Chapter 1

STRONGLY CORRELATED ELECTRONS: A DYNAMICAL MEAN FIELD PERSPECTIVE

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Abstract We discuss the role of the Mott transition in the strong correlation problem and describe new insights gained using dynamical mean field techniques (DMFT).

1. STRONGLY CORRELATED MATERIALS

The last two decades has witnessed a revival in the study of strongly correlated electron systems. A large variety of transition metal compounds, rare earth and actinide based materials have been synthesized. Strong correlation effects are also seen in organic metals, and carbon based compounds such as Bucky balls and carbon nanotubes. These systems display a wide range of physical properties such as high temperature superconductivity, heavy fermion behavior, and colossal magnetoresistance to name a few [1].

Strongly correlation effects are the result of competing interactions. They often produce at low temperatures several thermodynamic phases which are very close in free energy, resulting in complex phase diagrams.

As a result of these competing tendencies, strongly correlated electron systems are very sensitive to small changes in external parameters, i.e. pressure, temperature, composition, stress. This view is supported by a large body of experimental data as well as numerous controlled studies of various models of strongly correlated electron systems [1].

At the hart of the strong correlation problem is the competition between localization and delocalization, i.e. between the kinetic energy and the electron electron interactions. When the overlap of the electrons among themselves is large, a wave like description of the electron is natural and sufficient. Fermi liquid theory explains why, in a wide range of energies, systems such as alkali and noble metals behave as weakly interacting fermions, i.e. they have a Fermi surface, linear specific heat and a constant magnetic susceptibility and charge compressibility. The one electron spectra form quasi-particles and quasi-hole bands. The transport properties, are well described by Boltzmann theory applied to long lived quasi-particles, an approach that makes sense as long as $k_f l \gg 1$. Density functional theory in the local approximation, is able to predict most physical properties with remarkable accuracy.

When the electrons are very far apart, a real space description becomes valid. A solid is viewed as a regular array of atoms where each atom binds an integer number of electrons. These atoms carry spin and orbital quantum numbers, giving rise to a natural spin and orbital degeneracy. Transport occurs via activation with the creation of vacancies and doubly occupied sites. Atomic physics calculations together with perturbation theory around the atomic limit allows us to derive accurate spin -orbital Hamiltonians. The one electron spectrum of Mott insulators is composed of atomic excitations which are broaden to form bands which have no single particle character, known as Hubbard bands. In the large majority of known compounds the spin and orbital degrees of freedom generally order at low temperatures breaking spin rotation and spatial symmetries. However, when quantum fluctuations are strong enough to prevent the ordering, possible new forms of quantum mechanical ground states emerge.

These two limits, well separated atoms, and well overlapping bands, are by now well understood and form the basis of the "standard model" of solid state physics. One of the frontiers in strongly correlated electron physics problem, is the description of the electronic structure of solids, away from these well understood limits. The challenge is to develop new concepts and new computational methods, capable of describing situations where both itineracy and localization are simultaneously important. The "standard model " of solids breaks down in this situation and strongly correlated electron systems have anomalous properties such as resistivities which far exceed the Ioffe Regel Mott limit ${\rho_{Mott}}^{-1} \approx (e^2/h) k_f$, non Drude like optical conductivities, and spectral functions which are not well described by band theory [1]. To treat this problem one needs a technique which is able to treat Kohn Sham bands and Hubbard bands on the same footing, and which is able interpolate continuously between the atomic and the band limit. Dynamical Mean Field Theory (DMFT) is the simplest approach satisfying this requirement and will be used to describe some of recent advances in our understanding of the Mott transition problem [2].

