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Landau theory of the Mott transition in the fully frustrated Hubbard model in infinite dimensions

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Abstract. We discuss the solution of the Mott transition problem in a fully frustrated lattice with a semicircular density of states in the limit of infinite dimensions from the point of view of a Landau free energy functional. This approach provides a simple relation between the free energy of the lattice model and that of its local description in terms of an impurity model. The character of the Mott transition in infinite dimensions, (as reviewed by Georges, Kotliar, Krauth and Rozenberg, Rev. Mod. Phys. **68**, 13 (1996)) follows simply from the form of the free energy functional and the physics of quantum impurity models. At zero temperature, below a critical value of the interaction U, a Mott insulator with a finite gap in the one particle spectrum, becomes unstable to the formation of a narrow band near the Fermi energy. Using the insights provided by the Landau approach we answer questions raised about the dynamical mean field solution of the Mott transition problem, and comment on its applicability to three dimensional transition metal oxides.

PACS. 71.30.+h Metal-insulator transitions and other electronic transitions – 71.27.+a Strongly correlated electron systems; heavy fermions – 71.28.+d Narrow-band systems; intermediate-valence solids

1 Introduction

The idea of understanding lattice models of correlated electrons from a local perspective is a very intuitive one, and has been used repeatedly in many body physics over the years.

A well known example is the heavy fermion problem, where a broad band of conduction electrons interacts with more localized f electrons, *via* a magnetic Kondo exchange interaction. In the early days of the heavy fermion problem, a great deal of understanding was obtained by considering the screening of an isolated spin by a sea of conduction electrons, *i.e.* studying the single site Kondo effect, and then regarding the Kondo lattice as a collection of Kondo impurity models.

This view had some successes in explaining the origin of a non perturbative energy scale, the Kondo temperature, where the properties of the system change dramatically (for instance the susceptibility crosses over from Curie to Pauli behavior).

In an early paper, however, Nozières [1] pointed out, that the physics of the lattice problem is more complex than the single impurity problem since at least in the limit of low density of conduction electrons, there are not enough itinerant electron spins, to screen all the impurity spins in the lattice. In this case one cannot regard the lattice as a collection of single Kondo impurities. This issue is now known as Nozières' exhaustion problem. This is perhaps one of the earliest warnings that single impurity thinking can be misleading if it is applied uncritically to lattice problems involving a correlated degree of freedom at each site.

In the context of transition metal oxide physics, an impurity view of the d-electron spectral function was put forward by Zaanen, Sawatzky and Allen [2] and by Fujimori, Minami and Sugano [3], and led to a qualitative description of the spectra in these systems. In the light of the modern developments of the dynamical mean field theory, we would regard the early applications of impurity views to the physics of f and d electron systems as local (but not self consistent) impurity approximations to lattice models.

The last ten years have witnessed dramatic progress in the theory of correlated electron systems. The modern developments of a dynamical mean field theory [4] and its implementation *via* mappings onto impurity models [5,6], now allows us to use impurity models supplemented by a self consistency condition to study lattice models. The results are exact in the well defined limit of infinite lattice coordination [7].

We are now in a much better position to gauge the reliability of the arguments based on the Local Impurity Approximation by studying lattice models in the limit of large lattice coordination using Local Impurity *Self-Consistent* Approximations. If the self consistency condition does not play an important role, naive impurity

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based arguments are reliable. Since the dynamical mean field theory is exact in the limit of large lattice coordination, we can also understand which physical elements are absent in this limit (a most notable example is the feedback of the magnetic correlations on the single particle properties) and assess in which physical circumstances it provides reliable guidance to the physics of three dimensional real materials.

This paper is devoted to the problem of the Mott transition, *i.e.* the interaction driven metal insulator transition, and its description in terms of quantum impurity problems. We consider a half filled Hubbard model on a fully frustrated lattice [8] with a semicircular density of states in the limit of infinite lattice coordination. The term frustration refers to the degree of magnetic frustration in the parent Mott insulator.

Reference [8] reported that this model exhibits a Mott transition at a critical value of the ratio $\frac{U}{t}$. The correct description of the destruction of the metallic state at zero temperature as the Mott transition is approached by increasing U, was proposed by Zhang, Rozenberg and Kotliar (ZRK) [9] on the basis of the iterated perturbation theory (IPT) [5].

The calculations of ZRK revealed that while the approach to the Mott transition from the metallic side is driven by a collapse of the Fermi energy, as in Brinkman Rice [10] theory, it also exhibits new unusual features. The metal disappears into an insulator with a preformed (finite) Mott Hubbard gap. We will refer to this as the semicontinuous scenario to be distinguished from the competing, bicontinuous, scenario where the gap closes at the same point where the quasiparticle weight vanishes as discussed in page 30.

The complete picture, of the Mott Hubbard transition in infinite dimensions emerged with the work of Georges and Krauth [11,12] and Rozenberg *et al.* [13,14], who described the destruction of the insulating state at zero temperature, the first order finite temperature metal insulator transition, and the crossovers that govern the behavior above the finite temperature second order critical point. They produced a wealth of physical results, which were in surprisingly good qualitative agreement with experimental data [15]. The zero temperature scenario for the destruction of the metallic state was put on a firm footing by the development of the projective self consistent method [16]. This method overcame the difficulties associated with the presence of several energy scales, which had beset earlier treatments.

In spite of these developments, several questions about the solution of the Hubbard model in large dimensions were raised [17–20] and numerical studies were undertaken in an attempt to answer them [21–23]. This renewed interest and in particular the insightful questions of Nozières [19], motivates us to reexamine the problem from a new perspective, that of a Landau-like free energy functional of a "metallic order parameter", generalizing an approach used in our earlier studies of interacting random models with Dobrosavlevic [24].

Our discussion highlights the peculiar character of the Landau theory of the metal to insulator transition. This singular dependence of the mean field free energy on the metallic order parameter (and not the specific approximations such as IPT, QMC or exact diagonalization of finite systems which were used in the early studies of this problem) is responsible for the unusual features of the solution of the Hubbard model in infinite dimensions.

Our aim is partly pedagogical, we use the Landau functional to describe from a new perspective results that were obtained a few years ago. Besides clarifying the existing confusion in the literature of the subject, there is another purpose in writing a pedagogical note, there are not that many solvable models of the Mott transition in dimensions higher than one! We believe that there are still many lessons to be drawn from the solution in the limit of infinite dimensions, that can be of use in tackling more difficult problems, in the field of strongly correlated electron systems. We believe that the Landau-like approach which we advocate in this paper can be valuable in other dynamical mean field studies. Finally, while we believe that the nature of the Mott transition in fully frustrated systems in the limit of infinite dimensions, has been understood at the qualitative level, there still remains a large amount of quantitative work to be done on this problem. Our insights should be a helpful guide to further investigations.

This paper is organized as follows. After setting the notation in Section 2, summarizing the scenario describing the destruction of the metallic state in Section 3. We state the questions raised by this suggestion and describe the alternative (bicontinuous) scenario where the gap closes at the same point where the quasiparticle peak disappears in Section 4. Two technical tools are essential to justify the validity of the semicontinuous scenario, the Landau free energy functional is described in Section 5, and some results of the projective self consistent method are summarized in Section 6. Using these tools, we describe the energetics of the metal insulator transition, inspired by the questions of Nozières [18,19]. The Landau functional, provides us with a concrete bridge between the impurity model and the lattice model allowing us to use our knowledge of Kondo impurity physics to understand the Mott transition problem.

In Section 7, we use the Landau functional to describe the arguments of Fisher, Kotliar and Moeller [25] for the determination of the conditions for U_{c1}, the point where the insulator disappears. Near U_{c1} the physical picture is that of an impurity in a weakly coupled regime, Nozières exhaustion ideas are applicable in this case.

In Section 8 we recall the arguments of Moeller *et al.* [16] for the disappearance of the metal at the critical value U_{c2}. Here, the Mott insulator with a finite gap is indeed unstable towards the formation of a narrow metallic band at the Fermi level. The effective impurity description is in an intermediate coupling regime. From the perspective of our analysis based on a Landau functional, the semicontinuous scenario, *i.e.* the fact that $U_{c1} < U_{c2}$, is an unavoidable consequence of the different behaviors of quantum impurity models in weak and strong coupling limits.

