Dynamical mean-field studies of metal-insulator transitions

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We discuss the successes of the dynamical mean field (DMF) approach to metal insulator transitions in both the clean and the disordered limit. In the latter case, standard DMF equations are generalized in order to incorporate both the physics of strong correlation and Anderson localization effects. The results give new insights into the puzzling features of doped semiconductors.

1. Introduction

How a substance evolves from a metallic to a non metallic state is one of the most fundamental and richest problems in condensed matter physics.

In general, there are several mechanisms at play. Electron-electron interactions can drive a metal to insulator transition in a pure substance (Mott, 1990). This transition is named after Sir Nevill Mott who laid down the foundations for the physical understanding of this phenomenon. Another route was discovered by Anderson (1958) who realized that sufficiently strong disorder can drive a metal-insulator transition even in systems of non interacting electrons. The theoretical description of the situation when both effects are present is a central unsolved problem. For recent reviews see Lee & Ramakrishnan (1983) and Belitz & Kirkpatrick (1995).

Early treatments (Abrahams et al. 1979, Wegner 1976, Schäffer & Wegner 1980, Finkelshtein 1983, 1984) used direct analogies from the theory of magnetism and the scaling approach to critical phenomena. The technical apparatus of the approach was a field theoretical non linear sigma model and an expansion near two dimensions. The physical content of such theories was expressed concisely in terms of an extension (Castellani et al. 1987) of the Fermi liquid approach to disordered systems. These ideas were very successful in the description of the transport and thermodynamic properties of weakly disordered metals. The approach, however, encounter several difficulties in accounting for experimental observations in many systems. The origin of these difficulties can be traced to (1) strong interaction effects, and (2) strong statistical fluctuations. One important manifestation of this effect was the formation of local magnetic moments, objects which can not be understood from a weak correlation perspective. This aspect of the problem and its theoretical treatment were addressed in Paalanen et al. (1988) and Milovanović et al. (1989).

In the last few years, a new dynamical mean field approach to the strong correlation problem has been developed (Metzner & Vollhardt 1989, Georges & Kotliar 1992). It has explained many puzzling features of clean three dimensional transition metal oxides (for a review see Georges et. al. 1996). Very recently, it was extended (Dobrosavljević & Kotliar 1997) to incorporate the interplay of Anderson localization and correlations effects.

The mean field method is largely complementary to the scaling approach. While the latter concentrates on the long wavelength modes which presumably govern the immediate vicinity of the transition, the former focuses on the local charge and spin dynamics of the electrons. The latter is based on an expansion around the lower critical dimension, the former being formally valid in large dimensions. It is our view that a good mean field understanding of the metal to insulator transition problem is a necessary first step towards a comprehensive theory.

In this talk we will not focus on the technical aspects of the method which are thoroughly reviewed elsewhere. Instead we will attempt to give a simple description of the physical content of the approach, and of the results obtained by this method. Section 2 introduces the essential idea of the mean field method for a general periodic solid. It is our hope that its generality and local character will be of interested to the chemistry community which has stressed the importance of local bonding and correlations through the years. Section 5 discussed the extension to the disordered case. We stress the importance of statistical fluctuations and how they are captured by the mean field method. In section 3 we discuss the physics of the density driven Mott transition and explain why the mean field approach works so well for three dimensional compounds, stressing the role of orbital degeneracy. We then move to the physics of disordered interacting systems which was the focus of many years of Mott's research. Section 4 discusses our views on the puzzle posed by the differences between uncompensated semiconductors and disordered alloys. In section 5, 6 and 7 we elaborate on the physical content of the mean field approach and argue it captures some essential elements needed to resolve this puzzle. We conclude in section 8 with a comparison to other approaches and outline some directions for further work.

2. Dynamical mean-field theory (DMF) theory - the clean limit

To motivate the dynamical mean field (DMF) approach, it is useful to draw some analogies with a well established approach to the electronic structure problem, the density functional theory (DFT). The basic physical quantity in DFT is the density $\rho(r)$, and the free energy of a system is written as a functional of the density $F_{DFT}[\rho(r)]$. Its minimum gives the physical density of the system in question. In practice, the form of the functional F_{DFT} is unknown and various approximations such as the LDA (local density approximation) are used instead of the exact density functional.

The dynamical mean field approach is very similar in spirit, except that it adopts the local spectral function $A(\omega, r) \equiv -\frac{1}{\pi} ImG(r, r; \omega + i\delta)$ as the basic quantity. One then writes the free energy as a functional of this quantity, and its minimization leads to the dynamical mean field equations which give the one particle spectral function for the system of interest. One can motivate the extension from the density to the spectral function (which can be thought of loosely

as a kind of energy-resolved density) in the context of strongly correlated electron systems, by thinking about their photoemission (and inverse photoemission) spectra which demonstrate the existence of bands which have the character of atomic configurations (Hubbard bands), in addition to the ordinary quasiparticle bands which are analogous to those of the non interacting system. One can incorporate quasiparticle bands and Hubbard bands naturally in a single theoretical framework by resolving in energy, the local density, i.e. the local density is the integral of the local spectral function over frequency. By resolving in energy the localized and itinerant component of the electron, DMF approach treats coherent (quasiparticle like) and incoherent (Hubbard bands like) excitations on the same footing. It is a unified framework for the description of localized and itinerant electrons.