2. DYNAMICAL MEAN FIELD THEORY

The Hubbard model Hamiltonian, eq. (1.1), plays the role of the ”Ising model ” of strongly correlated electrons. It is the simplest model describing the competition between localization and itineracy.

$$H = -\sum_{<ij>,\sigma}(t_{ij}+\mu\delta_{ij})(c^+_{i\sigma}c_{j\sigma}+c^+_{j\sigma}c_{i\sigma})+U\sum_i n_{i\uparrow}n_{i\downarrow} \tag{1.1}$$

The essential parameters in the model are δ doping, or chemical potential μ T temperature U/t Magnetic Frustration ($t_{ij} = t$ n.n. , t' t" n.n.n.). We will denote the set of relevant parameters that can be varied as α. On a Bethe lattice with large coordination with $t_{ij} = (\frac{1}{\sqrt{(t)}})^{|i-j|}$ [3] the local properties can be computed from an Anderson impurity model[4]

$$H_{AIM.} = \sum_{K\sigma}\epsilon_K C^+_{k\sigma}C_{k\sigma}+\sum_{K\sigma}V_k(C^+_{k\sigma}f_\sigma+f_\sigma{}^+C_{k\sigma})+\epsilon_f f^+_\sigma f^+_\sigma+Uf^+_\uparrow f_\uparrow f^+_\downarrow f_\downarrow \tag{1.2}$$

with an hybridization function $\Delta(i\omega_n) = \sum_{K\sigma}\frac{V_K{}^2}{(i\omega_n-\epsilon_k)}$ obeying the self consistency condition:

$$t^2 G_{imp}(i\omega_n)[\Delta,\alpha] = \Delta(i\omega_n). \tag{1.3}$$

In the limit of large lattice coordination, all the physical quantities can be expressed in terms of the local quantities and the hopping matrix elements. This is convenient since it allows the evaluation of all the transport properties. A great deal of work has gone into solving and understanding the dynamical mean field equations (1.3) [2]. Furthermore the method is easily extended to treat situations with broken spin and spatial symmetries. An extension to treat realistic band structure and orbital degeneracy has recently been carried out [25][20][23]. In the following sections we will describe some of the insights that have emerged and some lessons that we learned about strongly correlated electron systems.

3. INSIGHTS FROM DMFT

3.0.1 DMFT phase diagrams, Frustration, Complexity and Universality. The low temperature phase diagram of even simple Hamiltonians treated within DMFT, has several distinct phases, and is fairly complex. Even the simplest, bare bones Hamiltonian (one band Hubbard model with partial frustration) described in the previous section, has at least a metallic antiferromagnetic phase and a paramagnetic insulating phase in addition to a paramagnetic metal phase and the antiferromagnetic insulating phase. The phase diagram of ref [8] shown in Fig 1.1 bears certain qualitative similarity of this phase diagram vis a vis the phase diagram of Vanadium Oxide, This observation lead Rozenberg et.

al. [8] to suggest several optical experiments which confirmed some qualitative predictions of DMFT.

It is important to emphasize, however, that the main lesson that should be drawn from the qualitative similarity, in the low temperature region, between the DMFT phase diagram of one of the simplest model of correlated electron systems and that of some real oxides, is the ability of the DMFT method to capture multiplicity of possible ordered states. The detailed nature of these phases, and the character of the transitions between them, depend on many details of the Hamiltonian describing the specific crystal structure and chemistry of the compound. To approach this problem, realistic versions of DMFT have been constructed and are being developed [25] [20].

The strong dependence of the low temperature phases and of the low temperature physical properties of each material on its crystal structure and chemical composition should be contrasted with the remarkable degree of universality that is predicted to occur at higher temperatures. All that is required to produce the high temperature features of the DMFT phase diagram, is a large degree of magnetic frustration to suppress the long range order and to allow for a localized phase with a large entropy entropy content. In systems without magnetic frustration, the onset of magnetism or other forms of order preempts us from accessing this strongly correlated regime. The origin of the magnetic frustration is crucial for understanding the low temperature part of the phase diagram, with its myriad of ordered phases, but is rather irrelevant in the high temperature regime, where thermal fluctuations average over all the various different configurations, leading to a more universal description which is captured by a relatively local approach such as DMFT in its single site or its clusters versions. In systems such as the titanates and in the Vanadium oxides, the origin of frustration arises from the orbital degeneracy which is unique to those materials. In the Nickel selenide sulfide mixtures, the crystal structure is such that a sizeable ring exchange term competes with the nearest neighbor superexchange interaction resulting in a reduced Neel temperature. Still, these systems display very similar phenomena around the Mott transition endpoint.

