

Strong correlations in low dimensional conductors. What are they, and where are the challenges?

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This paper is written as a brief introduction for beginning graduate students. The picture of electron waves moving in a crystalline potential and interacting weakly with each other and with crystalline vibrations suffices to explain the properties of technologically important materials such as semiconductors and also simple metals that become superconductors. In magnetic materials, the relevant picture is that of electrons that are completely localized, spin being left as the only relevant degree of freedom. A number of recently discovered materials with unusual properties do not fit in any of these two limiting cases. These challenging materials are generally very anisotropic, either quasi one-dimensional or quasi two-dimensional, and in addition their electrons interact strongly but not enough to be completely localized. High temperature superconductors and certain organic conductors fall in the latter category. This paper discusses how the effect of low dimension leads to new paradigms in the one-dimensional case (Luttinger liquids, spin-charge separation), and indicates some of the attempts that are being undertaken to develop, concurrently, new methodology and new concepts for the quasi-two-dimensional case, especially relevant to high-temperature superconductors.

I. INTRODUCTION

Quantum mechanics and statistical mechanics have provided us with the tools to understand the behavior of bulk matter. Nevertheless, except in the case where particles are independent, the problem of treating 10^{23} electrons is unmanageable by brute force application of the basic laws. A few concepts, and their mathematical implementation, were needed to enable us to develop both the qualitative and highly quantitative theories that nowadays explain the electronic and magnetic properties of solids. The computer revolution is in part the outcome of this understanding and of the massive experimental effort devoted to controlling semiconducting and magnetic materials, which are the basic elements of transistors, magnetic storage materials and other pieces of basic hardware.

What is there left to do then? All these successes may seem to indicate that we have the tools to understand the electronic and magnetic properties of any piece of solid matter. This is not so. This short overview, written primarily for the student with a first course in Solid State Physics, will summarize the traditional views of Solid State systems and move on to show how these views fail in a large class of materials. As we will see, high-temperature superconductors are one of the most famous examples of materials begging for understanding. But there are others. And the mysteries lay not only in the origins of the superconductivity itself, but also in normal state properties that one would have expected traditional Solid State Physics to explain. In fact, the failures of present day Solid State theory provide an intellectual challenge of the highest level. The Physics

of strong electron-electron interactions and of systems in low-dimensional spaces (one or two dimensions) is what is at stake. New concepts have already emerged. For example, we know now that in one dimension, single-electron momentum states are very bad representations of the true eigenstates, which are, instead, collective charge and spin excitations. In other words, in a one-dimensional solid, the electron splits into its spin and its charge degrees of freedom. This concept of spin-charge separation is only one example of the kind of new ideas, and corresponding tools that need to be developed. The close interplay between experimental facts and the development of new qualitative ideas, as well as the occasional need for heavy mathematical and numerical artillery, are characteristics of the field that we also wish to illustrate.

Although there is a vast number of topics in strongly correlated electron Physics, some of which have already led to Nobel Prizes, we will concentrate on those topics that we have worked on and that are closely related to the high-temperature superconductors, the subject of this issue of Physics in Canada. We first recall the standard approaches, show experimental results that are unexplainable within these schemes, briefly give general theoretical arguments that tell us why the standard approaches are expected to fail in these cases and conclude with remarks on theoretical models and new methods that are being developed. In a nutshell, it should be clear at the end of this review that ‘‘Strongly Correlated electrons’’ refers to a rather broad class of problems originating basically from either strong interactions or singular scattering processes in low dimension.

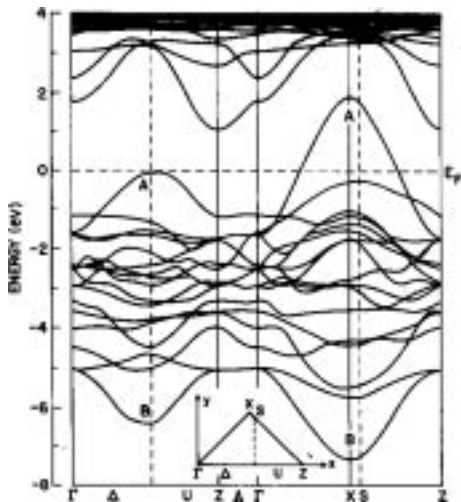


FIG. 1. Band structure of La_2CuO_4 , taken from Ref. [1]

II. THE STANDARD APPROACHES: QUASIPARTICLES AND LOCALIZED SPINS

The groundwork for successful theories of the electronic and magnetic properties of solids began in the early days of quantum mechanics. Bloch's theorem explained why single-electron eigenstates in periodic arrays are plane-wave like and can be described by a wavevector and an other quantum number, called the band index. In the case of magnetic insulators, the so-called Heisenberg model described the interactions of localized electrons interacting with each other through their spin degrees of freedom. These two dramatically opposite points of view, of delocalized vs localized electrons, have been usefully developed and applied to different types of materials. The present section illustrates the main concepts that have emerged.