To illustrate the generality of the method let us start from a Hamiltonian containing several orbitals per unit cell. We use a compact notation where the index $\alpha = (m, \sigma)$ combines the orbital m and the spin σ.

$$H_{lattice} = -\sum_{\langle ij \rangle} c_{i\alpha}^{+} t_{i\alpha,j\beta} c_{j\beta} + \sum_{i} \left(E_{\alpha\beta} - \mu \delta_{\alpha\beta} \right) c_{i\alpha}^{+} c_{i\beta} + \sum_{i} \Gamma_{\alpha\beta\gamma\delta} c_{i\alpha}^{+} c_{i\beta} c_{i\gamma}^{+} c_{i\delta}.$$

$$(2.1)$$

We now focus on a single unit cell, and integrate out all degrees of freedom except for those which reside in the selected unit cell. These are described by operators c_{α} and no longer carry a site index. The dynamics of the resulting problem is described by an impurity model which describes an impurity (c_{α}) coupled to a bath of fermions $(a_{b\mu})$

$$H_{imp} = \sum_{\alpha\beta} \left(E_{\alpha\beta} - \mu \, \delta_{\alpha\beta} \right) c_{\alpha}^{+} c_{\beta} + \sum_{i} \Gamma_{\alpha\beta\gamma\delta} c_{\alpha}^{+} c_{\beta} c_{\gamma}^{+} c_{\delta} + \sum_{b\mu} \epsilon_{b\mu} \, a_{b\mu}^{+} a_{b\mu}$$
$$+ \sum_{k} \left(V_{b\mu,\alpha} \, a_{b\mu}^{+} c_{\alpha} + h.c. \right) \qquad (2.2)$$

From the impurity model we can obtain all the local correlation functions, since by construction the local lattice Green's functions are identical to the impurity Green's function $\hat{G} = (G_{\alpha,\beta})$. We use a matrix notation so that the local Green's function is given by

$$G_{\alpha,\beta}(\tau - \tau') = -\langle T_{\tau} \, c_{\alpha}(\tau) c_{\beta}^{+}(\tau') \rangle \qquad (2.3)$$

This should be viewed as a functional of the parameters $\epsilon_{b\mu}$ and $V_{b\mu,\alpha}$. To determine these parameters we construct the "Weiss field" which describes the effect of the rest of the electrons on the selected cell, $\hat{G}_{0}^{-1}(i\omega_{n}) = (i\omega_{n} + \mu) \hat{I} - \hat{E} - \left(\sum_{b\mu} \frac{V_{b\mu,\alpha} V_{b\mu,\beta}}{i\omega_{n} - \epsilon_{b\mu}} \right)$, and the self energy of the impurity, $\hat{\Sigma}(i\omega_{n}) = \hat{G}_{0}^{-1}(i\omega_{n}) - \hat{G}^{-1}(i\omega_{n})$, viewed as a functional of $\epsilon_{b\mu}$ and $V_{b\mu}$. These parameters are determined by requiring that the bath and the local degrees of freedom describe the electrons in the original lattice problem. Namely we can construct the local Green's function from the lattice Green's function obtained by adding a k independent self energy to the non interacting lattice Green's function (obtained from 2.1 by setting the interaction terms to zero) or from the impurity model.

$$\hat{G}(i\omega_n) = \sum_k \left((i\omega_n + \mu)\hat{I} - \hat{t}(k) - \hat{\Sigma}(i\omega_n) - \hat{E} \right)^{-1} \qquad (2.4)$$

The reader will notice many common features between DMFT and the Bragg Williams theory of magnetism. However in fermionic problems a new feature emerges–the cavity field acquires nontrivial *time dependence*, allowing a nonperturbative treatment of *local dynamics*, which proves to be of crucial importance for strongly correlated electrons. In particular, the approach incorporates *incoherent* (inelastic) processes even on this mean-field level, as opposed to most other treatments. As a result, the formulation can be used even in the study of *non-Fermi liquid* metallic phases, for example in extended Hubbard models (Si and Kotliar 1993).

3. Dynamical Mean Field Theory of the Density Driven Mott Transition in Pure Systems

The Mott transition in transition metal oxides has received renewed theoretical and experimental attention. On the experimental side, new compounds have been synthesized (Tokura et al. 1993, Okimoto et al. 1995) and known compounds such as V_2O_3 and $NiSe_{1-x}S_x$ have been studied. On the theoretical side, new insights have been obtained from studying the one band Hubbard model in the limit of large lattice coordination. In this limit the pressure and temperature driven Mott transition as well as the density driven transition can be thoroughly analyzed.

Several quantitative comparisons between the physics of three dimensional transition metal oxides and the one band Hubbard model have already been performed (Kotliar & Kajueter 1996, Rozenberg et al. 1995). For example, the doping dependence of the electronic specific heat, the resistivity and the Hall coefficient in $La_xSr_{1-x}TiO_3$ can be explained by the one band Hubbard model without adjustable parameters after the values of U and D have been extracted from photoemission data (Kajueter et. al. 1996). Similarly, the single band Hubbard model can describe the temperature dependence of both, the optical and the DC-conductivity in V_2O_3 (Rozenberg et al. 1995).

The Mott transition with integer occupation has been the subject of extensive reviews (Georges et al. 1996). Here we focus on some qualitative aspects of the physics of the density driven Mott transition, the emphasis will be on the question: why does the mean field theory work so well for three dimensional transition metal oxides?

We start with a brief discussion of the qualitative content of the mean field theory of the doped Mott insulator. At low temperatures the mean field theory describes a Fermi liquid with a an energy scale (renormalized Fermi energy ϵ_F^*) which is proportional to the doping (i.e. deviation from half filling) δ. In infinite dimensions, the renormalized Fermi energy is proportional to the quasiparticle residue Z which also vanishes linearly in doping, $i.e. \epsilon_F^* = ZD$. In this regime, the linear term of the specific heat is inversely proportional to δ and the Hall coefficient is unrenormalized from its band structure value. The Fermi liquid description is valid up to a temperature scale T_0 that surprisingly scales as $\delta^{\frac{3}{2}}$, and is therefore quite small very close to the Mott transition (Kajueter et. al. 1996).