In Section 9 we argue that a more realistic consideration of the magnetic correlations in finite dimension, may change the character of the free energy functional and comment on the relevance of the dynamical mean field theory results to finite dimensional systems.

2 Lattice model and associated impurity Hamiltonian

We consider the Hubbard model on the Bethe lattice in the paramagnetic phase with coordination d and hopping $\frac{t}{\sqrt{\mathrm{d}}}$ at half filling.

$$H = -\sum_{\langle i,j\rangle\sigma} \frac{t}{\sqrt{d}}(c^+_{i\sigma}c_{j\sigma} + \text{c.c.}) + \sum_i U n_{i\uparrow}n_{i\downarrow}.$$

The half bandwidth is given by $D = 2t$ and we will use $D = 1$ as a unit of energy. The kinetic energy per site, K, can always be expressed in terms of the non local Green's function $G_{i,j}$. In the limit of large lattice coordination it can also be expressed in terms of the one particle Green's function:

$$\langle K\rangle = -\frac{1}{N_s}\sum_{\sigma,\langle i,j\rangle\omega} \mathrm{e}^{\mathrm{i}\omega 0^+} G_{i,j}(\mathrm{i}\omega)t_{i,j} = t^2 2T\sum_\omega G(\mathrm{i}\omega)^2. \tag{1}$$

In the limit of large dimensions the total energy per site, $E = \frac{\langle H\rangle}{N_s}$ reduces to:

$$E = T\sum_\omega [(\mathrm{i}\omega+\mu)G(\mathrm{i}\omega) - 1]\mathrm{e}^{\mathrm{i}\omega 0^+} + \frac{1}{2}\langle K\rangle. \tag{2}$$

The interaction energy per site is given by:

$$\langle U\rangle = E - \langle K\rangle = U\langle n_{i\uparrow}n_{i\downarrow}\rangle. \tag{3}$$

As is well known now [5], all the local correlation functions of the model can be obtained from an Anderson impurity model with hybridization function

$$\Delta(\mathrm{i}\omega) = \sum_k \frac{{V_k}^2}{\mathrm{i}\omega - \epsilon_k} \tag{4}$$

provided that $\Delta(\mathrm{i}\omega)$ obeys the self-consistency condition:

$$t^2 G(\mathrm{i}\omega)[\Delta] = \Delta(\mathrm{i}\omega). \tag{5}$$

Here, $G(\mathrm{i}\omega)[\Delta]$ is the Green's function of the SIAM (single impurity Anderson Model)

$$\sum_{K\sigma}\epsilon_K c^+_{k\sigma}c_{k\sigma} + \sum_{\mathrm{K}\sigma} V_k(c^+_{k\sigma}f_\sigma + {f_\sigma}^+ c_{k\sigma}) + U f^+_\uparrow f_\uparrow f^+_\downarrow f_\downarrow = H_{SIAM}. \tag{6}$$

viewed as a functional of the hybridization function $\Delta(\mathrm{i}\omega)$ which is the Hilbert transform of $\sum_k {V_k}^2\delta(\omega-\epsilon_k)$. Equations (2) and (1) express the total energy of the lattice model in terms of the *local* Green's function of the problem. We can therefore express the total energy in terms of the local spectral function $\rho(\omega) = \frac{-1}{\pi}\mathrm{Im}G(\mathrm{i}\omega = \omega + \mathrm{i}\delta)$ using the spectral representation $G(\mathrm{i}\omega_n) = \int \mathrm{d}\omega \frac{\rho(\omega)}{(\mathrm{i}\omega_n - \omega)}$ $= \int \frac{\mathrm{d}\epsilon D(\epsilon)}{(\mathrm{i}\omega_n + \mu - \epsilon - \Sigma(\mathrm{i}\omega))}$ with $D(\epsilon)$ the semicircular lattice density of states:

$$E = \int f(\omega)(\omega+\mu)\rho(\omega) + 2t^2\int\int \mathrm{d}\omega_1\mathrm{d}\omega_2 f(\omega_1)\frac{\rho(\omega_1)\rho(\omega_2)}{\omega_1-\omega_2}. \tag{7}$$

We will work in the grand canonical ensemble with the chemical potential chosen to be equal to $\mu = U/2$. $f(\omega)$ is the Fermi function.

3 Evolution of the spectral function at zero temperature

In this section, we describe the qualitative features of the evolution of the spectral function, as a function of interaction strength U/t which is obtained by solving the mean field equation (5) at zero temperature. These features were discovered in an IPT [9] study by Zhang, Rozenberg and Kotliar.

We start at large U with a paramagnetic insulating solution with a gap $\Delta(U)$. When U is reduced below a critical value of U, denoted by U_{c2}, (with $\Delta_{\mathrm{g}} \equiv \Delta(U_{c2}) \neq 0$) the paramagnetic Mott insulator becomes unstable against the formation of a metallic resonance at zero frequency.

The mathematical description of the ZRK scenario of the evolution of the spectral function when U_{c2} is approached from below is the following:

3.1 $\mathrm{Im}\,G(\omega, U) \neq 0$ for all $|\omega| < \frac{\Delta_{\mathrm{g}}}{2}$ and for all $U < U_{c_2}$ (finite spectral density everywhere in the metallic phase).

3.2 $\lim_{U\to U^-_{c_2}} \mathrm{Im}\,G(\omega, U) = 0$ for fixed ω such that $0 < |\omega| < \frac{\Delta_{\mathrm{g}}}{2}$ (Existence of a finite gap at the Mott transition point).

We now discuss more delicate issues, in which the frequency approaches zero while at the same time, U approaches the critical value U_{c_2}. More specifically, we define $\tilde{w} \equiv \frac{U_{c_2}-U}{U_{c_2}}$ and take the limits $\tilde{w}\to 0$ and $\omega \to 0$ such that $x \equiv \omega/\tilde{w}$ is fixed. This limit defines the scaling functions which were computed in reference [16].

3.3 $\lim_{U\to U^-_{c_2}} \mathrm{Im}\,G(\tilde{w}x, U) \neq 0$, *i.e.* there is a finite density of states at the Fermi level all the way up to the transition. In particular the pinning condition which leaves the density of states at zero frequency unrenormalized is obeyed everywhere in the metallic phase.

3.4 For a generic value of x $\lim_{U\to U^-_{c_2}} \mathrm{Im}\,\Sigma(\tilde{w}x, U)$ is finite. Notice however that since Fermi-liquid theory is valid below the Fermi energy in the metallic phase, for

a fixed value of U below U_{c2}

$$\lim_{\omega\to 0} \mathrm{Im}\Sigma(\omega, U) = 0. \tag{8}$$

3.5 There exists a $x_0 \sim O(1)$ such that

$$\lim_{U\to U_{c2}^-} \mathrm{Im}\Sigma\left(\sqrt{\tilde{w}}x_0, U\right) = \infty. \tag{9}$$

This incipient divergence and its significance was recognized in reference [9]: it represents the precursors of the Hubbard bands in the metallic phase. Its presence is unavoidable, since spectral features resembling the Hubbard bands are already well formed on the metallic side of the transition [5]. The divergence of the self energy occurs outside the Fermi liquid regime and should not be interpreted in terms of quasiparticle scattering. It should be understood as the precursor of the pole found at zero frequency in the paramagnetic insulator phase. This pole indicates that the paramagnetic insulating ground sate, is not smoothly connected to the non interacting Fermi gas.

It is important to stress, that in the metallic phase the density of states does not vanish for energies less than $\frac{\Delta_g}{2}$. This is a simple consequence of the self consistency condition of the dynamical mean field theory. The statement that the Mott Hubbard gap is finite at the Mott transition point, should be understood in terms of the previously described, highly non uniform, limiting procedure.