A. Quasiparticles, the Fermi surface and Fermi liquid theory

A mean-field (i.e. average) treatment of interactions leads to a picture where the many-electron wavefunction is simply an antisymmetrized product (because of Fermi statistics) of one-particle eigenstates of the type described by Bloch. The best available method to obtain these one-particle eigenstates today is the local density approximation (LDA), a method based on "density functional theory". The 1998 Nobel Prize in Chemistry was awarded for the development of the latter approach [4]. Fig. 1 gives the single-particle eigenenergies resulting from a LDA calculation for a compound in the high-temperature superconductor family, La_2CuO_4 . The horizontal axis represents wavevector along different directions and the different curves for the same wavevectors represent the bands. The zero-temperature many-body state is built by filling-in the lowest energy states, follow-

ing the constraints of the Pauli principle, until all electrons are accounted for. Hence, one would expect that one can draw a surface, in wavevector space, that separates filled from unfilled states. That is the so-called Fermi surface. When bands are either completely filled or completely empty, one has an insulator (or a semiconductor when the energy gap between the highest filled band and the lowest empty band is not too large). Otherwise, there are zero-energy excitations and the system conducts. Given that the last filled level in a metal lies in a band that spreads over a few eV in energy, room temperature ($1/40\text{eV}$) corresponds to energies that are minuscule on that scale and hence often beyond the precision of LDA calculations. Nevertheless, these small energies are often large enough to play an essential role in the observable properties of the system.

Suppose we put back the interaction, i.e. we compute matrix elements of the full Hamiltonian in the basis obtained from the LDA calculation. The Hamiltonian in that basis contains residual interactions between quasiparticles. Even if we cannot in practice carry out this program, the general form of the Hamiltonian is pretty clear on the basis of general considerations and on symmetry arguments. The residual interactions should be short-range since the LDA bands have taken screening into account for the most part. Furthermore, a wavefunction made of a single antisymmetrized product of states is not an eigenstate of the Hamiltonian that includes interactions. In a physical picture, particles scatter off each other, changing momentum and band quantum numbers. However, the Pauli principle strongly constrains phase space for final states. In fact, it can be proven to all orders in perturbation theory (assuming that it converges, which is not the case in one dimension or for strong interactions) that even in the presence of electron-electron interactions, the single-particle *excitations* near the Fermi surface are well described by a single-particle picture. These excitations are called quasiparticles. This is the first step in the so-called Landau Fermi liquid theory of metals. However complicated the band structure, the arguments given above suggest that for low-energy fermionic excitations, only the band near the Fermi surface is relevant, giving a conceptual framework to understand wide classes of materials. What will change from one material to the other is the effective mass of the excitations, or more generally, details of their energy dispersion, but the qualitative picture is quite universal.

Nowadays, one can see the quasiparticles experimentally in a rather direct manner. Indeed, synchrotron radiation has given us X-ray sources that are powerful enough to do Angle Resolved Photoemission Spectroscopy (ARPES). In these experiments, it is possible not only to measure the energy of the outgoing electron, it is also possible to resolve its momentum parallel to the surface, which is conserved when the electron is extracted by the X-ray from the material. For a system where energy eigenstates have a strong two-dimensional nature, that is all the quantum numbers that we need.

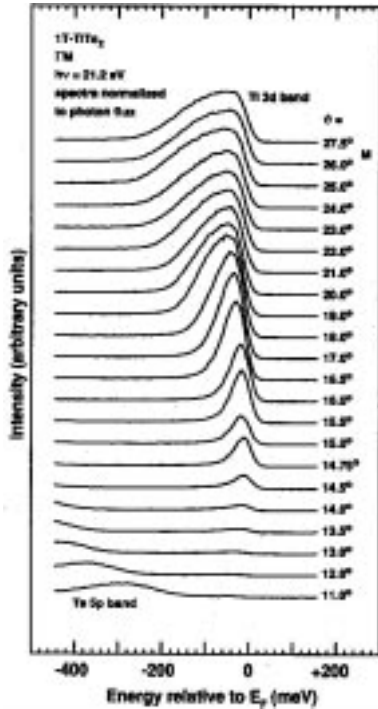


FIG. 2. ARPES spectra of $1-T-\text{TiTe}_2$, taken from Fig. 1 of Ref. [2]