The qualitative success of the mean field approach when applied to three dimensional transition metal oxides is due to the orbital degeneracy of three dimensional transition metal oxides. Orbital degeneracy causes a close competition between ferromagnetic and antiferromagnetic tendencies. The net spin-spin interaction is a sum of antiferromagnetic and ferromagnetic terms which tend to largely cancel. An illuminating example that can be studied exactly is a two site system was described by Kajueter and Kotliar (1997) mimicking a Ti ion in $LaTiO_3$. The basic scale of the problem is a bandwidth which is of order of 1 eV, but the splitting between different spin configurations turns out to be a much smaller (between 10^-3 and 10^{-4} eV).

If we insist on using a one band model which ignores the orbital degeneracy, to reproduce the gross features of transition metal oxides, one must introduce in the model terms that suppress the tendency towards magnetic order. In infinite dimension, this can be accomplished by choosing lattices with longer range hopping matrix elements which induce magnetic frustration or by adding and additional ferromagnetic interactions to the Hamiltonian to compensate for the antiferromagnetic exchange which is inherent to the Hubbard model on the hyper-cubic lattice. A Hamiltonian of the form:

$$H = -\sum_{ij,\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{J}{d} \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j \qquad (3.1)$$

with an additional ferromagnetic interaction J increasing as a function of x, can serve as a crude caricature of the $La_{1-x}Y_x TiO_3$ system. This compound is ferromagnetic for x near 1 but becomes antiferromangetic at small values of x. (Okimoto et. al. 1995).

While this approach is certainly too crude to describe details of the magnetic ordering, it expresses the fact that the localization tendencies in this system are not caused by, and are largely independent of, the magnetic ordering (which can be either ferromagnetic or antiferromagnetic). In the limit of large dimensions the J term does not affect the one particle properties, so the calculations of the effective mass performed in the absence of this term apply to this model as well. The Hamiltonian (3.1) was used by A. Georges & L. Laloux (1996) to model the Wilson ratio of liquid He_3, and by Obermeier et. al. (1996) to model the magnetic response of cuprate superconductors.

To summarize, the mean field theory works very well in systems where the charge and spin fluctuations are reasonably local. This is the situation in three dimensional transition metal oxides (as a result of orbital degeneracy) and in the disordered systems described in the next section.

While the qualitative success of dynamical mean field theory is easy to understand, the surprising quantitative agreement of this approach as applied to orbital degenerate systems was clarified only recently(Kotliar & Kajueter 1996, Kajueter & Kotliar 1997). It was shown that: the quantitative value of physical quantities such as the effective mass, and the optical gap, near the Mott insulating state with *one electron per site* which had previously been compared with experiments depend weakly on the band degeneracy (the differences are of less than 10 percent). On the other hand the high energy behavior of the spectral functions have a sizable dependence on the number of orbitals per site.

4. The metal to insulator transition in disordered systems: some outstanding puzzles

The presence of disorder adds a new dimension to the metal to insulator transition problem. The continuous nature of the metal to insulator transition was first demonstrated in this class of systems (for a general review of metal insulator transitions see Mott (1990)). As a result of a series of intensive experimental studies a basic picture of the behavior of physical quantities near the transition has emerged. In this section we describe briefly some aspects of the experimental picture which we regard as well established, but which still remain a challenge for the microscopic theory. For more comprehensive reviews of the experimental situation in this field see Paalanen & Bhatt (1991) Sarachik (1995) and v. Lohneyesen (1997).

It is well established the $T = 0$ conductivity vanishes as the transition (i.e. critical dopant concentration in doped semiconductors) is approached from the metallic side. We leave the immediate vicinity of the metal to insulator transition out of this analysis because the extrapolation to zero temperature is problematic (for a good discussion of this point see v. Lòhneysen (1997)). In the region where this extrapolation is unambiguous, the conductivity vanishes in a power law fashion. $\sigma \approx (n - n_c)^\mu$. In uncompensated materials (one electron or hole per dopant ion), the conductivity exponent takes an anomalously small value $\mu \approx 1/2$ (Paalanen et al. 1980). Such a small value of the conductivity exponent proved to be notoriously difficult to explain by any known theory. On the other hand, well compensated doped semiconductors (only partial filling of the impurity band) behave very differently; their conductivity vanishes with an exponent $\mu \approx 1$. Amorphous alloys behave the same way. In the presence of a strong magnetic field the conductivity vanishes with an exponent $\mu \approx 1$, in both compensated an uncompensated semiconductors (Dai et al. 1991, 1992). The presence of spin-orbit (SO) coupling (Dai et al. 1991, 1992) does not seem to be a determining factor for the behavior of the conductivity. Both Si:B (where SO coupling is strong) and Si:P (where SO coupling is weak) behave qualitatively in the same way. Uncompensated doped semiconductors also display an anomalous temperature dependence. In the metallic phase for concentrations not too close to the transition the conductivity *increases* as the temperature is lowered. This behavior can be reversed by applying strong magnetic fields, resulting in a decreasing conductivity at low T.

In our view these anomalies occur over a wide range of concentrations and are *not* restricted to a tiny critical region in the vicinity of the transition. For example, the anomalously small value of the conductivity exponent $\mu \approx 1/2$ describes the data all the way to $n \approx 4n_c$! It is then natural to conclude that the observed behavior should not be identified with an asymptotic critical behavior associated with a narrow critical region. Rather, it should be described by an appropriate *equation of state*, that is expected to follow from a relevant *mean-field* description of the problem. We also emphasize that the anomalies are associated with *uncompensated* systems, where we expect the effects of electronic correlation to be the strongest. It is thus natural to approach the problem from a DMF perspective. In this picture, many of the above features, but in particular the compensation (filling) dependence follow naturally.