The contrast between the highly universal behavior at high temperature and the dependence of low temperature properties on additional parameters in the Hamiltonian, was discussed in ref [29] in connection with the comparison of the physical properties of the Vanadium Oxide and the Nickel Selenide Sulfide mixtures. The phase diagram of the two dimensional organic compound κ BEDTTF [27], where the frustration originates in its underlying chiral triangular lattice of dimers, strengthen the validity of this point of view. Indeed many of the high temperature physical properties of this have been accounted for by the DMFT studies of McKenzie and Merino [14].

To summarize, since magnetic frustration and competition of kinetic and interaction energy is all that is required for obtaining the high temperature part of the "canonical " phase diagram of a correlated electron system where the transition between the localized and extended regime as a function of $\frac{U}{t}$ takes place via a first order transition [7][8], this is faithfully reproduced by the simplest model containing these ingredients treated within DMFT.

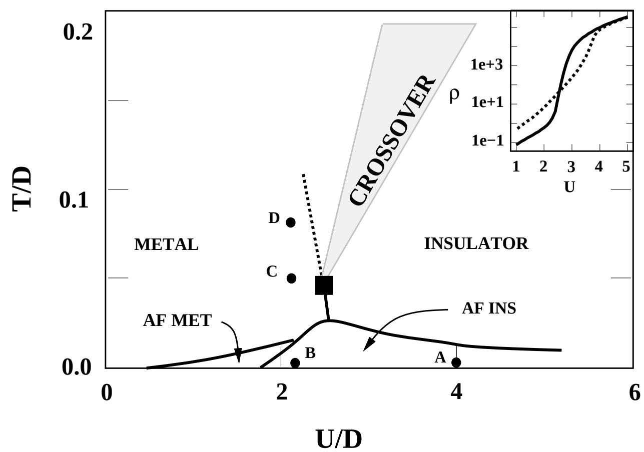

Figure 1.1 Schematic phase diagram of partially frustrated Hubbard model from ref [8], the inset illustrates the behaviour of the resistivity above but near the Mott endpoint

The phase diagram of ref [8] displays two crossover lines. The dotted line in fig 1 is a coherence incoherence crossover (i.e. the continuation of the U_{c2} line where metallicity is lost). The shaded area is a continuation of the U_{c1} line, where the temperature becomes comparable with the gap. Both were observed in the V_2O_3 and $NiSeS$ system [9] , [28]. Further justification for this point of view, and a refined description of the localization delocalization transition around the Mott transition endpoint was achieved by the development of a Landau like description [21] [22].

3.0.2 Coherent and Incoherent Spectra. The mapping of the Hubbard model onto an Anderson impurity model described in section 2. resulted in an important insight: that the one electron spectral function of the Hubbard model in the strongly correlated metallic region contains both atomic features (i.e. Hubbard bands) and quasiparticle features, in its spectra [4]. Further investigations revealed [5] that as the transition at zero temperature is approached there is a dramatic transfer of spectral weight from the low lying quasiparticles to the Hubbard bands, which results in a Mott transition point where the quasi-particle mass diverges, but a discontinuous gap opens in the quasi-particle spectra. These calculations, where in agreement with the pioneering work of Fujimori et. al. [6] who arrived essentially to the same picture on the basis of his experimental data.

3.0.3 Anomalous resisistivities. Figure 1.2 describes the anomalous resisitivities near these crossover regions. Notice the anomalously large metallic resistivity which is typical of many oxides [10]. While the curves in this figure far exceed the Ioffe Regel limit (using estimates of k_f from T=0 calculations) there is no violation of any physical principle. At low temperatures, a k space based Fermi liquid theory description works but in this regime the resistivity is low (below the Ioffe Regel limit). Above certain temperature the resistivity exceeds the Ioffe Regel limit but then quasiparticle description becomes inadequate. There is no breakdown or singularities in our formalism, the spectral functions remain smooth, (above the Mott transition endpoint), only the physical picture changes. At high temperatures we have an incoherent regime to which the Ioffe Regel criteria does not apply, because there no long lived excitations with well defined crystal momentum in the spectra. The electron is strongly scattered off orbitals and spin fluctuations, and is better described in real space. In this regime, there is no simple description in terms of k space elementary excitations, but one can construct a simple description and perform quantitative calculations if one adopts the spectral function as a basic object in terms of which one formulates the theory.