Fig. 2 presents the results for a compound that behaves as expected from the quasiparticle picture. The different curves correspond to different momenta. They give on the vertical axis a quantity proportional to the probability, times a Fermi function, that an electron of given momentum has the energy indicated on the horizontal axis. As one moves in the various directions of wavevector space, one reaches a point where the maximum intensity is very near zero energy (14.75^0 on the figure). The effect of the Fermi function is that for a probability that would be maximum *at* zero energy, the observed maximum is slightly *below* zero energy. At zero energy, the observed function is smaller than the value it would have had but it still has sizeable weight. In this way, one can thus map the wavevectors where there are no-longer electrons to photoexcite. This is the Fermi surface (Fermi line in $d = 2$). If there were no interaction between electrons, there would be only one energy allowed for a given momentum state. Clearly, here the probability for a given momentum is centered at a wave-vector-dependent position but it is nonvanishing for several energies. The width in energy for a given momentum cannot be accounted for simply by experimental resolution. Its existence is expected from the fact that quasiparticles have a lifetime. One can also check from the figure that the width in energy is becoming narrower as one approaches the Fermi surface. Also, although this is not shown here, at the Fermi surface the width decreases rapidly with temperature (like T^2).

B. Thermodynamics of the Fermi liquid, and phase transitions

So much for single-particle properties. What happens when one measures thermodynamic quantities such as the magnetic susceptibility or the specific heat? One is not adding or removing new particles in the system. The external probe is just emptying occupied states while filling unoccupied states: It is creating particle-hole excitations. In that case, Landau Fermi liquid theory predicts that the interactions have a mean-field-like effect that modifies the predictions one would obtain for noninteracting particles. For example, the specific heat is linear in temperature and proportional to the density of single-particle excitations, like in a free electron gas. The spin susceptibility should then be temperature independent, like the Pauli susceptibility of free electrons, and, in a naive picture, it should also be proportional to the density of single-particle excitations. In reality, Fermi liquid theory tells us that there is an enhancement factor $(1 + F_0^a)^{-1}$, where F_0^a is a measure of the interaction.

Interactions, quite generally, are the cause of phase transitions. The case $F_0^a = -1$ above corresponds to $(1 + F_0^a)^{-1} = \infty$, which means a divergent static spin susceptibility. That is a clear signal for the onset of ferromagnetism. The ferromagnetic state breaks spin rotational invariance. Another example of phase transition caused by interactions, is the superconducting transition, which breaks global gauge invariance. This is discussed further by J. Carbotte in this issue. The origin of the interactions leading to phase transitions may be quite subtle. For example, in the case of conventional superconductors, the retarded electron-phonon interaction leads to an effective attraction between quasiparticles that is ultimately responsible for the superconducting state. Finding and characterizing all possible states of matter caused by interactions is a field of endeavour in itself.

C. What about the Heisenberg model?

While band theory works well with most materials with only s and p derived bands, in certain cases, mostly with d and f electron materials, it is totally inappropriate. One of the most famous examples is V_2O_3 . The band structure predicts it should be a metal. Instead, at low pressure and low temperature it is an antiferromagnetic insulator. In other words, electrons do not move (that defines the insulator) unless they are kicked really hard, and spins, on the other hand, order in an up-down pattern on alternating sites (that is called an antiferromagnet). As we shall discuss more later, this failure of band theory comes from the fact that interactions in these materials are larger than kinetic energy effects, leading to a breakdown of perturbation theory. In the jargon, this is a “strong coupling” effect. Despite the difficulties of deriv-

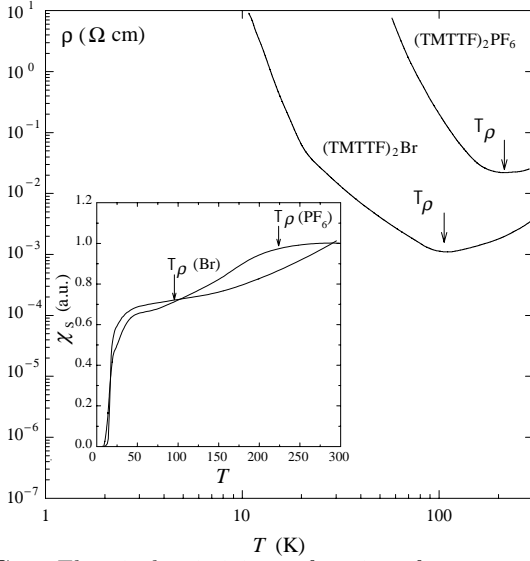


FIG. 3. Electrical resistivity as function of temperature for two members of the $(\text{TMTTF})_2\text{X}$ series. Inset: Temperature-dependent spin susceptibility, from Ref. [5].

ing from first principles the Hamiltonian in the reduced Hilbert space involving only spin degrees of freedom of the last filled states, again one can use general symmetry principles to write down model Hamiltonians. Solving these is a non-trivial task that has been successfully accomplished by many people for many years in the field of magnetism. Numerous neutron scattering experiments have verified in details the predictions of these models in many cases.