In contrast to the transport properties, the thermodynamic quantities χ and

γ vary smoothly (Paalanen et al. 1988) as a function of concentration across the transition, and seem to diverge at low temperatures both on the insulating and on the metallic side of the transition. The NMR experiments (Paalanen et al. 1985, Alloul & Dellouve 1987) portray a strongly inhomogeneous picture. There is a wide distributions of Knight shifts on the Phosphorus sites. As the transition is approached a large number of sites acquire knight shifts that are larger than the measurable range indicating the formation of local moments. The knight shift on Si is a smoother function of concentration(Stoddart et al. 1992) suggesting that the metal insulator transition takes place in the phosphorus impurity band.

Underlying this experimental picture is a broad distribution of energy scales which makes the metal-insulator transition in disordered systems very different than in the clean case. In addition, this behavior reflects unusually developed *spatial fluctuations* of the electronic system. While such behavior does not normally occur in ordinary metals, it is a natural consequence of the incipient *localization* of the electronic states – which by definition cannot happen in a uniform fashion.

5. Statistical DMF theory

We have argued that in presence of disorder, the situation is qualitatively more complex than in the clean limit. Clearly, it is necessary to extend the DMF ideas in order to capture the crucial effects of disorder – the spatial fluctuations of the order parameter. In the following we present a simple pedagogical derivation of the statistical DMF theory, and discuss some of its main features.

We follow an approach very similar to the Thouless-Anderson-Palmer (1977) formulation of the mean field theory of spin glasses. Specifically, we treat the correlation aspects of the problem in a dynamical mean-field theory fashion, but allow *spatial variations* of the order parameter in order to allow for Anderson localization effects. The theory is then exact in the noninteracting limit, and reduces to the standard dynamical mean field theory in absence of disorder. The approach can be applied to any lattice model of interacting fermions. For simplicity, we consider a simple single-band Hubbard model with random site energies given by the Hamiltonian

$$H = \sum_{ij}\sum_{\sigma}(-t_{ij} + \varepsilon_i \delta_{ij})c^{\dagger}_{i,\sigma}c_{j,\sigma} + U\sum_i c^{\dagger}_{i,\uparrow}c_{i,\uparrow}c^{\dagger}_{i,\downarrow}c_{i,\downarrow}. \qquad (5.1)$$

Following the general spirit of the DMF theory, we focus on a particular site i of the lattice, and integrate all the other sites. This procedure is formally exact, but the resulting local effective action takes an arbitrarily complicated form (Dobrosavljević & Kotliar 1994), containing n-point vertices of all orders. However, within the DMF approach, one retains only the contributions *quadratic* in Fermion fields, and the local effective action assumes the form

$$S_{eff}(i) = \sum_{\sigma}\int_o^{\beta}d\tau\int_o^{\beta}d\tau' c^{\dagger}_{i,\sigma}(\tau)(\delta(\tau - \tau')\,(\partial_{\tau} + \varepsilon_i - \mu)$$

$$+\Delta_{i,\sigma}(\tau,\tau'))c_{i,\sigma}(\tau') + U\int_o^{\beta}d\tau n_{i,\uparrow}(\tau)n_{i,\downarrow}(\tau). \qquad (5.2)$$

Here, we have used functional integration over Grassmann fields $c_{i,\sigma}(\tau)$ that rep-

resent electrons of spin σ on site i, and $n_{i,\sigma}(\tau) = c_{i,\sigma}^\dagger(\tau)c_{i,\sigma}(\tau)$. The *"hybridization function"* $\Delta_i(\tau,\tau')$ is given by

$$\Delta_i(\omega_n) = \sum_{j,k=1}^{z} t_{ij}^2 G_{jk}^{(i)}(\omega_n). \tag{5.3}$$

The sums over j and k runs over the z neighbors of the site i, and

$$G_{jk}^{(i)}(\omega_n) = < c_j^\dagger(\omega_n)c_k(\omega_n) >^{(i)} \tag{5.4}$$

are the lattice Green's functions evaluated with the site i removed. In general, these objects can be expressed through ordinary lattice Green's function as

$$G_{jk}^{(i)} = G_{jk} - \frac{G_{ji}G_{jk}}{G_{ii}}. \tag{5.5}$$

We emphasize that the above construction is carried out for a *fixed realization* of disorder defined by a given set of random site energies $\{\varepsilon_i\}$. The DMF truncation, which keeps only the quadratic contributions to the effective action is *exact* for:

(A) infinite coordination $(z \to \infty)$ (Dobrosavljević & Kotliar 1993, 1994), or

(B) non-interacting electrons for arbitrary coordination (Anderson 1958).

Note that in the case (A) the sum in the definition of $\Delta_i(\omega_n)$ runs over infinitely many neighboring sites, so that the hybridization function is replaced by its *average value*. As a result, the all the spatial fluctuations in the "cavity" representing the environment of a given site are suppressed, prohibiting Anderson localization effects. For noninteracting electrons, the resulting theory reduces to the well known "coherent potential approximation" (Elliott et al. 1974).

Since one of the main goals of the statistical DMF theory is to incorporate Anderson localization effects, we concentrate on finite coordination lattices. In this case, Δ_i can be considered to be a *functional* of the lattice Green's functions G_{jk}, evaluated for fixed disorder, i. e.

$$\Delta_i = \Delta_i [G_{jk}]. \tag{5.6}$$

At strong disorder, Δ_i will exhibit pronounced fluctuations from site to site, reflecting a distribution of local environments "seen" by the electrons.

