many treatments of the quantum-mechanical many-body problem give the misleading impression that they are indeed methods for obtaining approximations to the exact solution of the Schrödinger equation.*

A better approach is to develop approximate schemes for calculating, for idealized systems, reduced quantities that do not provide complete information of the system but still allow us to calculate experimentally accessible quantities, such as Green functions or response functions. This route is successfully taken by density-functional theory (DFT) [12], which uses the many-body electron density as a variable, or by the dynamical mean-field theory, which is based instead on Green functions. The great success of DFT is that, via the Kohn-Sham equation, the problem of finding the electron density of the original many-electron system is reduced to that of calculating it for an auxiliary one-electron problem, whose Hamiltonian has to be determined self-consistently. The electrons in the auxiliary problem feel a one-electron potential whose strength and shape is determined not only by the nuclei which define the lattice but also by all the other electrons – which is why self-consistency is needed. Of course, even though DFT is in principle an exact ground-state theory, we know only approximate forms of the DFT potential, such as the local-density approximation (LDA) and its extension. Nevertheless, if the approximate form is good enough, we can perform *ab-initio* calculations, i.e., calculate many properties of a system specified only by the atomic positions and the type of atoms. In an emergent world, it would, however, be very surprising if the LDA always worked. The reason is a fundamental one. If objects qualitatively different from the quasi-electrons, on which the LDA is built, can form, this approach is bound to fail even qualitatively. This is what happens in strongly correlated materials. Remarkably, however, the LDA is so successful that DFT can be considered the *standard model* of solid state physics that is used to understand and even predict the properties of whole classes of materials. Strongly correlated systems are not only characterized by the fact that the LDA fails to describe them. More importantly, their properties are very sensitive to small changes in external fields or doping, and hence they are characterized by surprisingly large effects, such as colossal magneto-resistance, high-temperature superconductivity, and the like. This suggests that a variety of different layers can easily form in which new fundamental entities exist and interact. Hence, for strongly correlated systems, it is particularly unlikely that a single approximation can be sufficient for explaining all phenomena.

One exemplary failure of the LDA is the Mott metal-insulator transition. Within the LDA, metals have partially filled bands while insulators are characterized by a band gap. The latter can also arise because of long-range magnetic order. The same concept of metal and insulator remains in place if we use approaches in which many-body effects are taken into account on a static mean-field level such as the Hartree-Fock (HF) method. Thus the existence of materials with partially filled bands that are paramagnetic insulators is a paradox in the context of LDA or HF. It can, however, be understood using a simple model, the *Hubbard model*

$$H = -t \sum_{\sigma} \sum_{\langle ii' \rangle} c^{\dagger}_{i\sigma} c_{i'\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \,. \tag{2}$$

In this model, the metal-insulator transition at half-filling is a consequence of a large t/U ratio, i.e., an on-site Coulomb repulsion which is large with respect to the band-width, determined by the hopping t. Although the mechanism behind the paramagnetic insulating phase had been proposed about 60 years ago by Nevil Mott, it is only recently, through the dynamical mean-