We stress that the results discussed above, were derived by non perturbative means. The mapping of the Hubbard model in large dimensions, onto the impurity model can be done using the cavity construction [4] which does not involve any expansion in U. Furthermore, to reach the conclusions discussed above, non perturbative treatments of the impurity model and the self consistency condition are required.

In the next section we mention a perturbative expansion, the skeleton expansion, which expresses the self-energy as a power series in U and in terms of the fully renormalized Green's function,

$$\mathrm{Im}\Sigma(U, \omega) = \sum_{\alpha,m} I_{\alpha,m}(\omega). \tag{10}$$

Here, $I_{\alpha,m}$ denotes the contribution of a specific Feynman skeleton graph, labeled α and of order m in the interaction strength U, to the imaginary part of the self-energy evaluated at a frequency ω.

The convergence properties of this series are not well understood [30,31]. Since the Anderson impurity model with a hybridization function which is non vanishing at zero frequency, has a singlet ground state which is a smooth function of U, it may converge for very small U. It is also known that the series diverges when U is sufficiently large and the lattice model supports a paramagnetic insulating phase.

In the ZRK scenario, since the graphs of the the skeleton series for $I_{\alpha,m}(\omega)$ are evaluated in terms of U and G which has a very small spectral weight at low frequencies

$$\lim_{U\to U_{c_2}} I_{\alpha,m}(\omega) = 0 \tag{11}$$

for all $\frac{\Delta_g}{2} > |\omega| > 0$,

But equations (8, 9) imply that the function which the skeleton expansion represents in some form, behaves very differently in various frequency reanges. So even if the skeleton expansion converges pointwise in the open interval $(0, U_{c2})$ the convergence in this interval cannot be uniform. Finally, we notice that exactly at the point U_{c2}, the quasiparticle peak has zero weight. The system is in the paramagnetic insulating phase where the skeleton series is known to diverge.

The lack of uniformity in the frequency domain, is the mathematical manifestation of the collapse of the Fermi energy, as we approach the transition. Below that scale a power series in the interaction has to be well-behaved because at low frequencies the system resembles a correlated metal, which is smoothly connected to the non interacting system by Fermi liquid theorems. At high frequencies, the system resembles a paramagnetic insulator, which has a doubly degenerate ground state at each site. For such a system skeleton perturbation theory is known to diverge, because a doublet cannot be smoothly connected to a singlet ground state.

4 Critiques of the ZRK scenario

Some of the findings in the ZRK paper described in the previous section were expected. For example, the gradual narrowing of the resonance as the Mott transition is approached, is the result of the Brinkman Rice mass enhancement [10]. Other aspects of the ZRK scenario, however, were new counterintuitive and surprising. The instability of a Mott insulator *with a finite gap*, towards metalization was unexpected (previously, such an instability was only expected to take place when the gap was infinitesimal). Also the incipient divergence of the self energy, at a relatively high energy scale $\sqrt{\tilde{w}}D$ had not appeared in earlier slave boson studies.

The alternative scenario for the Mott transition in frustrated systems, is a bicontinuous one (*i.e.* continuous from the metallic and the insulating side) In this scenario the gap closes from the insulating side at the same critical value of the interaction at which the resonance vanishes upon approaching the transition from the metallic side. This bicontinuous scenario was shown to occur within the slave boson formulation of Kotliar and Ruckenstein [26] after including Gaussian fluctuations on top of the mean field theory [27,28] and within a large N model of the metal to charge transfer insulator [28]. The natural extension of this scenario to finite temperatures gives a smooth crossover between a metal and an insulator, excluding a first order phase transition between a metallic and an insulating phase but other extensions are possible [29].

Several authors raised questions about the physical meaning and the internal consistency of the ZRK scenario and raised the possibility [17–20,22] that the alternative, bicontinuous scenario might be realized in the frustrated large d Hubbard model with the semicircular density of states.

Nozières [19] expressed the surprising nature of the evolution of the spectral function at zero temperature in

two different ways. First an energetic argument: if one is near the Mott transition, transfer of a small amount of spectral weight ϵ from high to low energy across a Mott Hubbard gap $\Delta_{\rm g}$ costs $\epsilon\Delta_{\rm g}$ while the kinetic energy gain is only of order $\epsilon^2 D$. For the transition to take place, these two terms have to balance (*i.e.* $\Delta_{\rm g}$ has to be of order ϵD) thus ruling out the possibility of a preformed Mott Hubbard gap.

The second argument makes use of Nozières exhaustion principle (which we interpret in the present context as saying that the Kondo quenching of a spin in a dilute bath of conduction electrons does not result in a substantial energy gain). Near the Mott transition, the ZRK spectral function has very few carriers, while there are many spins. The system is in the exhaustion regime, where very little Kondo energy can be gained, and is therefore unlikely to be energetically stable. Full Kondo compensation, which is necessary to form the resonance, and the Fermi liquid state is unlikely.

Recently Kehrein argued [20], that under the assumption that the sekelton expansion converges pointwise in the open interval $(0, U_{\rm c2})$, the scenario presented in the previous section is inconsistent. From equation (11) he concludes

$$\sum_{\alpha,m} \lim_{U\to U_{\rm c2}} I_{\alpha,m}\left(\omega = x_0\sqrt{\tilde{w}}\right) = 0. \tag{12}$$

He then interchanges the order of the infinite summation and the limiting procedure. Using equation (10) he obtains $\lim_{U\to U_{\rm c2}^-} \Sigma\left(\sqrt{\tilde{w}}x_0, U\right) = 0$ contradicting equation (9).

This exchange of limits, is not allowed, even when the skeleton expansion converges pointwise for all frequencies, and even if the total spectral weight of each graph can be bounded uniformly as is stated in footnote 14 of reference [20].

The exchange of limits is mathematically justified only when the series (10) converges *uniformly*. The skeleton expansion cannot converge *uniformly* as one approaches the Mott transition since it diverges at $U_{\rm c2}$, which in the ZRK picture, is in the paramagnetic insulating phase.

Recently Lange [30] analyzed the soluble strong coupling limit of an Anderson impurity for arbitrary U. He showed explicitly that while the skeleton expansion may fail to converge, particularly, at high frequencies, an IPT-like treatment, gives the exact answer for this model.

The rest of this paper addresses the questions of Nozières. The goal is to explain why at some point it becomes energetically favorable to metallize a paramagnetic insulator while it still has a finite gap. We also clarify how the energetics of lattice models can be estimated using impurity models. For these purposes, we develop a framework based on a Landau like functional to connect lattice and impurity physics in the next section.

5 Landau functional

To address the questions about energetics and to illuminate the analogies and differences between the dynamical mean field theory and the more standard Landau theory of phase transitions it is useful to introduce the free energy functional [24]:

$$F_{\rm LG}[\Delta] = -T\sum_{\omega} \frac{\Delta(\mathrm{i}\omega)^2}{t^2} + F_{\rm imp}[\Delta]. \tag{13}$$

where $F_{\rm imp}$ is the free energy of the impurity model defined by (6) which can be represented as a functional integral:

$$\mathrm{e}^{-\beta F_{\rm imp}} = \int \mathrm{d}f^+\mathrm{d}f\ \mathrm{e}^{-L_{\rm loc}[f^+,f]-\sum_{\omega,\sigma}\sigma f_\sigma^+(\mathrm{i}\omega)\Delta(\mathrm{i}\omega)f_\sigma(\mathrm{i}\omega)}. \tag{14}$$

Here, $L_{\rm loc}$ is the action of a local f level with the hybridization set to zero.

One should regard equation (13) as a Landau Ginzburg Functional of the "Metallic Order Parameter" $\Delta(\mathrm{i}\omega)$. At zero temperature, the function $\Delta(\mathrm{i}\omega)$ is non zero in both phases, but it has very different low frequency behavior in the metallic and in the insulating phase.