Finally, in order to obtain a closed set of DMF self-consistency conditions, we need to specify a procedure that relates the lattice Green's functions G_{jk} to the solution of the local dynamical problem, as defined by the local effective action $S_{eff}(i)$. We first note that the local action $S_{eff}(i)$ is identical to that describing an Anderson impurity (AI) model (Anderson 1961, Hewson 1993) embedded in a sea of conduction electrons described by a hybridization function $\Delta_i(\omega_n)$. The solution of this AI model then uniquely defines the corresponding self energy Σ_i, which is given by

$$\Sigma_i(\omega_n) = i\omega_n + \mu - \varepsilon_i - \Delta_i(\omega_n) - (G_{ii}^{loc}(\omega_n))^{-1}, \tag{5.7}$$

where the local Green's function

$$G_{ii}^{loc}(\omega_n) = < c_i^\dagger(\omega_n)c_i(\omega_n) >_{loc}, \tag{5.8}$$

is evaluated with respect to the local effective action $S_{eff}(i)$.

Next, we follow an "exact eigenstate" strategy, and define the "bare" lattice Green's functions G_{ij}^o as the exact lattice Green's functions evaluated for the same realization of disorder $\{\varepsilon_i\}$, in absence of interactions. The "full", i. e. interaction-renormalized lattice Green's functions are within statistical DMF theory then defined by

$$G_{ij} = G_{ij}^o[\varepsilon_i \to \varepsilon_i + \Sigma_i(\omega_n)], \qquad (5.9)$$

closing the set of DMF self-consistency conditions.

We emphasize that a similar relationship relates the *exact* interaction-renormalized lattice Green's functions to their noninteracting counterparts. However, in the exact formulation, the self energies describing the interaction renormalizations are in general *nonlocal in space*, as well as in frequency. Having this in mind, we can describe the statistical DMF theory as a requirement for these interaction dependent self energies to assume a strictly *local* character.

For an arbitrary lattice, an iterative procedure for solving the above set of statistical DMF equations could be obtained by

(i) making an initial guess for the form of $\Delta_i(\omega_n)$,
(ii) solving the corresponding AI models on every lattice site,
(iii) use the resulting Σ_i-s to calculate the full lattice Green's functions,
(iv) calculate the new values of $\Delta_i(\omega_n)$ and go back to step (ii).

This procedure can be carried out for an arbitrary lattice in any dimension, but the procedure can be fairly time consuming due to the need to compute all the off-diagonal components of the lattice Green's functions G_{ij}. However, similar computations have already been carried out to study the interplay of correlations and disorder in a Hartree-Fock (HF) approach (Yang & MacDonald 1993). Interestingly, such a lattice HF treatment for a fixed disorder realization can be obtained as a further simplification of the statistical DMF theory, if the local Anderson impurity models are themselves solved at the same level. Of course, an exact solution of the statistical DMF equations goes well beyond such a HF treatment, since it can describe *inelastic* processes, which are expected to be of particular importance at finite temperature and in metallic non Fermi liquid phases.

In practical terms, it is important to identify specific models where the solution of the statistical DMF equations can be simplified. The situation is particularly simple in the case of a Bethe lattice (Cayley tree). Because the absence of loops on such lattices, only *local* Green's functions $G_{jj}^{(i)}(\omega_n)$ appear in the expression for $\Delta_i(\omega_n)$. Furthermore, in this case the objects $G_{jj}^{(i)}(\omega_n)$ can be computed from a local action of the form *identical* as in Eq. (5.2), *except* that in the expression for $\Delta_j(\omega_n)$, the sum now runs over $z - 1$ neighbors, excluding the site i. We thus conclude that the objects $G_{jj}^{(i)}(\omega_n)$ are related by a *stochastic* recursion relation, that involves solving Anderson impurity models with random on-site energies ε_i. In the non-interacting limit, the recursion relations can be written in close form, and reduce to the exact solution of the disordered electrons on a Bethe lattice (Abou-Chacra et al. 1971).

6. Order parameters for the metal to insulator transition: the disordered case

In attempting to describe any phase transition, a crucial step is to identify appropriate *order parameters* that can characterize the qualitative differences between the different phases of the system.

Since the basic focus of the dynamical mean field approach is the one particle Green's function, it is useful to write down an explicit expression for the Greens function of a lattice system with a one body Hamiltonian H_{ij} and a general two body interaction term in terms of a self energy $\Sigma_{ij}(i\omega)$.

$$[G^{-1}(\omega_n)]_{ij} = [\delta_{ij}i\omega_n - H_{ij} - \Sigma_{ij}(\omega_n)]. \tag{6.1}$$

Here, we have used a matrix notation, for a fixed realization of disorder, so that the self energy $\Sigma_{ij}(\omega)$ describes the interaction induced renormalizations of the Green's function. A quasiparticle picture emerges under a fairly general assumptions of regularity of the interaction self energy at low frequencies. In this case

$$\Sigma_{ij}(\omega) \approx \Sigma_{ij}(0) + ([Z^{-1}]_{ij} - 1)\omega_n + O(\omega_n^2). \tag{6.2}$$

and the Greens function at low frequencies assumes a very transparent form

$$G(\omega_n) = \sqrt{Z}G^{QP}(\omega_n)\sqrt{Z} \tag{6.3}$$

with the quasiparticle Green's function defined as

$$[G^{QP}]^{-1} = \omega_n I - \sqrt{Z}(H + \Sigma(0))\sqrt{Z}. \tag{6.4}$$

Introducing the low energy eigenvalues of the quasiparticle Hamiltonian E_n and their corresponding eigenvector $|n>$, we can write

$$G(x, x') \approx \sum_n \frac{< x|\sqrt{Z}|n >< n|\sqrt{Z}|x' >}{(\omega - E_n)}. \tag{6.5}$$

So far we have just repeated the derivation of the disordered Fermi liquid framework of dirty metals (Castellani et al. 1987). In that reference those concepts were used to interpret the field theoretical coupling constants of Finkelshtein's non linear sigma model in terms of Fermi liquid parameters. Implicit in that framework was the assumption that the spatial fluctuations, or the sample to sample fluctuations were not too large. This assumption is valid for weak disorder. The main advance of the dynamical mean field approach is the ability to deal with strong spatial fluctuations.