III. EXPERIMENTAL EVIDENCE FOR FAILURES OF STANDARD SOLID STATE THEORY IN LOW-DIMENSIONAL CONDUCTORS.

What do we mean by low dimensional conductors? In practice they can be formed, for example, by organic molecules stacked onto each other, or by copper oxygen planes separated by ions, as in the case of high-temperature superconductors. Despite the horrendous complexity of these structures, the Pauli principle and the general arguments given above tell us that for low-energy Physics we can concentrate only on the LDA bands that are very close to the Fermi energy. It turns out that, in many realizable cases, there is only one such band. Furthermore, the eigenstates in that band may turn out to be very different depending on which axis one is looking from. In these very anisotropic cases, it is as if electrons moved preferentially in one or two dimensions, the latter being the case for the high-temperature superconductors. Let us see what non-Fermi liquid Physics can arise in the $d = 1$ and $d = 2$ cases.

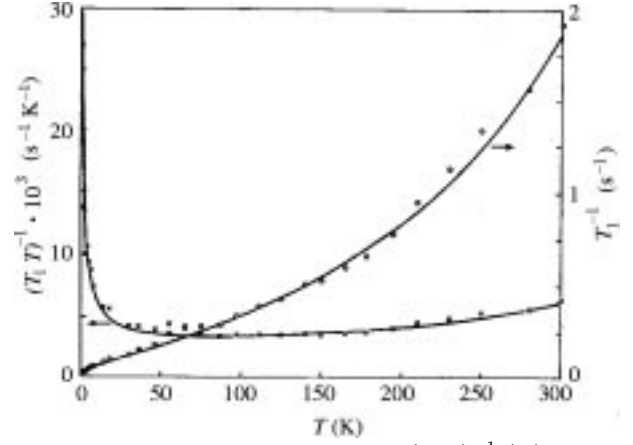


FIG. 4. Temperature dependence of $(T_1T)^{-1}$ (\times) and T_1^{-1} (\circ) for $\text{TTF}[\text{Ni}(\text{dmit})_2]_2$. The continuous line corresponds to the Luttinger liquid prediction, from Ref. [7].

A. One dimension: spin-charge separation in the organics

When electrons of opposite momentum are confined to move in one spatial direction, they cannot avoid each other and their interaction will be in some way enhanced in comparison with isotropic systems. As we will explain in the theory section, quasiparticles are absent in one dimension, and one has instead a Luttinger liquid where harmonic collective oscillations of both spin and charge are the true elementary excitations.

Here we present two clear experimental examples of the failure of the quasiparticle picture. Consider the normal phase of the $(\text{TMTTF})_2\text{X}$ series of quasi-one-dimensional organic conductors (here, TMTTF stands for the tetramethylfulvalene molecule and $\text{X} = \text{PF}_6, \text{Br}, \dots$, for an inorganic monovalent anion) [5]. As shown in Fig. 3, there is a clear upturn in electrical resistivity at temperature T_ρ , which depicts a change from metallic to insulating behavior. Below T_ρ , charge carriers become thermally activated. In a band picture of insulators, the same thermally activated behavior should be present for spins since the only way to create spins in a band insulator is to excite quasiparticles across the gap between the filled and the empty bands. For the compounds shown in Fig. 3, spin excitations instead are unaffected and remain gapless. This is shown by the regular temperature dependence of the spin susceptibility χ_s at T_ρ (inset of Fig. 3).

Among other experimental tools that are quite useful in probing signs of unusual behavior in low-dimensional organic conductors is Nuclear Magnetic Resonance, especially the temperature dependence of the nuclear spin-lattice relaxation rate, denoted as T_1^{-1} . Nuclear and electronic spins being coupled through the hyperfine interaction, the measurement of T_1^{-1} can give valuable information about electronic spin excitations. While $(T_1T)^{-1}$ is temperature-independent in a Fermi liquid, the correct theory in one dimension for $(T_1T)^{-1}$ takes the form [6]:

$$(T_1 T)^{-1} = C_1 T^{K_\rho - 1} + C_0 \chi_s^2(T), \quad (1)$$

where the exponent $K_\rho \geq 0$ stands for the ‘stiffness’ constant of collective charge degrees of freedom. It gives rise to a power-law enhancement of $(T_1 T)^{-1}$, which comes from antiferromagnetic spin correlations. For one-dimensional insulating compounds like $(\text{TMTTF})_2\text{X}$, charge degrees of freedom are frozen so that $K_\rho = 0$. The resulting behavior $T_1^{-1} \sim C_1 + C_0 \chi_s^2$ turns out to be invariably found in all these insulating materials down to low temperature, where three-dimensional magnetic or lattice long-range order is stabilized [6]. Among the very few quasi-one-dimensional organic materials that do not show long-range ordering, the case of $\text{TTF}[\text{Ni}(\text{dmit})_2]_2$ is interesting [7]: This system remains metallic down to very low temperature and a power law enhancement ($K_\rho \approx 0.3$) of $(T_1 T)^{-1}$ is maintained from 300K down to 1K or so (Figure 4).