Only the anomalously large magnitude of the resisitivity (which follows from a Greens function which has branch cuts rather than well defined poles), is universal as can be seen by comparaison of the detailed temperature dependence at half filling (as in fig 1.2) and away from half filling as in figures (1.3) and (1.4). The temperature dependence of the transport in the high temperature incoherent regime, depends on whether the system is at integer filling or doped, as can be shown numerically [12] and analytically [11]. in the example of the doped Mott insulator. The low temperature and the high temperature Anomalously large resistivities also occur in strongly coupled electron phonon systems, as discussed in ref [13].

3.0.4 Anomalous Transfer of Spectral Weight. Another manifestation of the same physics is the anomalous transfer of spectral weight which is observed in the one electron and in the optical spectra of correlated systems as parameters such as doping or pressure are varied. This surprising aspect of strong correlation physics was noted and emphasized by many authors[16]. Transfer of spectral weight can also take place as a function of temperature. For example the ”kinetic energy ”which appears in the lo energy optical sum rule can have sizeable temperature dependence, an effect that was discovered experimentally by [17] and explained theoretically by DMFT calculations [18]

Once more thinking about this problem in terms of well defined quasiparticles is not useful. It is more fruitful to formulate the problem in terms of spectral functions describing on the same footing coherent and incoherent excitations. The relative weights of these components in the spectra evolves

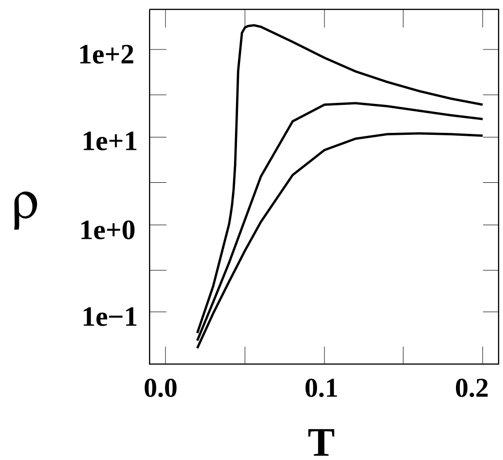

Figure 1.2 $\rho_{dc}(T)$ around the coherence incoherence crossover near the finite temperature Mott endpoint. $U/D = 2.1, 2.3, 2.5$ (bottom to top), obtained with the IPT method from ref [8].

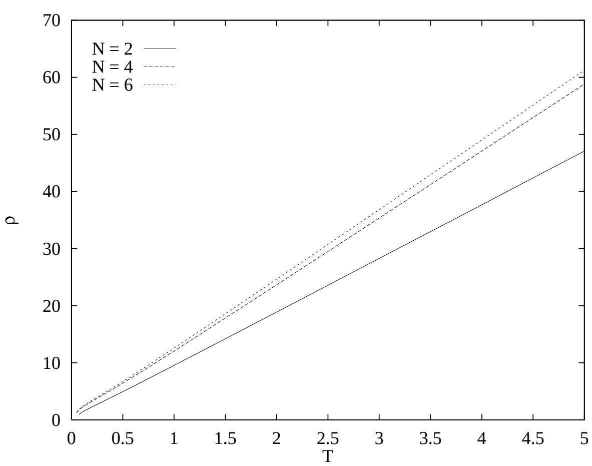

Figure 1.3 $\rho_{dc}(T)$ in units of $z\hbar a/e^2$, vs T (in units of D) for different values of orbital degeneracy N for a fixed doping $\delta = .1$ obtained with the NCA method which is valid at high temperatures, from the work of Palsson [11].