The results of the next section indicate very different behavior for typical and average quantities, reflecting large spatial fluctuations. These differences may be the source of the finite scale divergences that were encountered in the field theoretical approach (Finkhelstein 1983, 1984) which, from the very begining, carries out an average over the disorder.

We now use the previous developments to introduce the order parameters which are relevant to the DMF theory. We begin with defining the local density of states at zero frequency

$$\rho_i = -\frac{1}{\pi}ImG_{ii}(0+), \tag{6.6}$$

and the corresponding local quasiparticle density of states

$$\rho_i^{QP} = -\frac{1}{\pi}ImG_{ii}^{QP}(0+).$$
(6.7)

Their ratio defines the second order parameter

$$Z_i = \frac{\rho_i}{\rho_i^{QP}}.$$
(6.8)

which could be dubbed the local quasiparticle weight. In the DMF framework, all the previous equations simplify because the self energy is local ($\Sigma_{ij}(\omega_n) = \delta_{ij}\Sigma_i(\omega_n)$) and Z_i can directly be calculated from the expression

$$Z_i = \left[1 - \frac{\partial}{\partial\omega}Re[\Sigma_i(\omega_n)]|_{\omega_n=0+}\right]^{-1}.$$
(6.9)

When these parameters are mostly uniform, i.e. site independent their averages are precisely two of the coupling constants in the field theoretical approach of Finkelshtein. In the statistical mean field approach we focus instead on whole distributions (or on typical values) of these parameters.

We now turn to the physical interpretation of the order parameters, or more precisely their statistical distribution. The low energy physics is described by two parameters, ρ_i and Z_i, which are associated with the height and the width of the resonance in the spectra of the local impurity problem. Physically, ρ_i can be interpreted as a the density of states for adding or removing and electron from a specific site; Z_i is related to the energy scale (or timescale) over which the quasiparticle picture applies. On the metallic side of the transition, the electron behaves as a local magnetic moment up to a time scale proportional Z_i^{-1}, but as a delocalized quasiparticle over longer timescales. The vanishing of Z_i signals the conversion of quasiparticle degrees of freedom into local moments, which takes place at the Mott transition.

To gain further insight into the physical content of these order parameters, we concentrate on transport properties. The fundamental difference between a metal and an insulator is defined by the ability of the electron to leave a given lattice site – to delocalize. In early work (Anderson 1958) Anderson pointed out that, at least for noninteracting electrons, this property could be examined by evaluating the *lifetime* of an electron on a given site. Very generally, the inverse lifetime simply measures the width of the the local resonance level. We thus expect

$$\frac{1}{\tau_i} \sim \text{Im}\,(G_{ii}(0+))^{-1}.$$
(6.10)

Within DMF, the local Green's function takes the form

$$G_{ii}(\omega_n) = [i\omega_n + \mu - \varepsilon_i - \Delta_i(\omega_n) - \Sigma_i(\omega_n)]^{-1},$$
(6.11)

and since for Anderson impurity models (see for example Hewson 1993) $\text{Im}\,\Sigma_i(0+) = 0$, we conclude that the desired local lifetime can be directly related to the local hybridization function as

$$\frac{1}{\tau_i} \sim \text{Im}\,\Delta_i(0+).$$
(6.12)

We thus expect $\text{Im}\,\Delta_i(0)$ to vanish whenever the system is insulating, but to

remain finite in a metallic regime. We emphasizing that the *same* qualitative behavior should be expected for the local density of states (LDOS) ρ_i as can be readily seen from Eq. (5.3). We can thus use the LDOS as an order parameter that discriminates a metal from an insulator. In a random system, ρ_i will fluctuate from site to site, and we need a whole distribution function to fully characterize the approach to the transition.

In particular, in the Mott insulator, there is a "hard" gap of order U on every lattice site, so even the *average* DOS discriminates the Mott insulator from the metal. The situation is more complex as the Anderson insulator is approached. Here, the local spectrum is composed of a few delta-functions (discrete, bound states), separated by gaps, but the average DOS remains *finite*. In contrast to the Mott insulator, in the Anderson insulator the sizes and positions of the local gaps *fluctuate*, but in both cases a *typical* site has a gap at the Fermi energy. A natural order parameter is therefore the *typical* DOS, that is represented by the *geometric average*

$$\rho_{typ} =< \rho >_{geom}= \exp\{< \ln \rho_i >\}. \tag{6.13}$$

This quantity is found to *vanish* at the Anderson transition, in contrast to the *average* DOS, which is not critical.

On the metallic side of the transition, the distribution function of a second quantity, the local quasiparticle (QP) weight, is necessary to characterized the low energy behavior near the transition. Important information is obtained from the typical value of the random variable Z_i, defined as

$$Z_{typ} = \exp\{< \ln Z_i >\}, \tag{6.14}$$

which emerges as a natural order parameter from previous studies of the Mott transition.

Finally, we define the *averaged* QP DOS by

$$\rho_{av}^{QP} =< \rho_i^{QP} > . \tag{6.15}$$

This object is very important for thermodynamics, since it is directly related to quantities such as the specific heat coefficient $\gamma = C/T$, or the local spin susceptibility χ_{loc}. Note that in absence of interactions, ρ_{av}^{QP} reduces to the usual (algebraic) average DOS, which is not critical at a $U = 0$ Anderson transition, but it is strongly enhanced in the vicinity of the Mott transition.