field theory [6, 7], that we can indeed describe that physics quantitatively. DMFT yields an approximate solution of the Hubbard model in which spatial correlations are neglected and only dynamical effects are taken into account. The DMFT solution of the Hubbard model shows that with increasing t/U the quasiparticle masses increase and eventually diverge; the Mott transition is associated with the corresponding divergence of the real part of the self energy.
It is remarkable that a model as simple as the Hubbard model, bare of all the complications or details of the real material, can be of any relevance for systems as different as NiO, $\mathrm{LaTiO_3}$ and $\mathrm{KCuF_3}$. LDA-based studies on weakly correlated materials suggest that this cannot possibly be the case. When the LDA works, we typically need the full details of the electronic structure to explain the structure of the Fermi surfaces, the lattice, or the chemical bond. In fact, model Hamiltonians might grasp the substance of a phenomenon, such as the nature of the Mott transition, but they are not sufficient to account for the varieties of its manifestations, and eventually will fail in explaining new paradoxes that are found when this variety is explored. The Mott mechanism can explain the existence of Mott insulators, but it does not tell us why $\mathrm{SrVO_3}$ is metallic while the very similar $\mathrm{YTiO_3}$ and $\mathrm{LaTiO_3}$, are insulators, or why the gap is much larger in $\mathrm{YTiO_3}$ than in $\mathrm{LaTiO_3}$, although they have a similar LDA band width. Even if we know that Mott physics is the right starting point, we have to augment the simple Hubbard model to describe reality. But how? If we could solve it, the original Hamiltonian contains all details, but, as we have discussed, they are too many, and thus they tell us nothing. The crucial point is to disentangle the important features from all the irrelevant details. This is the true challenge in condensed-matter physics. In the case of $\mathrm{SrVO_3}$, $\mathrm{YTiO_3}$ and $\mathrm{LaTiO_3}$, it turns out that structural distortions and a tiny crystal field splitting of t_{2g} levels play the crucial role [13]. Not surprisingly, there is no systematic way of determining which details do matter for explaining a certain behavior in a given system. This process relies on our intuition about the mechanisms, and it brings the work of a physicist rather close to that of an artist, requiring proper taste and judgement. The good news is that for Mott-like system the DMFT method turns out to be a very flexible approach. It has been combined with DFT in the LDA+DMFT approach [14], whose steady development in the last ten years allows us to solve more and more realistic Hubbard-like models and thus to test ideas and approximation in a realistic context. And it is not difficult to imagine that in the next 20 years LDA+DMFT codes will probably become as flexible and versatile as modern DFT codes. We have to keep in mind that, although this constitutes impressive progress, as in the case of the LDA, it is very unlikely that a single approximation will solve all the paradoxes. New ones will certainly be found, and will require us to extend the theory, to think differently, to go away from the well known path, to look for new mechanisms. The end of physics is unlikely to come any time soon.

2 Paradigmatic cases

At the focus of this year's school are two paradigmatic examples of emergent phenomena, antiferromagnetism and electron-phonon driven superconductivity. We briefly reconstruct the main steps that led to the unraveling of their mystery and discuss their emergent aspects.

2.1 Antiferromagnetism

At the beginning of the 20th century, magnetism was the subject of intense debate. The theoretical scenario was dominated by the ingenious concept of Weiss' molecular field theory of ferromagnetism [15]. Of course magnetic moments in matter could only be understood quantum mechanically and it was Heisenberg, who proposed that the ferromagnetic coupling between magnetic moments is due to the *Coulomb exchange* between electrons [16]. The latter yields an interaction of the form

$$H = \frac{\Gamma}{2} \sum_{ii'} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i'} \,, \tag{3}$$

with $\Gamma < 0$. Néel [17] extended Weiss' theory to the case of a site-dependent molecular field and found the antiferromagnetic state as the mean-field solution of the $\Gamma > 0$ Heisenberg model below a critical temperature, T_{N}. Antiferromagnetism is one of the precious exceptions to the rule that condensed-matter physics is essentially led by experiment: The experimental proof of the existence of antiferromagnetism came only much later, in 1951, when Shull and Smart measured via elastic neutron scattering sharp new Bragg peaks below a critical temperature in the transition-metal oxide MnO [18]. Even in the case in which they are actually predicted, however, emergent phenomena are rarely as simple as in the original theoretical proposal. The paradox at the time was that the exact solution of the antiferromagnetic one-dimensional Heisenberg chain, obtained by Bethe, yields a ground state with total-spin zero, a condition not satisfied by the Néel antiferromagnetic state. Later on, this paradox was solved by the observation of Anderson that, in a perfect antiferromagnet, quantum fluctuations would restore the symmetry, but in a real system weak perturbations, defects, or an external magnetic field can suppress them; these quantum fluctuations however imply the existence of cooperative excitations, *spin waves*. This is a consequence of the Goldstone theorem, which states that soft bosonic excitations have to be present whenever a continuous symmetry is broken. Antiferromagnetism turns out to be, indeed, a representative example of a so-called *broken symmetry* state, a state in which the electrons choose not to have the same symmetry of the Hamiltonian that govern their behavior, in this specific case the continuous spin-rotation symmetry of the Heisenberg model Eq. (3). Remarkably, some of the ideas developed in the context of broken symmetry, such as *Goldstone bosons*, were taken over by high-energy physics [5], and have driven the search for the Higgs boson [19]. It is worth pointing out another emergent aspect associated with the Heisenberg model that brings us back to the basics of quantum mechanics. Where do the local spins $\boldsymbol{S}_i$ come from? There are apparently no such local spins in the orginal Schrödinger Hamiltonian, the ToaE of solid-state physics. The existence of local spins becomes immediately clear, however, if we consider an idealized atom described by the Hamiltonian