Differentiating the free energy with respect to $\Delta(\mathrm{i}\omega)$ we obtain the mean field equation (5). The derivative of the first term is $-2\frac{\Delta(\mathrm{i}\omega)T}{t^2}$. Combining it with the results of differentiating the impurity free energy in (14)

$$\frac{\delta F_{\rm imp}}{\delta\Delta(\mathrm{i}\omega)} = T\Sigma_\sigma\langle {f_\sigma}^+(\mathrm{i}\omega)f_\sigma(\mathrm{i}\omega)\rangle = 2TG(\mathrm{i}\omega)[\Delta]. \tag{15}$$

we obtain equation (5).

We will show below, by means of an explicit calculation, that $F_{\rm LG}[\Delta]$ evaluated at the saddle point (5) gives the correct energy of the lattice problem. $F_{\rm LG}[\Delta]$ allows us to consider the free energy of arbitrary hybridization functions (*i.e.* away from self consistent solutions), and to interpolate between various stationary points.

It also has a nice physical interpretation by analogy to the mean field free energy of a spin system regarded as a function of the Weiss field h:

$$\beta F_{\rm LG}[h] = \beta\frac{h^2}{2J} - \log[\mathrm{ch}[2\beta h]]. \tag{16}$$

The first terms in (16) and (13) are the cost of forming the Weiss fields around a site. The second terms are the energies of a site (spin in the classical case, electron in the quantum case) in the the presence of the the Weiss field around it.

Note that our order parameter $\Delta(\mathrm{i}\omega)$ is always non zero but has a qualitatively different form at low frequencies on either side of the transition. This is analogous to the density in the liquid gas transition. At zero temperature, there is a qualitative difference between a metal and an insulator, which appears naturally in this formalism. The metallic phase is characterized by a hybridization function which is nonzero at low frequencies, as opposed to insulating phases for which the hybridization function vanishes at low energy [33].

We stress the difference between the Landau functional (13) and expression (7). Both (7) and (13) give the correct energy if one evaluates them at the *exact local spectral*

function or the *exact hybridization* function respectively. However, (13) is a stationary functional, *i.e.* upon differentiation it produces the correct dynamical mean field equations. On the other hand, (7) is not stationary (its derivative with respect to ρ is nonzero at the physical spectral density) and therefore it does not give the correct mean field equations. It is not a Landau functional, it can only be used to obtain the ground state energy if one knows the correct spectral function but it cannot be used to determine the spectral function itself.

We now prove, that the Landau free energy, evaluated at the saddle point value of the order parameter, indeed gives the total energy of the lattice model. In the process we make the correct connection between the various contributions to the energy of the lattice model and the energy of the corresponding impurity model.

The lattice Hamiltonian contains two terms, K and U. When $\Delta(\mathrm{i}\omega)$ (or correspondingly the one particle Green's function) changes, both $\langle K\rangle$ and $\langle U\rangle$ change. $F_{\mathrm{LG}}[\Delta]$ has two terms, $-T\sum_\omega \frac{\Delta(\mathrm{i}\omega)^2}{t^2}$ and $F_{\mathrm{imp}}[\Delta]$, but it would be incorrect to associate $F_{\mathrm{imp}}[\Delta]$ directly with the kinetic energy of the lattice model. At a stationary point and at $T=0$, the correct connection is:

$$F_{\mathrm{imp}}[\Delta] = \frac{3}{2}\langle K\rangle + \langle U\rangle. \tag{17}$$

Notice that since we work at zero temperature, the free energy and the energy are identical. The impurity energy is composed of three parts, the local correlation $\langle U\rangle$, the hybridization energy $2\sum_{k\sigma} V_k\langle f^\dagger_\sigma c_{\sigma k}\rangle$ which is given by $4T\sum_\omega \Delta(\mathrm{i}\omega)G(\mathrm{i}\omega)$ (extra factor of 2 comes from spin) and the change in kinetic energy of the conduction electrons, which is defined as $\sum_{k\sigma}\epsilon_k(\langle c^\dagger_{\sigma k}c_{\sigma k}\rangle_\Delta - \langle c^\dagger_{\sigma k}c_{\sigma k}\rangle_{\Delta=0})$ and is therefore given by

$$\begin{aligned}
2T\sum_{\omega,k}\frac{{V_k}^2\epsilon_k}{(\mathrm{i}\omega-\epsilon_k)^2}G(\mathrm{i}\omega) &= -2T\sum_\omega \Delta(\mathrm{i}\omega)G(\mathrm{i}\omega)\\
&\quad +2T\sum_\omega \frac{1}{2}\left[\frac{-\mathrm{d}}{\mathrm{d}\mathrm{i}\omega}(\Delta(\mathrm{i}\omega)G(\mathrm{i}\omega)\right]\mathrm{i}\omega\\
&= -T\sum_\omega \Delta(\mathrm{i}\omega)G(\mathrm{i}\omega).
\end{aligned}$$

Combining the three terms, we arrive at equation (17). The first term in the functional in equation (13) is given by

$$-T\sum_\omega \frac{\Delta(\mathrm{i}\omega)^2}{t^2} = \frac{-1}{2}\langle K\rangle > 0. \tag{18}$$

The positivity of this term is essential if we want to interpret it as the cost of forming the Weiss field. Clearly once the Weiss field is formed the impurity energy is negative. (Notice that we are in the half filled situation where $\Delta(\mathrm{i}\omega)$is purely *imaginary*).

Notice that while local quantities have a straightforward interpretation in terms of the impurity model, nonlocal quantities such as the kinetic energy require more care. This is why we stated very clearly how the self-consistent local impurity approximation embeds the impurity model in a medium and gives well defined relations between the kinetic and potential energy of the lattice model, and the energy of the Anderson impurity model, equations (1, 18, 17) and (13) are exact in the limit of large dimensions.

The previous discussion highlights the self consistent character of the Local Impurity Self-Consistent Approximation, whereby the energy is composed of two terms, cost of the Weiss field and the energy gain of the impurity in the presence of the Weiss field. This is very different from the reasoning within the local impurity approximation, which would equate the energy of the lattice to the number of sites times the impurity energy.

Nozières [18,19] reduced the validity of the semicontinuous or the continuous scenario to the following question: does one gain Kondo energy once per spin or once per electron in the resonance (described by the small fraction of electrons contained in the low energy part of the bath)?

To answer this question an unambiguous expression of the energy of the lattice models in terms of the energy of impurity models in the *putative trial states* is required. Expression (13), unambiguously describes the energy per lattice site, *i.e.* the energy per spin, in a self consistent local impurity framework substantiating the semicontinuous scenario.

We can now describe in a precise manner the energetics near the critical points $U_{\mathrm{c}1}$ and $U_{\mathrm{c}2}$. Their existence highlights an essential difference between the classical and the quantum Landau Ginzburg functionals. While in the classical case the Landau functional is an *analytic* function of the magnetization and of the Weiss field which has a straightforward power series expansion, this is not the case in the quantum case.

Free energies obtained by "integrating out" massless degrees of freedom (fermions with a Fermi surface) are non analytic. Here we will deal with the manifestation of this problem in infinite dimensions. We note however that while this problem is most extreme in infinite dimensions, some manifestation of this problem in weaker form may be relevant to the treatment of quantum phase transitions in finite dimensions.

An important lesson to be learned from this analysis is that the quantum Landau Ginzburg functional is non analytic in the field Δ. The source of non analyticity can be traced to the presence of a Fermi surface, and in infinite dimensions can be given a sharp formulation following Nozières' analysis of the Kondo model.

6 Projective self consistent analysis

In the next sections we address a number of questions concerning the stability of the paramagnetic insulating state $\Delta_0(\omega)$. When we evaluate the free energy functional in the perturbed state $\Delta_0(\omega)+\delta\Delta_{\mathrm{L}}(\omega)$ (i) do we gain or lose energy? (ii) and how much? (iii) What is the physical origin of the energy gain?

For this purpose we analyze the low energy behavior of the Landau functional, using the projective self consistent

method, a technique designed to isolate the low energy physics of impurity models in a bath which is self consistently determined (as in the solution of lattice models in the limit of large lattice coordination)

The goal of this section is to set up the notation associated with this reduction to low energies. The results quoted here will be used in the next few sections to isolate and discuss the singular dependence of the Landau free energy on the metallic order parameter. The projective self consistent method was developed in references [16,25,34] where it was used to calculate the value of U_{c2} and the scaling functions at the Mott transition point.