B. Two dimensions: The pseudogap.

We have already shown the band structure of La_2CuO_4 in Fig. 1. The last occupied band is essentially a linear combination of copper and oxygen orbitals corresponding to two-dimensional (planar) arrangements of CuO_2 atoms. Thus, one expects that electrons relevant for transport are essentially confined to two dimensions. This is confirmed by the highly anisotropic transport properties of these materials, as discussed by T. Timusk in this issue. The Fermi level crosses the last occupied band, so we expect a metal.

But in reality, La_2CuO_4 is an antiferromagnetic insulator! This is because of strong interactions. When La^{3+} cations located away from the conducting planes are replaced by Sr^{2+} cations, electrons are removed from the CuO_2 planes and $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ becomes eventually a high-temperature superconductor. The generic phase diagram for high-temperature superconductors appears elsewhere in this issue. There are many high-temperature superconductors, and they all have in common CuO_2 planes that can be doped. The physical properties of these planes are quite similar from one compound to the next. From being antiferromagnetic when there is one electron per CuO_2 unit, they become superconductors when doped with holes (or with electrons in certain compounds). With hole doping, the superconducting T_c first increases. That is called the underdoped region. Then, a maximum T_c is reached at ‘optimal doping’, decreasing thereafter in the ‘overdoped’ region.

Let us look at the underdoped regime, above T_c . To see if the standard Fermi-liquid approach applies in this regime, we resort to ARPES. It is experimentally difficult to do ARPES in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, so we use results obtained from the CuO_2 planes of the so-called Bi2212 high-temperature superconductor. In Fig. 5(a), the solid line shows the location of the Fermi line expected from band structure calculations. Fig. 5(b), illustrates the

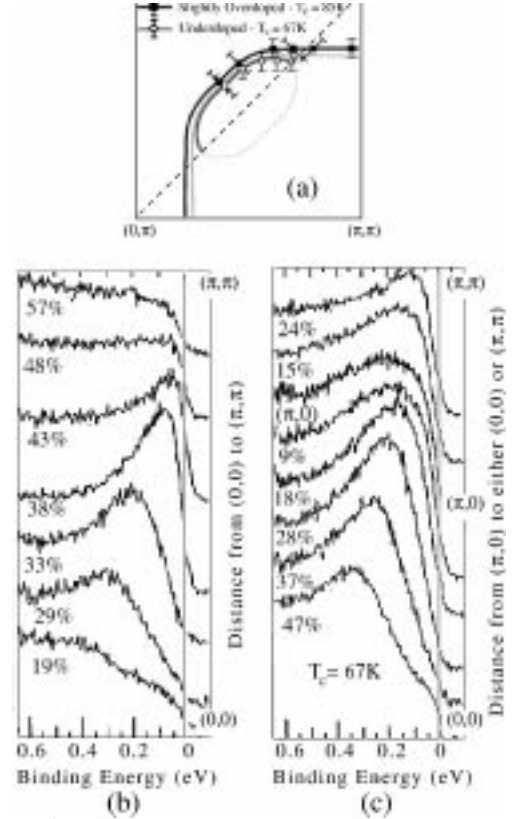


FIG. 5. ARPES spectra of O_2 -reduced $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$, taken from Ref. [3]

ARPES spectrum obtained for various wavevectors along the $(0,0)$ to (π,π) direction. At the wave-vector location expected from band structure, one finds the properties expected for a state at the Fermi surface, namely at zero energy the photoemission intensity is a sizeable portion of the value at the peak position. The surprise arises when one looks along the $(\pi,0)$ to (π,π) direction, Fig 5(c). None of the photoemission curves has the features expected from a state at the Fermi surface. It is as if the Fermi line had disappeared. This is the co-called pseudogap phenomenon. It is as if an energy gap had opened on part of what should have been the Fermi line (hence the ‘pseudo’ prefix, since zero-energy excitations are left elsewhere in wave-vector space). If you think about it from a quasiparticle picture, this is completely crazy. Take an energy band in a two-dimensional system. The allowed wavevectors cover a finite region of the two-dimensional k_x, k_y plane. That is the Brillouin zone. Plot the energy corresponding to a given wavevector in the z direction. That gives a singly connected surface. Now, cut this surface by a plane parallel to the k_x, k_y plane. The intersection of that plane with the energy surface can only be of two types. Either it is a line that links one edge of the Brillouin zone to another (or the same) edge, or it is a closed line inside the zone. The two possibilities can exist at the same time: In other words, there may be several Fermi lines in the Brillouin zone. But ac-