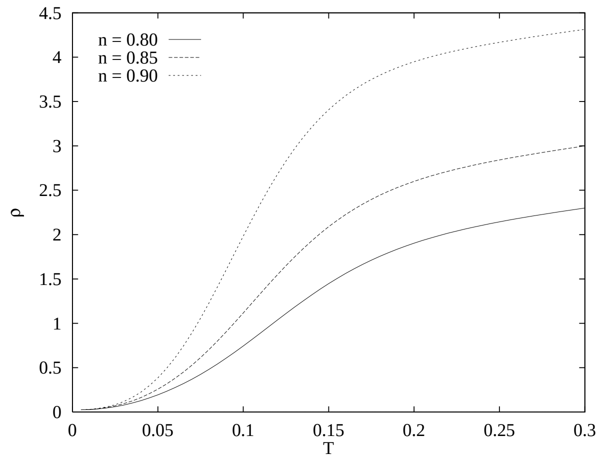

Figure 1.4 $\rho_{dc}(T)$ vs T in units of $z\hbar a/e^2$, vs T (in units of D) obtained with the IPT method, for different dopings at $\frac{U}{D} = 2.8$ from ref [11].

smoothly with temperature and leads to sizeable variations in the integrated optical intensity. This fundamental role of the spectral function, becomes even more prominent, in the Landau theory approach to the Mott transition where we allow the greens function to fluctuate away from its physical saddle point value, in order to explore different non perturbative states which may not be accessible in perturbation theory in the interaction strength.

4. STRONGLY CORRELATED ELECTRON SYSTEMS, RENORMALIZATION GROUP FLOWS AND OUTLOOK

To understand better the DMFT description of the high temperature regime, and its connection with the underlying critical points of self consistent impurity models, it is illuminating to make a comparison with the theory of quantum critical points.

In this theory, [15] a phase transition at zero temperature at a critical value of a control parameter x_c, cause anomalies in a finite region of the temperature control parameter phase diagram (see fig 1.5). This region is the quantum critical regime. In the language of the renormalization group (RG), in this region, the renormalization group trajectories are very close to the fixed point describing the critical point. If the initial conditions depart from the critical surface, the renormaliation group trajectories at sufficiently low temperatures are driven towards two different fixed points describing the two stable phases.

In a strongly correlated regime, it is fruitful to think of the phase diagram of a model Hamiltonian, as one varies several independent parameters, so the

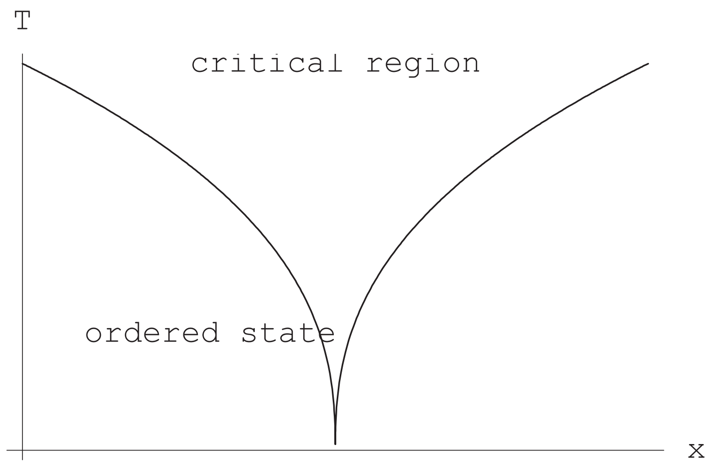

Figure 1.5 Schematic view of a phase diagram of a system undergoing at x_c a quantum phase transition as a function of a control parameter x. The anomalous region is the quantum critical regime [15].

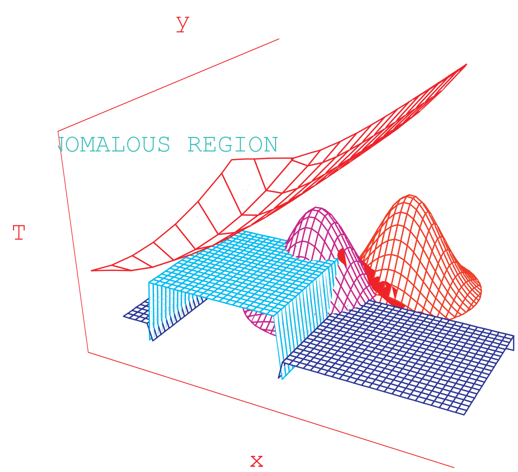

Figure 1.6 Schematic view of the DMFT phase diagram of a strongly correlated electron system. x and y are multidimensional control parameters, there are many underlying low temperature phases separated by first and second order phase transitions. The anomalous region is the finite temperature manifestation of the localization delocalization crossover rather than the result of proximity to one particular instability.