We start with a Mott paramagnetic insulating solution, $\Delta_0(\omega)$, *i.e.* a solution to the mean field equations (5) with a finite gap and we add to it a perturbation $\delta\Delta_{\rm L}(\mathrm{i}\omega) = \sum_{\varepsilon_k} \frac{{V_k^{\rm L}}^2}{\mathrm{i}\omega - \epsilon_k}$ localized in the low energy region (*i.e.* the variables ε_k are much smaller in absolute value than the Mott Hubbard gap).

Notice that since Δ_0 is the exact insulating solution, (*i.e.* a stationary point of the functional (13)) the expansion of the energy in the small addition $\delta\Delta_{\rm L}(\omega)$ starts with quadratic terms We will therefore only write the terms which are quadratic in $\delta\Delta_{\rm L}(\mathrm{i}\omega)$, and ignore the linear variations which have to cancel in the final answer [32].

Furthermore we take $\delta\Delta_{\rm L}(\omega)$ as entirely concentrated in the region of low energies, since changes at high energies will be shown to be unimportant (see discussion of this point in page 34). Using a Schrieffer Wolff [35] transformation on the Hamiltonian, we can reduce (6) (to order ${V_k^{\rm L}}^2$) to a Kondo like Hamiltonian

$$H_{\rm K}(\delta\Delta_{\rm L}) = E_{\rm ins} + J_s(U,t)\sum_{kk'} V_k^{\rm L} c_k^\dagger \boldsymbol{\sigma} c_{k'} V_{k'}^{\rm L}\mathbf{S} + \sum_k \epsilon_k c_{k\sigma}^+ c_{k\sigma}. \tag{19}$$

$E_{\rm ins}$ is the energy of the Mott insulator, the subscript k, runs over the low energy conduction electrons. We introduced the local conduction electron:

$$c_{{\rm L}\sigma} = \sum_k 2\frac{V_k^{\rm L} c_{k\sigma}}{D\sqrt{Z}} \tag{20}$$

and $\mathbf{S}$, the local renormalized impurity spin $S^a = \frac{1}{2}{\sigma^a}_{\sigma\sigma'} X_{\sigma\sigma'}$ acting on the low energy spin degrees of freedom. $|\downarrow\rangle_a$, $|\uparrow\rangle_a$. These are defined formally as ground states $|\downarrow\rangle_a$, $|\uparrow\rangle_a$, of the Anderson impurity model with hybridization function Δ_0 [16]. X are Hubbard operators, acting on those spin degrees of freedom.

$J_s(U,t)$ is a monotonically decreasing function of U/t which depends explicitly on the insulating solution Δ_0. An explicit expression is given by: $J_s \equiv {}_a\langle\uparrow| f_\downarrow \frac{1}{H_a - E_g^a} f_\uparrow^\dagger |\downarrow\rangle_a$ [16].

Since we intend to compute the energy change to order $\delta\Delta_{\rm L}(\mathrm{i}\omega)^2$, we need in principle the effective Hamiltonian obtained by the Schrieffer Wolff [35] transformation to order ${V_k^{\rm L}}^4$. It has the form:

$$H_{\rm low}^{(3)} = \frac{D}{2}J_1^{(3)}\mathbf{S}\cdot\mathbf{s}_{\bar\epsilon{\rm L}} + \frac{DJ_2^{(3)}}{8}\sum_\sigma (c_{{\rm L}\sigma}^\dagger c_{\bar\epsilon{\rm L}\sigma} + c_{\bar\epsilon{\rm L}\sigma}^\dagger c_{{\rm L}\sigma}) \tag{21}$$

$$+ \frac{D}{2}{J_3}^{(3)}\mathbf{S}\cdot\mathbf{s}_{\rm L} + \frac{D}{16}{J_4}^{(3)}\left(n_{{\rm L}\uparrow} - \frac{1}{2}\right)\left(n_{{\rm L}\downarrow} - \frac{1}{2}\right) \tag{22}$$

with $c_{\epsilon L\sigma} \equiv 2\sum_k \tilde V_k \epsilon_k c_{k\sigma}$ and $\mathbf{s}_{\bar\epsilon} \equiv \frac{1}{4}(c_{\bar\epsilon\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_\beta + c_\alpha^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{\bar\epsilon\beta})$. The coefficients $J^{(3)}$, have been evaluated numerically [34] but they are not necessary for our purposes since the expectation value of the fourth order Hamiltonian (22) in the ground state is zero, hence contributions to the energy to order $\delta\Delta_{\rm L}(\mathrm{i}\omega)^4$ only arise from a second order computation using equation (19).

It is also instructive to record the explicit form of the low energy part of the Anderson model f operator after the canonical transformation is performed:

$$F_\sigma = -\frac{J_s}{2}D\sqrt{Z}\sum_{\sigma'} S^a {\sigma^a}_{\sigma,\sigma'} c_{{\rm L}\sigma'} \tag{23}$$

Z is a very important quantity, the total low energy spectral weight of the trial state:

$$Z = \frac{4}{D^2}\int \delta\Delta_{\rm L}(\omega')\mathrm{d}\omega' = \sum_k 4\frac{{V_k^{\rm L}}^2}{D^2}\cdot \tag{24}$$

It is proportional to the quasiparticle residue of Fermi liquid theory. The proportionality constant between the low energy spectral weight and the quasiparticle residue was evaluated in reference [16].

We now isolate the dependence of the Landau functional on $\delta\Delta_{\rm L}(\mathrm{i}\omega)$, from equation (13), namely,

$$E_{\rm L}(\delta\Delta_{\rm L}) = \frac{-T}{t^2}\sum_\omega \delta\Delta_{\rm L}(\mathrm{i}\omega)^2 + E_{\rm K}(\delta\Delta_{\rm L}) \tag{25}$$

$E_{\rm K}$ is the usual expression for the energy of a Kondo impurity model

$$E_{\rm K}(\delta\Delta_{\rm L}) = \langle H_{\rm K}\rangle[V_k^{\rm L}] - \langle H_{\rm K}\rangle[V_k^{\rm L} = 0]. \tag{26}$$

While one can make qualitative arguments about transfer of spectral weight by regarding $E_{\rm L}(\delta\Delta_{\rm L})$ as a *function* of Z one should always keep in mind that $E_{\rm L}$ is really a *functional* of the whole hybridization function Δ (or, if we restrict ourselves to low energy variations, of $\delta\Delta_{\rm L}$). In fact, we shall show in the following sections that the free energy functional (25) takes very different values for hybridization functions having the same value of Z but different aspect ratios or shapes. The physical reason underlying this is the different behavior of the Kondo energy depending on whether the model (19) is in the weak coupling or the strong coupling limit. This will have significant implications for the Mott transition in the limit of infinite dimensions.

7 Energetics near U_{c1}

In this section we describe the energetics of making a "very small " perturbation (very small is defined by the requirement that the corresponding effective Kondo problem (19) is weakly coupled) to the Mott insulating solution. The goal is to determine the location of U_{c1}, the point where the insulator ceases to exist because it becomes linearly unstable against such a small perturbation [25].