It is instructive to discuss the behavior of these order parameters in the previously studied limiting cases. In the limit of large lattice coordination, the spatial fluctuations of the bath function $\Delta_i(\omega_n)$ are unimportant, and there is no qualitative difference between typical and average quantities. In the Mott insulating phase of a periodic solid, there is a gap in the density of states, while there is a finite density of states on the metallic side of the transition. As the MIT is approached from the metallic side, ρ_{typ} remains finite, but Z_{typ} is found (Dobrosavljević & Kotliar 1993,1994) to linearly go to zero.

Another well studied limit is that of noninteracting electrons on the Bethe lattice, which is known (Abou-Chacra et al. 1971, Efetov 1987, Mirlin & Fyodorov 1991) to display an Anderson transition. The average DOS is *finite* both in the insulating and in the metallic phase, and is non critical at the transition. Similarly, by definition $Z_{typ} = 1$ in this noninteracting limit, so it also remains non critical. On the other hand, the typical density of states ρ_{typ} is finite in the metal and

zero in the Anderson insulator. This quantity is critical, and is found to vanishes exponentially with the distance to the transition.

The definitions of the the order parameters that we have proposed are *not restricted* to the statistical DMF framework, which is simply used as a specific calculational scheme. The same definitions can in principle be used in other approaches that can calculate local *unaveraged* values of the local DOS $\rho_i(\omega_n)$ or the local part of the frequency dependent self energy $\Sigma_{ii}(\omega_n)$ due to the interactions.

7. Results

The dynamical mean field theory maps the insulating phase of the model onto a collection of Anderson impurity models each one of them is embedded in an insulating bath. An Anderson impurity in an insulator, away from particle hole symmetry, can either have a doublet ground state when the coupling to the enviroment is weak or a singlet ground state when the coupling to the bath exceeds a critical value. In this strong coupling limit (Dobrosavljević & Kotliar 1992*b*), a *bound state* is pulled from the continuum formed by the bands of the insulator. From these general consideration, we obtain a two fluid picture of the insulating phase: there are sites which have a local moment down to zero temperature while other sites quenched their spin by exchanging it with a strongly coupled neighbor.

The number of sites in a doublet state, in the insulating phase of the system form "Mott droplets" . Based on our experience on the Mott transition in clean systems, we expect a larger density of states when the system undergoes a metal to insulator transition into an insulating phase with a large number of doublets. This result in at least two different regimes depending on whether the insulating phase has a high or low concentration of sites in doublet states.

We have considered a $z = 3$ (Dobrosavljević & Kotliar 1997). Bethe lattice, in the limit of infinite on-site repulsion U at $T = 0$ and fixed average density n in the presence of a uniform distribution of random site energies ε_i of width W. To calculate the probability distributions of ρ_j and Z_j we used a simulation approach, where the probability distribution for the stochastic quantity $G_j^{(i)}(\omega_n)$ is sampled from an ensemble of N sites, as originally suggested by Abou-Chacra et al. (1971). In order to solve Anderson impurity models for given bath functions $\Delta_j(\omega_n)$ we use the slave boson (SB) mean-field theory (Barnes 1977, Read & Newns 1983, Coleman 1987), which is known to be qualitatively and even semi-quantitatively correct at low temperature and at low energies. In agreement with heuristic arguments, we expect the results to be a strong function of the density n. In order to illustrate this behavior, we have carried out explicit calculations for both low electron density $n = 0.3$, and high electron density $n = 0.7$ (i.e. close to half filling). We emphasize that in the clean limit ($W = 0$) the behavior is qualitatively identical for the two values of the density, and the system remains metallic, with only the value of the effective quasiparticle mass $m^* \sim Z^{-1}$ being a function of n. Qualitatively different behavior is found as the disorder is introduced.

We first describe the evolution of the probability distribution of the local quasi-particle weights Z_i, as the disorder is increased. The sites with $Z_i \ll 1$ represent (Milovanović et al. 1989, Dobrosavljević & Kotliar 1993,1994) disorder-induced
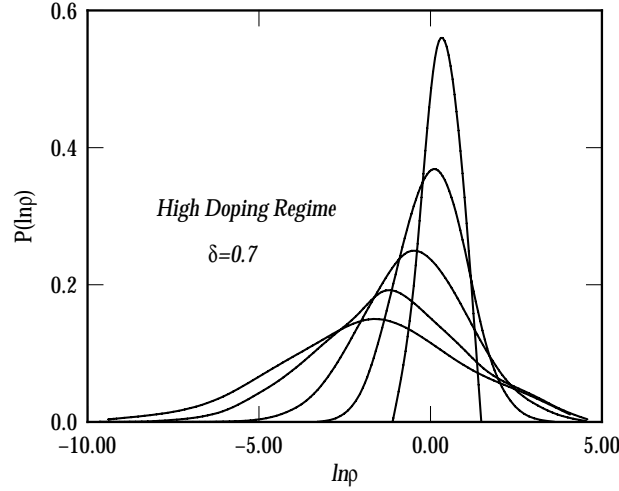
Figure 1. DOS statistics in the low filling (high doping) regime. The full distributions $P(\ln \rho)$ are presented for increasing amounts of disorder. We find that the *maximum*, i. e. $< \ln \rho >$ shifts, as the transition is approached. Note also the extremely large *width* of the distribution, so that ρ now spans many orders of magnitude.

local magnetic moments, and as such will dominate the thermodynamic response (see the definition of ρ_{QP}). For weak disorder we expect relatively few local moments and the quasiparticle weight distribution is peaked at a finite value. As the disorder is increased, the distribution of Z_i-s broadens. At a critical value of the disorder $W = W_{nfl}$, the form of this distribution assumes a singular form (Bhatt & Fisher 1992, Dobrosavljević et al. 1992a, Miranda et al. 1996, 1997) , leading to anomalous thermodynamic response characterized by a diverging magnetic susceptibility χ and specific heat coefficient γ. This behavior was found both for high and low density, in remarkable agreement with experiments carried out on for uncompensated and compensated doped semiconductors. Interestingly, a similar transition to a non Fermi liquid metallic phase, well before the MIT, has been found from the field-theoretical approaches in $2 + \varepsilon$ dimensions (Finkelshtein 1983,1984; for a review of subsequent work on this issue, see the review by Belitz & Kirkpatrick (1994)).