cording to these simple geometrical considerations, there is no other possibility. If you cover the Brillouin zone with ARPES measurements, you find that in the underdoped high-temperature superconductors the Fermi line does something worse than disagreeing with band structure calculations. It disappears in thin air! That is a total no-no in both standard approaches. Remember that in the standard approaches, either you have quasiparticles and there is a Fermi line, or you have an insulator and there is no single-particle state at all at zero energy.

Other manifestations of the pseudogap, especially in transport, are discussed elsewhere in this issue.

IV. WHY DO THE STANDARD APPROACHES FAIL?

The failure of the standard approaches in low dimension is not a total surprise from a theoretical standpoint. On the contrary, for a long time there have been papers discussing the peculiarities of low-dimensional systems. For example, consider the Mermin-Wagner theorem, which states that a spontaneous breaking of a continuous symmetry (e.g. a rotation) cannot occur in low dimension.

To be more specific on what that means, let us give an example. In three dimensions, Heisenberg antiferromagnets exist at finite temperature. In two dimensions, thermal fluctuations forbid such order from occurring at finite temperature. A rough argument for that is as follows. At long wavelengths, the energy associated with a change in the relative angle between neighboring spins, θ , will be proportional to $(\nabla\theta)^2$, or $q^2\theta_{\mathbf{q}}\theta_{-\mathbf{q}}$ in Fourier space. The mean square of the local angle is given by the integral over all wavevectors of $\langle\theta_{\mathbf{q}}\theta_{-\mathbf{q}}\rangle$. Using the classical fluctuation-dissipation theorem, this means that $\langle\theta^2\rangle \propto \int d^d q (k_B T/q^2)$. That integral diverges logarithmically in two dimensions, which proves *ad absurdum* that long-range order cannot exist. At zero temperature, the above argument fails and antiferromagnetic long-range order may exist. In one-dimension, quantum fluctuations have a similar detrimental effect and, even at zero temperature, antiferromagnetic or superconducting long-range order does not exist.

All this classical and quantum fluctuation business is bad news for the quasiparticle approach. Indeed, even though long-range order does not set in, below a temperature of the order of what would have been the mean-field transition temperature, there are collective modes that spread over large distances, making the material appear ordered over large scales. This strongly scatters quasiparticles, and in some instances it may lead to short lifetimes, or even to pseudogap phenomena [11].

So much for doing all at once. Let us consider first the effects of low-dimension in weak to intermediate coupling, and after that the effects of strong interactions. In weak to intermediate coupling, things behave very differently

according to dimension. Dimension still plays a role in strong coupling, but some strong-coupling effects depend little on spatial dimension.

A. The effects of low dimension in weak to intermediate coupling

1. One dimension

General considerations on phase space and the Pauli principle tell us that in high dimension, the scattering rate of quasiparticles at the Fermi surface is proportional to $(T/E_F)^2$. Since the relative width of the Fermi function is of order T/E_F , it makes sense to expect that thermodynamic properties will not much be influenced by the $(T/E_F)^2 \ll T/E_F$ width of the quasiparticles. In one dimension, this argument fails. The width in perturbation theory is proportional to T , like the Fermi function. Right from the start, this invalidates the Fermi-liquid starting point. In addition, response functions diverge as $\ln T$ at low temperature. More specifically, what makes one dimension so special lies in the shape of the Fermi surface, which consists of two points ($\pm k_F$). Electron and hole states that are created by electron-electron scattering close to $\pm k_F$ lead to elementary superconducting (Cooper) and density-wave ($2k_F$ electron-hole) pairings; these are not only singularly enhanced at low temperature, but their confinement in k -space produces strong interferences between them that persist to all orders in perturbation theory. A striking outcome of this interference is an instability of the Fermi liquid towards the formation of a quite different quantum state called a Luttinger liquid.

The point of view has to change completely. The appropriate theoretical tools here bear the name of renormalization group [19] or bosonization [8]. They lead to the same final picture: It is best to consider spin and charge collective modes as the elementary excitations. In the resulting “Luttinger liquid” picture [9], which replaces the Fermi liquid as a general limiting case in one dimension, the spin and the charge of would-be quasiparticles separate, becoming the true elementary excitations that propagate at different velocities. We have illustrated experimental manifestations of this phenomenon in organic conductors in the previous section. The cases where the compounds were insulators displayed extreme examples of spin-charge separation. These compounds have a commensurate band filling and their insulating behavior is a manifestation of one-dimensional Mott localisation, a more general topic on which we return in the discussion on the effects of strong interactions.