The cost of modifying the Weiss field (first term in (25)), is computed by inserting explicitly the expression $\delta\Delta_{\rm L}(i\omega_n) = \sum_k \frac{{V_k^{\rm L}}^2}{i\omega_n - \varepsilon_k}$, doing the Matsubara sums, and taking the zero temperature limit, and is given by:

$$\frac{2}{t^2} \sum_{\varepsilon_{k'}>o, \varepsilon_k<0} \frac{{V_k^{\rm L}}^2 {V_{k'}^{\rm L}}^2}{(\varepsilon_{k'} - \varepsilon_k)} \cdot \tag{27}$$

Next we evaluate equation (26) in second order perturbation theory to compute the energy gain

$$E_{\rm K}(\delta\Delta_{\rm L}) = - \sum_{\varepsilon_{k'}>0, \varepsilon_k<0} \frac{\left(J_s V_k^{\rm L} V_{k'}^{\rm L}\right)^2 \langle\phi_0|\mathbf{S}\cdot c^+_{k\sigma}\boldsymbol{\sigma} c_{k'\sigma} c^+_{k'\sigma}\boldsymbol{\sigma} c_{k\sigma}\mathbf{S}|\phi_0\rangle}{(\varepsilon_{k'} - \varepsilon_k)} \cdot \tag{28}$$

$|\Phi_0\rangle$ is a Fermi sea, *i.e.* a ground state of $\sum_k \varepsilon_k {c^+}_{k\sigma} c_{k\sigma}$. Evaluating (28) we get

$$E_{\rm K}(\delta\Delta_{\rm L}) = {J_s}^2 \frac{3}{2} \sum_{\varepsilon_{k'}>0\, \varepsilon_k<0} \frac{{V_k^{\rm L}}^2 {V_{k'}^{\rm L}}^2}{(\varepsilon_{k'} - \varepsilon_k)}.$$

Therefore, the energy gained by a *weakly coupled Kondo impurity* embedded in the perturbed Weiss field is

$$E_{\rm K}(\delta\Delta_{\rm L}) = -T[\sum_{\omega} \delta\Delta_{\rm L}(i\omega)^2] \frac{3}{4} {J_s}^2 \cdot \tag{29}$$

Balancing cost and gain then gives the condition for U_{c1}, namely $\frac{1}{t^2} = \frac{3}{4} J_s^2(U,t)$. Recalling that $t = \frac{D}{2}$ we have rederived the equation that determines U_{c1} first obtained in reference [25]:

$$\frac{1}{D^2} = J_s^2(U,t) \frac{3}{16} \cdot \tag{30}$$

Since the closure of the gap, necessarily implies instability towards metalization, the U that solves equation (30) is an upper bound to the value of U at which the gap closes [36].

An advantage of the Landau formulation is that the trial states $\delta\Delta_{\rm L}(i\omega)$ do not have to be normalized to unity, *i.e.* the condition $1 = \sum_\omega \frac{\Delta(i\omega)}{t^2} e^{i\omega 0^+}$ does not have to be satisfied. However, if for esthetic reasons one wants to exhibit trial states which do satisfy a proper normalization, this can be easily done without altering significantly the energy of the state by adding a small perturbation $\delta\Delta_{\rm H}$ centered at high energies near the gap edge. Since Δ_0 was stationary, the cost associated with this addition is of the form

$$\Delta E \approx \frac{(a_1 \sum_{\varepsilon_k} {V_k^{\rm L}}^2 + a_2 V_{\rm H}^2) V_{\rm H}^2}{D} \cdot \tag{31}$$

with a_1 and a_2 numbers of order unity. Since $V_{\rm H}^2$ is of order Z, but the denominator D is much larger than the corresponding denominator in equations (27, 28) it is clear that this term does not contribute substantially to the energy balance and the condition for the insulator to become unstable is still controlled by the equation involving low energy denominators (27, 28).

The first argument of Logan and Nozières, which stated that we can only gain energy from the metalization process when the gap has closed is in complete agreement with our detailed calculations, but is only valid for trial states, relevant to the determination of U_{c1}. Under the assumption that the trial state is in the weak coupling regime, we can regard the changes in the spectral function as small continuous deformations of the insulating solution. This kind of perturbations destabilize the insulating solution only when the gap closes.

We can now address the second point raised by Logan and Nozières. What is going on from the point of view of Nozières exhaustion principle: a few electrons cannot gain a great deal of Kondo energy when they have to screen a lattice of spins. We see that this argument is qualitatively correct when applied to the dynamical mean field theory provided that the conduction band is weakly coupled to the spin. Indeed, if we regard the variables ϵ_k in equations (27) and (29) to be of order D, (and not of order ZD), the changes in energy are indeed of order $Z^2 D$

More generally, we note that the partial screening of magnetic moments, is a very common situation in the full solution of the non linear dynamical mean field equations (5). It occurs in the correlated regime at *finite temperatures* when the condition $\Delta(i0^+) = -it$ is strongly violated.

8 Energetics near U_{c2}

A most interesting aspect of the large d solution is the instability of the Mott insulating state with a finite gap to the formation of a narrow metallic band at the Fermi energy. This takes place at a critical value $U_{c2} > U_{c1}$, as we now show.

We are interested in the energetics of this problem which we shall consider from the point of view of the free energy (7) and (13). We first consider the energetics of the problem by inserting a spectral function $\rho(\omega) = \rho_0(\omega) + \delta\rho(\omega)$ in the functional (7). ρ_0 describes the Mott insulating state, and $\delta\rho$ is comprised of two pieces, one removing spectral weight Z from the gap edge at $-\Delta_{\rm g}$ and one that adds it at zero energy.

Since the functional (7) is quadratic, the evaluation of the energy difference between this state (our candidate for metallic state) and the Mott insulating state ρ_0 is straightforward. It consist of a linear part in $\delta\rho$, δE_1 and

a quadratic part in $\delta\rho$, δE_2. These are given respectively by:

$$\delta E_1 = \int \mathrm{d}\omega_1 \delta\rho(\omega_1)\Big[\omega_1 f(\omega_1) + 2t^2 \int \mathrm{d}\omega_2 \rho_0(\omega_2)\frac{f(\omega_1)-f(\omega_2)}{\omega_1-\omega_2}\Big] \quad (32)$$

$$\delta E_2 = 2t^2 \int\int \mathrm{d}\omega_1 \mathrm{d}\omega_2 f(\omega_1)\frac{\delta\rho(\omega_1)\delta\rho(\omega_2)}{\omega_1-\omega_2}\,. \quad (33)$$

It is now straightforward to evaluate δE_1, which as expected turns out to be positive representing a *cost* of energy and given by

$$\delta E_1 = Z\left[\Delta_{\mathrm{g}} + 2t^2\int_0^\infty \mathrm{d}\epsilon\rho_0(\epsilon)\frac{-\Delta_{\mathrm{g}}}{[\epsilon+\Delta_{\mathrm{g}}]\epsilon}\right]. \quad (34)$$

We can now see the breakdown of the exhaustion arguments when applied to the impurity model *relevant to* $U_{\mathrm{c}2}$. If $\delta\rho$ were indeed a "small" (in the sense of the previous section) perturbation, it would then be true that the contribution from δE_2 is negative but small, of the order Z^2 and that to obtain a net gain from $\delta E_1 + \delta E_2$ one would require the gap to be of order Z rather than finite. However the perturbation that we are considering (which is a perfectly legitimate trial state, for the large d Hubbard model) is *not small*. The low energy part ($\delta\rho = \delta\rho_{\mathrm{L}} + \delta\rho_{\mathrm{H}}$) has height one and is described by the scaling function $\delta\rho_{\mathrm{L}}(\omega) = \frac{1}{D}\phi\left(\frac{\omega}{ZD}\right)$. The contribution from δE_2 is *of order* Z and is given by

$$\delta E_2 = Zt\int\int \mathrm{d}\omega_1 \mathrm{d}\omega_2 f(\omega_1)\frac{\phi(\omega_1)\phi(\omega_2)}{\omega_1-\omega_2}\,. \quad (35)$$

Now it is completely clear that the gain in kinetic energy, δE_2 is of the same order as the positive contribution δE_1 so an instability to the metallic state when the insulator has a finite gap can take place. To see that it *does take place* we need to resort to the variational functional (13).

To demonstrate this point we take an insulating solution with a finite gap with U slightly bigger than $U_{\mathrm{c}1}$. According to the analysis of the previous section this is stable against a perturbation $\delta\Delta_{\mathrm{L}}$ which is in the weak coupling regime. On the other hand this state can be unstable against a perturbation $\delta\Delta_{\mathrm{L}}$ described by a Kondo model in an intermediate coupling regime. In this section we will concern ourselves with a perturbation $\delta\Delta_{\mathrm{L}}(\omega)$ *with height of order unity* .