parameter space in this case is multidimensional. We describe this schematically, in figure 1.5 by two axis x and y . Examples of coordinates in the relevant space are parameters which control the degree of magnetic frustration, or parameters which control the relative stability of two competing phases. The phase diagram of a correlated system in this parameter space is more complex and is described by several competing phases and first and second order phase transitions separating them as shown schematically in 1.6. Inside this complex phase diagram, but probably in a physically inaccessible region, are transition lines reminiscent of the Mott transition in fully frustrated models. The shaded region at high temperature, is not directly controlled by the vecinity to a single unstable fixed point. There are two many instabilities which are nearby, and at the temperature scale considered, they are all two close in energy to be able to nudge the RG trajectory towards a specific critical trajectory (wich has a relatively small basin of attraction). DMFT is able to describe this intermediate behavior at high temperatures by means of a weakly k dependent but frequency dependent Weiss field. This results in the anomalies described in the previous subsections. Of course, at lower temperatures some form of ordering is established and more conventional behavior is restored. A somewhat analogous, but much more extreme situation (macroscopic rather than finite number of competing states), occurs in glassy systems. In the context of glassy DMFT is known to describe successfully many experimentally observed phenomena [26].

One can also think of the intermediate asymptotic regime of the disordered phase at finite temperatures in a functional integral representation. If there are several competing instabilities one is forced to introduced several Hubbard Stratonovich fields to describe them. Theories of individual phase transitions would have a phase diagram such as the one in fig 1.5a, with a Hubbard stratonovic fields condensing at a special ordering wavevector. However as long as all the instabilities are competing on the same footing, the Hubbard Stratonovich fields have low energy but no specific wavevector. In this case a local picture, with a q independent Hubbard Stratonovich master field, reproduces the correct physics at high temperatures.

It is useful to think of the program of performing realistic electronic structure calculations for correlated materials in the light of the previous discussion. The Hamiltonian describing the electrons at short distances is known and easily written down. This is the formal starting point of all electron first principles calculations. However, to describe the physics at a lower energy scale Λ, one would like to eliminate the degrees of freedom which have energies much larger than that scale, and derive an effective Hamiltonian which is more transparent and contains only the relevant or active degrees of freedom. The effective Hamiltonian at that scale, is the model Hamiltonian which is usually written down by the solid state physicist on physical grounds. As Λ is reduced a renormalization group flow in the space of all Hamiltonians is defined. Different initial conditions at short distances describe different materials, different pressures, lattice spacings concentration etc..

If one starts with conditions that correspond to weakly correlated systems (e. g. atomic numbers involving s or p electrons, high densities etc.) the RG flows are relatively simple and converge at low energies to reach simple fixed points describing band metals or insulators.

On the other hand when we start from more correlated situations (e.g. open shells, containing relatively localized d or f electrons, lower densities), the R.G. trajectories are diverging from one another, reflecting the diversity of phases nearby. This situation calls for quantitative methods for realistic modelling of the material in question. One of the most serious difficulties in carrying out the Wilson RG program described above, is the continuous change in the *form* of the effective Hamiltonian from scale to scale. A typical example is the formation of a heavy fermion liquid state at a coherence energy scale. At high energies the effective Hamiltonian contains atomic configurations and conduction electrons, at low frequencies only heavy quasiparticles are the relevant degrees of freedom. In spite of these difficulties, an R.G analysis taking account some quantum chemistry in the initial conditions has been carried out *in the local approximation* aided by developments in DMFT, see e.g. ref [19].

While following the R.G. flows down to very low temperatures and predicting physical properties in the most strongly correlated situations may prove to be very difficult, we optmistically hope that cluster DMFT, with small sizes will be accurate in a wide range to interesting situations (not too close to phase transitions, not too low temperatures). This view is supported by the recent success of S. Savrasov [20] in describing within realistic DMFT some of the most puzzling properties of δ Pu, a strongly correlated electron system.

Acknowledgments

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