2. Two dimensions

Contrary to the one-dimensional case, the quasiparticle picture does not fail automatically in two dimensions. For example, the compound in Figure 2 is a two-dimensional Fermi liquid. Theoretically, in two dimensions there are only weak logarithmic corrections to the standard phase space arguments of Fermi liquid theory. Stronger corrections occur when the Fermi surface has so-called nesting properties [10], or when one enters a fluctuation regime. Let us consider the latter case. The fluctuation regime may occur over a broad temperature range in two dimensions, basically from a temperature of the order of the mean-field transition temperature, all the way to zero temperature. Let ξ be the length over which the collective mode fluctuations are correlated. In the fluctuation regime, the scattering rate for quasiparticles at the Fermi surface is proportional to $\frac{T}{v_F} \int d^{d-1}q (q^2 + \xi^{-2})^{-1} \propto T\xi^{3-d}/v_F$. In $d = 2$, this becomes ξ/ξ_{th} , where $\xi_{th} \equiv \hbar v_F/k_B T$ is the thermal de Broglie wavelength. Since the correlation length ξ diverges much faster as $T \rightarrow 0$ than ξ_{th} , this implies a divergent scattering rate. It is difficult to have a stronger contradiction of the quasiparticle picture. Physically, when the correlation length ξ becomes much larger than the thermal de Broglie wavelength, the quasiparticles are moving in a locally ordered background. Then a pseudogap, precursor of the $T = 0$ ordered state, opens up at the Fermi surface [11]. As temperature decreases, it may open on certain segments of the Fermi surface before it opens on other segments. That is a consequence of the fact that the scattering rate, proportional to $T\xi/v_F$, may be very different on different parts of the Fermi surface. Close to half-filling in particular, the Fermi velocity nearly vanishes at certain points of the Fermi surface while it is large at other points.

B. The effects of very strong interactions

When interactions are very strong, electrons avoid getting close to each other by localizing. When an odd number of electrons is localized on each atom, the charge does not move and the only degree of freedom left at low energy is essentially the spin. Note the contrast with the quasiparticle picture where a half-filled band is a metal. The low energy Physics in these system, where electrons are localized by interactions, is then essentially governed by variations of the Heisenberg Hamiltonian described above. Many years ago, Mott imagined what would happen to a system as the strength of the interaction is increased. The transition from extended quasiparticle states to localized states produced by large interaction effects is referred to as the Mott transition. It is a first order transition whose Physics has become better understood in recent years [12], thanks to the development of calculational methods in the limit of infinite dimension [13].

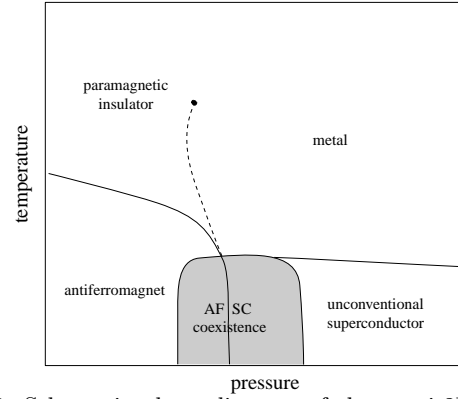


FIG. 6. Schematic phase diagram of the quasi-2D organic compound κ -(ET) $_2$ Cu[N(CN) $_2$]Cl, from Ref. [16]

In the Mott insulator, many properties are not strongly dependent on dimension, in particular when they concern high energy. That is why infinite-dimensional methods have been useful. Nevertheless, precursor effects caused by collective mode fluctuations have been seen in models of Mott insulators in low dimensions [14]. These effects do not occur in infinite dimension.

The Mott transition does not break any symmetry, and it may occur in any dimension. For example, V $_2$ O $_3$ may exhibit such a transition, although questions regarding the effects of lattice symmetry change and of orbital degeneracies are still open [15]. A clearer example of a Mott transition has been discovered recently in two-dimensional organic conductors [16]. The phase diagram is illustrated on Fig. 6. The system is half-filled. The horizontal axis represents pressure. From a model point of view, increased pressure means larger overlap between atomic orbitals and hence increased kinetic energy. Indeed, at low pressure on this diagram, the system is either a paramagnetic insulator at high temperature, or an antiferromagnetic insulator at low temperature. At higher pressure, one crosses a first order transition that leads to a metallic state at high temperature and to a d -wave superconductor at low temperature.