We will take the perturbation with the scaling form

$$\delta\Delta_{\mathrm{L}}(\omega) = D\phi_1\left(\frac{\omega}{ZD}\right) \quad (36)$$

with $\phi_1(0)$ of order unity. It is instructive, following reference [16], to write the low energy Kondo Hamiltonian corresponding to such a perturbation in a way that makes completely clear that the condition of unit height of $\delta\Delta_{\mathrm{L}}(0)$ corresponds to an effective impurity model in the intermediate coupling regime (Kondo energy comparable to electron kinetic energy).

$$H_{\mathrm{K}} = ZJ_s(U,t){c_{\mathrm{L}}}^{+}\boldsymbol{\sigma}c_{\mathrm{L}}\mathbf{S} + \sum_\sigma \sum_{-ZD<\epsilon_k<ZD}\epsilon_k c^+_{k\sigma}c_{k\sigma}. \quad (37)$$

It describes a band of narrow electrons with bandwidth ZD interacting with an orbital the local electron of equation (20) which is properly normalized ($\{c^\dagger_{\mathrm{L}}c_{\mathrm{L}}\}=1$), *via* a Kondo exchange $ZJ_s(U,t)$. The Kondo problem in (37) has a coupling $J_{\mathrm{eff}} = ZJ_s\left(\frac{U}{D}\right)$ and an effective bandwidth $D_{\mathrm{eff}} = ZD$. As a result $\frac{J_{\mathrm{eff}}}{D_{\mathrm{eff}}}$ is independent of Z, so the Kondo impurity is in the intermediate coupling regime. Therefore $\langle\mathbf{S}_{\mathrm{L}}\mathbf{S}\rangle < 0$ where we defined the local conduction electron spin operator by

$$\mathbf{S}_{\mathrm{L}} = \frac{1}{2}{c^\dagger}_{\mathrm{L}}\boldsymbol{\sigma}c_{\mathrm{L}}. \quad (38)$$

Notice that, while the value of the expectation value of the scalar product of the impurity spin and the local spin operator depends on the full form of the scaling function and has only been calculated numerically [16], the fact that it is non zero depends only on the intermediate coupling nature of the associated impurity model in equation (37).

We now insert the variation $\Delta_{\mathrm{trial}} = \Delta_0 + \delta\Delta_{\mathrm{L}}$, with $\delta\Delta_{\mathrm{L}}$ given by equation (36) into the Landau function (13) and compute explicitly the quantity

$$m \equiv \lim_{Z\to 0}\frac{\partial F_{\mathrm{LG}}[\Delta_{\mathrm{trial}}]}{\partial Z}. \quad (39)$$

If m is positive, there is a finite net cost to forming the resonance, if it is negative then it is energetically favorable to metallize. From the chain rule, we find

$$m = -2T\sum_{\mathrm{i}\omega_n}\left[\frac{\delta\Delta_{\mathrm{L}}(\mathrm{i}\omega_n)}{t^2} - G_{\mathrm{L}}(\mathrm{i}\omega_n)\right]\frac{\mathrm{d}}{\mathrm{d}Z}\delta\Delta_{\mathrm{L}}(\mathrm{i}\omega_n). \quad (40)$$

We now insert the spectral representation of the low energy part of the impurity Green's function $G_{\mathrm{L}}(\mathrm{i}\omega)[\delta\Delta_{\mathrm{L}}] = \int \mathrm{d}\epsilon\frac{\rho_{\mathrm{L}}(\epsilon)}{(\mathrm{i}\omega_n-\epsilon)}$, with $\rho_{\mathrm{L}}(\epsilon) = \frac{1}{D}\phi\left(\frac{\epsilon}{ZD}\right)$, into equation (40) to obtain

$$m = 4D\int_{-\infty}^0 \mathrm{d}x\int_0^\infty \mathrm{d}y\frac{1}{(x-y)}\Big[\left(\frac{D}{t}\right)^2\phi_1(x) - \phi(x)\Big]\phi_1{}'(y)y. \quad (41)$$

We next assume a trial state such that $\phi_1'(y) \equiv 0$ at small y and $\phi_1'(y) = c$ between $W1$ and $W2$. Then equation (41) simplifies to:

$$m \approx -4Dc\int_{W2}^{W1}\mathrm{d}y\, y\int_{-\infty}^0 \mathrm{d}x\frac{1}{(x-y)}[4\phi_1(x)-\phi(x)]. \quad (42)$$

For $W1$ and $W2$ large, we thus arrive at:

$$m \approx 4cD(W1-W2)\int_{-\infty}^0 \mathrm{d}x[4\phi_1(x)-\phi(x)]. \quad (43)$$

ϕ is of course a complicated functional of ϕ_1. However, to estimate a *lower* bound to the instability point we only need the integral of ϕ which we calculated in Appendix B. Using those results, and the fact that both ϕ_1 and ϕ are even we obtain the condition for U_{c2} first derived in reference [16]:

$$1 - \frac{(DJ_s(U))^2}{2}\left[\frac{3}{8} - \langle \mathbf{S}\cdot\mathbf{S}_{\rm L}\rangle\right] < 0. \qquad (44)$$

Here, $\mathbf{S}_{\rm L} = \frac{1}{2} {c^+}_{{\rm L}\sigma} {\sigma^a}_{\sigma,\sigma'} c_{{\rm L}\sigma'}$ is the local conduction electron spin.

The proof of the instability of an insulator with a finite gap results from comparing conditions (30, 44) which imply the strict inequality:

$$U_{c1} < U_{c2}. \qquad (45)$$

This follows once we recognize that while $\langle \mathbf{S}\cdot\mathbf{S}_{\rm L}\rangle$ depends on ϕ_1 and can only be computed numerically after solving a non linear self consistent problem, the fact that it is non zero and negative is immediate, from the fact that it describes an impurity in the intermediate coupling regime. Since $J_s(U)$ is a monotonically decreasing function of increasing U, the solution of equation (30) has a lower value than the solution of equation (44).

Notice that the derivation is free from ad-hoc assumptions. The projective self consistent analysis is applied in the region where this method is valid, *i.e.* for a bath with clear separation of energy scales. The formulation in terms of the Landau like functional (13) is useful, because it allows the introduction of *trial* states, which can be analyzed more easily than the solution of the full non linear dynamical mean field equations (5).

We end the section by recapitulating the logic leading to the inequality (45). We start with the Mott insulator and slowly decrease the value of U. In Section 7 we asked the question when is the insulating solution unstable to a small perturbation. The answer is an implicit equation for U, equation (30). Its solution, which we denote U_{c1} is certainly bigger or equal than the value of U at which the gap closes, since when the gap is closing the insulator is definitely unstable against small perturbations. Then we consider a trial state corresponding to an impurity model in an intermediate coupling regime. The condition for instability against this specific trial state, is given by equation (44). While the specific value of $\langle \mathbf{S}\cdot\mathbf{S}_{\rm L}\rangle$ depends on the trial state, the fact that the Mott insulator is unstable at a value of U strictly larger than U_{c1} and therefore posessing a finite gap, relies only on the fact that $\langle \mathbf{S}\cdot\mathbf{S}_{\rm L}\rangle < 0$. This is always true for impurity models which are in the intermediate coupling regime. The trial state we used gives us *a lower bound* to the true value of U_{c2}, since improving the scaling function might result in a better trial state which can destabilize an insulator at an even larger value of U. (This optimization was done numerically in reference [16]).

We therefore have proved that an upper bound for the U which is needed for gap closure is strictly smaller than a lower bound for the U at which the insulator becomes unstable against metalization.

Within the context of the Landau analysis we do not have to worry about the normalization of $\delta\Delta_{\rm L}(\omega)$. To exhibit the instability against a normalized trial state, one can proceed as we did in page 34.

Notice the two significant differences with respect to the previous section:

a) The cost of forming the required Weiss field (while still given by the first term in equation (25) and therefore having an identical form to that considered in the previous section (see Eq. (27)) is now of order Z (and not Z^2 as in the previous section) because the height of the spectral function at the origin is of order unity.

b) The gain in energy from the free energy of the impurity model is now also of order Z. This is not surprising because each individual term in the Hamiltonian of the Kondo impurity is of order Z.