As the level of disorder is increased further, a metal insulator transition is reached at the second critical value of disorder $W = W_c$. At this point, the typical quasiparticle weight Z_{typ} vanishes, a behavior reminiscent of the clean Mott transition. While this behavior is found at both high and low density, the examination of the second order parameter ρ_i reveals striking density dependence in the vicinity of the transition. The difference are most clearly displayed by plotting the evolution of the *distribution function* $P(\rho_i)$ as a function of doping. At low filling $n = 0.3$, we find that the with of this distribution becomes extremely large, spanning many decades, reflecting huge spatial fluctuations of the electronic wave-functions, as shown in Fig. 1. At the same time, the most probable value ρ_{typ} is found to dramatically decrease, vanishing linearly with the distance to the transition. In contrast to this result, a very different behavior is found at high density $n = 0.7$. As we can see from Fig. 2, in this case the distribution *width* again broadens, albeit in a somewhat slower fashion, as the transition is
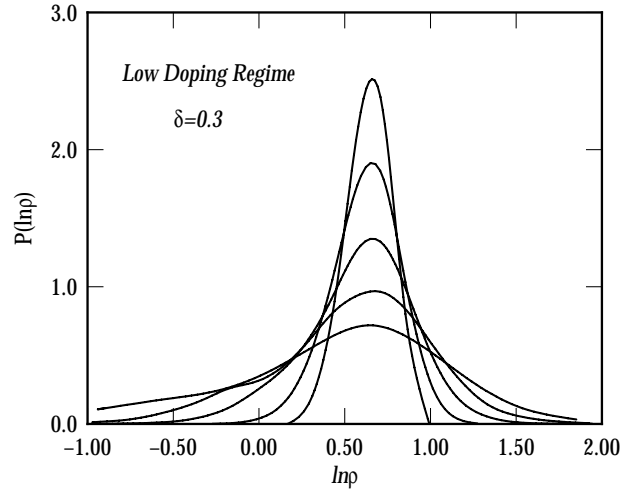
Figure 2. DOS statistics in the high filling (low doping) regime. W show the probability distribution for $\ln \rho$, as a function of disorder. We clearly see that while the distribution broadens, $< \ln q > \approx cons.$

approached. However, in this case the most probable value ρ_{typ} is only weakly modified with increasing disorder, and is found to approach a *finite* value at the transition. Recalling that the statistics of ρ_i are intimately related to *transport*, our results strongly suggest that kinetic coefficients such as the conductivity will strongly depend electron filling, as the MIT is approached. These expectations should be confirmed by explicitly calculating the critical behavior conductivity at different values of the density.

Finally, we mention an important feature of the insulating state in presence of both the strong electronic correlation and disorder. By explicit calculations of both the average and the typical density of states we have demonstrated that the introduction of disorder, fills the Mott gap with localized electronic states. The average DOS is therefore finite in the insulator. Nevertheless, the MIT still retains a definite Mott character, with a finite fraction of electrons turning into localized magnetic moments, and the typical quasiparticle weight Z_{typ} vanishing at the transition. Our results explicitly show that the metal insulator transition in presence of both interactions and disorder is a qualitatively new type of transition, having well defined signatures of *both* the Anderson and the Mott route to localization.

8. Conclusions

The metal to insulator transition continues to be one of the central problem in condensed matter physics. Building on the fundamental concepts introduced by Mott and Anderson there have been several attempts at the construction of a microscopic theory. We have summarized in this contribution some aspects of the dynamical mean field approach to this problem.

Deeply rooted in local physics, it combines the chemical and physical aspects of the problem. We regard the construction of a mean field theory as an essential first step before a more complete treatment including Gaussian and non linear

fluctuations is carried out. In the clan limit the DMF description of the Mott transition has already given insights into puzzling aspects of transition metal oxide physics.

Since the approach emphasizes the local environment, it has a conceptually very simple extension to the disorder case: the statistical dynamical mean field theory. The theory explicitly incorporates both the Mott and the Anderson route to localization, and thus provides a consistent description of the transition, interpolating between the respective limits of no disorder and no interaction. This key feature seems to be missing in a recent field theoretical formulation of the Anderson-Mott transition (Kirkpatrick & Belitz 1994, 1995).

The statistical mean field theory reproduces many remarkable features of doped semiconductors. A transition to a Griffiths phase (Bhatt and Fisher 1992, Dobrosavlevic et. al. 1992, Lakner et. al. 1994) where local moments coexist with conduction electrons down to arbitrary low temperature precedes the true metal to insulator transition. The local properties such as the density of states depend in a distinct fashion on the level of doping (compensation). The metal to insulator transition in the low doping region (uncompensated) has a larger typical density of states and is closer to a Mott transition than the corresponding transition at larger doping levels (compensated situation). The latter contains ingredients from both the Anderson and the Mott transition.

There are several issues that deserve further investigation. A detailed study of the transport properties has to be carried out. One should also elucidate the interplay of the short wavelength fluctuations with long wavelength modes. The latter are presumably described by the non linear sigma model approaches that have been investigated near two and six dimensions. A second element still missing form the mean field theory is the inclusion of short range magnetic correlations. In our view these are the most pressing problems that need to be address on the road to a comprehensive theory of the Mott-Anderson transition.

Acknowledgements:

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