$$H = U n_{\uparrow} n_{\downarrow} \,.$$

This Hamiltonian has four eigenstates, which can be labeled as $|N, S, S_z\rangle$, where N is the total number of electrons and S_z, the z component of the total spin,

$$\begin{array}{rcr} |0,0,0\rangle &=& |0\rangle \\ |1,\frac{1}{2},\uparrow\rangle &=& c_\uparrow^\dagger|0\rangle \\ |1,\frac{1}{2},\downarrow\rangle &=& c_\downarrow^\dagger|0\rangle \\ |2,0,0\rangle &=& c_\uparrow^\dagger c_\downarrow^\dagger|0\rangle \end{array}$$

These states result from the electron-electron interaction and the Pauli principle. In this simple example the energy of the atomic states depends only on the total number of electrons; thus we label it with $E(N)$, with $E(0) = 0$, $E(1) = 0$, and $E(2) = U$. If the atom is full or empty, its total spin is zero; if instead the idealized atom is occupied by one electron, it behaves as a local $S = 1/2$. Let us consider now a half-filled system described by the one-band Hubbard model, Eq. (2), in which a set of idealized atoms of the type just discussed form a lattice. In this model the electrons can, in principle, hop from site to site, gaining kinetic energy $\propto -t$; each hopping process will, however, cost the Coulomb energy

$$E(2) + E(0) - 2E(1) = U\,.$$

If the ratio between kinetic energy gain and Coulomb energy loss, $\propto t/U$, is small enough double-occupations are unlikely and each site is filled on average with ~ 1 electron. Then spins remain stable in the crystal, and the overall effect of the virtual excitations to $N = 0$ and $N = 2$ states is an effective exchange interaction between the spins. We can calculate the effective exchange coupling by downfolding the $N = 0$ and $N = 2$ high-energy states; if we follow this procedure [20] we find an effective antiferromagnetic Heisenberg interaction with

$$\Gamma = -\frac{4t^2}{U}\,.$$

This is an example of the *kinetic exchange* mechanism. It plays an important role in the physics of transition-metal oxides. We are now in the position to discuss emergence at work. The first lesson is that spins are by themselves emergent objects. They are the result of the interplay of the Pauli principle and Coulomb repulsion. Furthermore, within the kinetic exchange mechanism, they interact because of virtual excitations to high-energy states, in this case those with $N = 2$ and $N = 0$. Then, below a certain temperature T_N, because of the interactions between these emergent entities, a new cooperative emergent state, the antiferromagnetic Néel state, arises; an example of emergence built on emergence. Finally, spins only “live” on certain energy scales. At energy scales comparable with t/U excitations to empty and doubly occupied states (charge fluctuations) become likely and it is no longer possible to describe the system by a simple Heisenberg model; this happens, for example, when we want to study the Hubbard bands in photoemission spectra. Thus, increasing the energy or the temperature we cross the boundary to a different layer and change the effective theory. In the higher layer of theory the spins are the fundamental particles and the Heisenberg model becomes an effective theory of everything. In the lower layer we have to account for the charge degrees of freedom, and the effective theory of everything is the Hubbard model.

2.2 Superconductivity

The discovery of metals with infinite conductivity [21] by Kamerlingh Onnes in 1911 came as a genuine surprise. It took almost 60 years to find an explanation, years in which brilliant minds tried hard to solve the riddle and yet failed. This failure by itself is a strong indication that superconductivity is an emergent phenomenon. Many experimental facts were added along the way; we just mention two of the most significant. The first was the Meissner effect in 1933 [22], the spontaneous expulsion of a magnetic field, somewhat similar to perfect diamagnetism. The most crucial observation was perhaps the discovery of the isotope effect in 1950 [23]. From the theory side, the decisive development was the concept of electron pairs as developed by Leon Cooper in late 1956 [24]. Cooper realized that, in the presence of an arbitrarily weak electron-electron attraction, $-V$, two electrons with energy just above the Fermi surface of a metal will form a bound-state that could destabilize the Fermi surface itself. Cooper's pair creation operator is defined as

$$b_{\mathrm{CP}}^{\dagger} = \sum_{\boldsymbol{k}} \lambda_{\boldsymbol{k}} c_{\boldsymbol{k}\downarrow}^{\dagger} c_{-\boldsymbol{k}\uparrow}^{\dagger}.$$