C. And high-temperature superconductors in all that?

The high-temperature superconductors are Mott insulators at half-filling. Doping eventually leads to a d -wave superconducting state. Their electronic properties are also highly two-dimensional, in particular in the underdoped region. They thus manifest all the complexities described above. The high energy (100 meV) pseudogap described in Section IIIB above, is likely to be a strong-coupling pseudogap, in other words a pseudogap originating from the Physics of doped Mott insulators. However, closer to the superconducting phase transition, in the more metallic regime, one expects a fluctuation-induced pseudogap. Indeed, in photoemission, one can

often identify a lower energy pseudogap that seems to occur in a fluctuation regime. A more detailed discussion appears in Ref. [17].

V. THEORETICAL METHODS AND CHALLENGES

One of the most widely studied model Hamiltonians of correlated electrons is the so-called one-band Hubbard Hamiltonian:

$$H = - \sum_{\langle ij \rangle \sigma} t_{i,j} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} . \quad (2)$$

In this expression, the operator $c_{i\sigma}$ destroys an electron of spin σ at site i . Its adjoint $c_{i\sigma}^\dagger$ creates an electron and the number operator is defined by $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. The symmetric hopping matrix $t_{i,j}$ determines the band structure, which here can be arbitrary. Occupation of a site by both a spin up and a spin down electron costs an energy U due to the screened Coulomb interaction. This Hamiltonian is clearly a caricature of reality, but what is important is that it has a minimal number of parameters and it allows one to describe the two limiting cases of delocalized and localized electrons, as well as the Mott transition between these two limits. Consider the case where the band is characterized by a single parameter t representing hopping between neighboring sites. At weak coupling, when $U/t \ll 1$, one can apply the standard quasiparticle approach. At strong coupling, when $U/t \gg 1$, one can show how this Hamiltonian becomes, at low energy and half-filling, the Heisenberg Hamiltonian for spins. Hence, it is a good starting point in both the strong and weak coupling limits as well as in the intermediate coupling regime, characteristic of high-temperature superconductors, where neither of the two standard approaches work. At half-filling, the high-temperature superconductors become antiferromagnetic insulators that are well described by the Heisenberg model. At low energy and away from half-filling, the Hubbard model becomes a variant of the so-called $t - J$ model, widely studied also in the context of high-temperature superconductors.

It is hard to know from first principles if U/t will be large or small for a given system. But there are heuristic guides coming from Chemistry and from so-called “constrained LDA calculations”. In general, the Hubbard Hamiltonian is an effective Hamiltonian. It is even useful in some cases to let $U < 0$ to study models of s -wave superconductivity. Despite the fact that the Hubbard model was proposed almost 40 years ago, it is only recently that it has become to be understood at intermediate coupling and in low dimension. Various methods have been developed to study this model. In one dimension, an exact solution was found by Bethe Ansatz [18], from which physical information is unfortunately quite difficult to extract. The linear dispersion of the one-dimensional electron gas in one dimension is at the

root of an analogy with relativistic field theories which explains the success of field theoretic methods like the renormalization group [19], bosonization [20] and Conformal Field Theory [20]. In two and more dimensions, let us mention Slave-boson approaches [21], renormalized perturbation theory approaches [22], strong-coupling perturbation expansions [14] and the two-particle self-consistent approach [11]. Finally, infinite-dimensional methods have provided a dynamical mean-field theory methodology [13] that has been very useful in understanding the Mott transition. This approach can also be extended to lower dimensions. In $d = 2$ however, the effect of antiferromagnetic fluctuations are not included yet in this methodology, which limits somewhat the applicability of the method to high-temperature superconductors.

A major factor for progress is that it is now possible to do reliable numerical calculations that allow us to both develop physical intuition and check the validity of approximation methods. Exact diagonalizations are possible in any dimension but are restricted to a small number of electrons [23]. In one dimension, Density Matrix Renormalization Group [24] has provided a revolutionary method to obtain reliable results. In two dimensions, Quantum Monte Carlo simulations [25] remain a tool of choice. Such simulations have allowed us, for example, to choose between various analytical approaches that were giving different answers to the pseudogap question in weak to intermediate coupling [17].

How can we understand electronic systems that show both localized and propagating character? Why do both organic and high-temperature superconductors show broken-symmetry states where mean-field-like quasiparticles seem to reappear? Why is the condensate fraction in this case smaller than what would be expected from the shape of the would-be Fermi surface in the normal state? Are there new elementary excitations that could summarize and explain in a simple way the anomalous properties of these systems? Do quantum critical points play an important role in the Physics of these systems? Are there new types of broken symmetries? How do we build a theoretical approach that can include both strong-coupling and $d = 2$ fluctuation effects? What is the origin of d -wave superconductivity in the high-temperature superconductors? These are but a few of the basic open questions left to answer in this field.

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