Since a Cooper pair is, to first approximation, a boson, Cooper pairs can in principle all occupy the same state, as it happens in Bose-Einstein condensation. Based on these ideas, Bardeen, Cooper and Schrieffer elaborated the theory of superconductivity. They identified the superconducting state as a coherent state, the eigenstate of Cooper's pair annihilation operator b_{CP}. In Fock space such state can be easily written in product form

$$|\Psi_{\mathrm{BCS}}\rangle = e^{b_{\mathrm{CP}}^{\dagger}}|0\rangle = \prod_{\boldsymbol{k}} \left(1 + \lambda_{\boldsymbol{k}} c_{\boldsymbol{k}\uparrow}^{\dagger} c_{-\boldsymbol{k}\downarrow}^{\dagger}\right)|0\rangle,$$

where $|0\rangle$ is the electron vacuum. The microscopic mechanism that leads to the pairing in conventional superconductors is the electron-phonon coupling; for electrons right above the Fermi surface the resulting electron-electron coupling is attractive. The BCS Hamiltonian has then the form

$$H_{\mathrm{BCS}} = \sum_{\boldsymbol{k}\sigma} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k}\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'} c_{\boldsymbol{k}\uparrow}^{\dagger} c_{-\boldsymbol{k}\downarrow}^{\dagger} c_{\boldsymbol{k}'\downarrow} c_{-\boldsymbol{k}'\uparrow},$$

where $\varepsilon_{\boldsymbol{k}}$ is the dispersion of the electrons, and $V_{\boldsymbol{k},\boldsymbol{k}'}$ the electron-electron interaction. In the simplest version of the BCS theory one can assume that the coupling $V_{\boldsymbol{k},\boldsymbol{k}'}$ is isotropic. Thus we can make the following approximation

$$V_{\boldsymbol{k},\boldsymbol{k}'} \sim \begin{cases} -\overline{V} & \text{for} \quad |\varepsilon_{\boldsymbol{k}}|, |\varepsilon_{\boldsymbol{k}'}| < \varepsilon_D \\ 0 & \text{otherwise} \end{cases}$$

where ε_D defines the small energy window in which the potential is attractive. The superconducting gap $\Delta(T)$ is then given by the solution of the BCS gap equation; at $T = 0$

$$\Delta(0) = 2\varepsilon_D e^{-1/\rho_\sigma(\varepsilon_F)\overline{V}}, \tag{4}$$

where $\rho_\sigma(\varepsilon_F)$ is the density of states per spin at the Fermi level, and $\rho_\uparrow(\varepsilon_F) = \rho_\downarrow(\varepsilon_F)$. There is a universal relation between the gap and the critical temperature,

$$\frac{2\Delta(0)}{T_c} \approx 3.528.$$

In superconductivity the continuous symmetry that is broken is the gauge symmetry related to the conservation of charge; in the broken symmetry state the *phase* of the wavefunction is the new physical parameter. The Cooper pairs are emergent objects, which interact to form a macroscopic condensate: the superconducting state.

Nowadays, we call superconductors that can be explained within the BCS theory and its simple extensions *conventional superconductors*. This does, however, not mean that they do not hold surprises. The discovery of MgB_2 in 2001 [25], with a T_c as high as 40 K, was totally unanticipated, in particular in such a comparatively simple binary compound. It immediately sparked an intense search for similar conventional materials with perhaps even higher T_c. Remarkably, MgB_2 is not an exotic material; at the time of the discovery it was available to many laboratories. In principle we did, once more, have the theory – we could have predicted it. But again, nobody thought in advance that MgB_2 could be such a remarkable system. And even if we had used our theoretical tools, would we have predicted that MgB_2 is a high-T_c conventional superconductor? Probably not: it turns out that MgB_2 is less simple then one might think. To understand it we have to account for multiple bands and gap anisotropies, typically neglected in the standard version of the theory of conventional superconductors. Thus this is a case in which details that are usually negligible play an essential role.

Another, totally different surprise had arrived earlier, in 1986, with the discovery of superconductivity with $T_c = 40$ K in La_2CuO_4. The finding was so unexpected that the title of the paper [26] that won Bednorz and Müller a Nobel prize conveys the author's doubts: *Possible high T_c superconductivity in the Ba-La-Cu-O system.* In a relatively short time, an entire family of CuO_2-layered superconducting materials was identified, the high-temperature superconducting cuprates (HTSCs). Within the HTCS family, the maximum value of T_c rose rapidly to ~ 130 K. It quickly became clear that these new materials differ substantially from conventional superconductors and the mechanism for high-temperature superconductivity remains a puzzle. There is no doubt, however, that the pairing has d-wave symmetry. More recently, in 2006, superconductivity was discovered in LaOFeP [27], and many other iron-based superconductors were quickly identified. Once more, a different class of superconductors, iron pnictides, had been *experimentally* found, and new puzzles have to be solved; within iron pnictides a T_c as high as 57 K has been reached.

The lesson that emerges is that a superconducting state can manifest itself in very different systems, ranging from superfluid ^{3}He, to MgB_2, high-temperature superconducting cuprates, and neutron stars. While the phenomenon itself is in all cases similar, its microscopic origin, i.e., the lower layer of the theory, varies strongly from case to case. The challenge is to identify in each case the proper connection between these layers of theory.

3 Overview of the school

This year's school aims to give a broad introduction to the physics of emergent phenomena in condensed matter and to the modern approaches to dealing with them. We focus primarily on the two paradigmatic manifestations of emergence that we have just discussed, magnetism and superconductivity. In order to understand these phenomena, we start with the fundamentals. The lecture of Bob Jones discusses density-functional theory from a historical perspective, stressing the aspects relevant to the study of emergence. The lecture of Erik Koch extends the scope to many-electron states, from introducing the formalism of second quantization to discussing the Mott- and BCS-states. The fundamental aspects of magnetism and exchange phenomena in a model context are presented in the lecture of Eva Pavarini. Robert Eder then introduces the variational cluster approximation to the spectral properties of the Hubbard model, the *drosophila* of strong correlation physics, using a self-energy functional.

Reflecting our focus on magnetism, a group of lectures is dedicated to magnetism in real materials and to numerical methods to solve complex spin models. The lecture of Sasha Lichtenstein retraces the path from Stoner to Hubbard models of magnetism, emphasizing modern DMFT-based approaches to understanding real materials. Treating extended magnetic systems requires highly efficient methods for successful finite-size extrapolations. Werner Krauth introduces the Monte Carlo approach and discusses methods for determining and reducing correlation times. The lecture of Stefan Wessel shows how to use Monte Carlo techniques for simulating quantum spin models. Turning to finite systems, Jürgen Schnack illustrates the state-of-the-art in describing and designing molecular magnets, intriguing systems that could become crucial building blocks for future quantum computers.

A school on emergent phenomena in condensed matter systems would not be complete without the view from experiment. Bridging magnetism and superconductivity, Bernhard Keimer took the challenging task to cover recent advances and open problems in our understanding of the high-temperature superconducting cuprates, with a special focus on the role of spin fluctuations.

The next group of lectures is dedicated to the various aspects of conventional and unconventional superconductivity, the second focus of our school. The lecture of André-Marie Tremblay illustrates theoretical progress on the theory of strongly correlated superconductivity. Warren Pickett then explains the challenges in designing real superconducting materials, highlighting some of the puzzles they pose or have posed. Two lectures are dedicated to the theory of conventional superconductors. Rolf Heid discusses the mechanism of conventional superconductivity and shows how to calculate the electron-phonon coupling *ab initio* using density functional perturbation theory. These results are the input to Eliashberg theory, which is introduced in the lecture of Giovanni Ummarino. The case of superfluidity is discussed in the lecture of David Ceperley, introducing the path-integral picture of degenerate quantum systems.

The final group of lectures focuses on wave function based methods. Shiwei Zhang shows us how to study models and real materials using the auxiliary-field quantum Monte Carlo approach. Ulrich Schollwöck gives an introduction to the density-matrix renormalization group approach, while Jens Eisert explains how to analyze ground states using concepts of quantum information.

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