The difference between the determination of U_{c1} and U_{c2} can then be traced to the different behavior of the impurity model in the weak coupling and the intermediate coupling regime. To illustrate this idea in a much simpler setting, we analyze a very simple free energy function in Appendix A.

9 Implications and outlook for finite dimensions

Our analysis so far was confined to zero temperature. However the proof of existence of two coexistent solutions (one metallic and one insulating) in a finite interval of interaction strength at zero temperature, has immediate consequences for the finite temperature phase diagram. Away from the phase boundaries, the Landau functional, is a smooth functional of the hybridization function. Since we have two coexistent solutions, at a finite distance of each other [37], at zero temperature, by continuity the two solutions persist at finite temperature.

At finite temperatures there is no qualitative difference between the metal-like and the insulating-like solution. Just the low frequency density of states is quantitatively different (large in the metal, small in the insulator). The coexistence of two solutions at zero temperature results in a first order phase transition at finite temperatures since entropy favors the paramagnetic insulating solution.

In the temperature interaction strength phase diagram of the frustrated Hubbard model references [11–14] the points U_{c1} and U_{c2} are the end points of two lines $U_{c1}(T)$ and $U_{c2}(T)$ which cross at a finite temperature second order point at $(U_{\rm MIT}, T_{\rm MIT})$.

Rozenberg *et al.* [15] observed that the $U_{c1}(T)$ and $U_{c2}(T)$ can be continued above $T_{\rm MIT}$, where they become crossover lines. The physical interpretation [15], as crossover lines, was remarkable similar, to that of the zero temperature points where they originated. At $U_{c1}(T)$ the gap becomes comparable to the temperature and activation results. At $U_{c2}(T)$ the Fermi liquid coherence disappears [15].

The limit of full frustration is rare. However, it turns out that for reasons having to do with orbital

degeneracy, crystal structure, and longer range multi-spin interactions, many three dimensional transition metal oxides undergoing a metal to insulator transition, are very nearly frustrated, and finite temperatures easily stabilize the paramagnetic insulator phase.

The continuation of the zero temperature paramagnetic metal to paramagnetic insulator transition to finite temperatures, then becomes immediately relevant for answering a long standing question of whether one can account for the phase diagram of $NiSe_{2-x}S_x$ or of V_2O_3 in purely electronic terms without including explicitly the coupling to the lattice. The answer suggested in references [11,13,15] was positive, provided one includes a sufficient degree of magnetic frustration.

The original discussion relied on approximate methods such as the IPT, QMC, or exact diagonalization, which were open to criticism. We have stressed in this article that at zero temperature there are two coexisting solutions in a range of interaction strengths U, which allows us to conclude (without recourse to approximations), that the qualitative features found in references [13,15] in IPT are not artifacts of the approximation, but genuine features of the solution of the dynamical mean field equations (5). The character of the phase diagram, is a consequence of the analytic structure of the free energy functional. One can view, the different approximation methods, as providing different approximate values to the coefficients of the Landau Ginzburg functional of the order parameter. As long as the functional has the correct analytic structure, the qualitative features of the solution are preserved (of course, approximate methods can only give approximate values of $T_{\rm MIT}$, $U_{\rm c1}(T)$ $U_{\rm c2}(T)$ etc.). Approximations such as the fully self consistent skeleton method fail because they do not capture the correct analytic properties of the free energy functional, *i.e.* they miss the paramagnetic insulating phase.

The dynamical mean field solution of the Hubbard model has allowed us to study and understand the *finite temperature* consequences of the existence of a Brinkman Rice quantum critical point [10] $U_{\rm c2}$, where spatial coherence is lost. This quantum critical points is always inaccessible because no system is fully frustrated and some form of magnetic order always sets in before reaching the critical point at zero temperature. The DMFT has been of extraordinary value in revealing the hidden origin of the anomalous temperature dependence [15] of many properties. The *observable* anomalous finite temperature properties, of the paramagnetic phases close to the Mott transition point, are connected, *via* DMFT, to the presence of a zero temperature quantum critical point.

Having established the physical *relevance* of the paramagnetic metal to paramagnetic insulator transition in magnetically frustrated systems, we turn to the broader and more interesting question of how reliable the DMFT description of this transition is.

Conventional mean field theories of classical phase transitions are qualitatively valid from infinite dimensions down to a finite upper critical dimension. The situation is very different in dynamical mean field theory. As currently formulated, in the paramagnetic insulating phase, this theory omits a physically relevant scale, the magnetic exchange energy. The dynamical mean field picture of metalization, as a result, cannot capture the competition between intersite magnetic correlations and the Kondo effect.

In a simplistic picture of the DMFT, which views the central site as a strongly correlated electron f, and the neighbor as a non interacting bath electron c, the f site will have a well formed moment S (which captures the localized character of the electron) while the nearby sites are represented by a conduction band which is narrowed to represent the correlated but itinerant character of the original electrons. Since the bath is uncorrelated, it can only describe a moment, by becoming infinitely narrow. This does not happen in reality, as a result of magnetic correlations, which in three dimensions, ultimately trigger some form of magnetic order. The qualitative success of the dynamical mean field approach depends crucially on the weakness of the intersite magnetic correlations compared to the renormalized Fermi energy $\epsilon_{\rm F}^*$.

Since in the dynamical mean field theory, the effective Fermi energy vanishes at zero temperature and at the critical point, the situation at first sight looks hopeless. However the experimental confirmations of the existence of an underlying quantum critical point at $U_{\rm c2}$ arise from the finite temperature behavior. As long as the degree of frustration and the temperature is sufficiently high so that the relevant magnetic energy scale is smaller than the temperature, (or when the distance from the critical point is sufficiently large so that the renormalized Fermi energy is larger than the magnetic exchange), we are in a situation where many of the qualitative predictions of the dynamical mean field theory are applicable. some of these predictions have actually been observed experimentally [15,38]. Underlying these successes are some unique features of the dynamical mean field theory which are not shared by ordinary mean field theories. A single dynamical mean field solution can contain information about a large number of energy scales. As the corresponding dynamical mean field theory of spin glasses, it works well in frustrated situations. This should be contrasted with static mean field theories, which usually do not work well when there are several competing ground states.

We now turn to the outstanding open issue of how the findings of the dynamical mean field theory are modified when one is at sufficiently low temperatures, or sufficiently close to the transition so that the magnetic correlations have to be taken into account. The considerations presented in this note suggests significant departures from the results of ynamical mean field theory.

In infinite dimensions, near $U_{\rm c1}$ we have complete decorrelation of $\mathbf{S}$ and $\mathbf{S}_{\rm L} = {c_{\rm L}}^\dagger \boldsymbol{\sigma} c_{\rm L}$. Near $U_{\rm c2}$ however we have a finite value of $\langle \mathbf{S} \cdot \mathbf{S}_{\rm L} \rangle$ because a band which is infinitely narrow, can be polarized without any cost, and we succeed in getting some finite energy from the *spin correlations* between neighboring sites all the way to the transition.

This can not be accomplished once we have a finite exchange among nearby sites (an effect which is formally $1/d$ and therefore invisible in the large d paramagnetic phase but becomes of order one once we allow for magnetic long range order). Now the Kondo interaction between the central spin $\mathbf{S}$ and $\mathbf{S}_{\rm L}$ will compete with the exchange interactions with the nearby spins. As a result the free energy becomes a smoother function of the hybridization. If there is some kind of Kondo effect going on at the transition it will now occur in a regime of weaker coupling strength. The same conclusion can also be reached from the point of view of the itinerant electrons. If we now accept that the self energy can contain k dependence the pinning condition $\rho(0) = \frac{1}{D}$ is now eliminated. The possible Weiss fields can now be more like those considered in the discussion in Section 7.

For these reasons we believe that the destruction of the insulator near $U_{\rm c1}$ which we described in Section 7 may play a more fundamental role in finite dimensions or in partially frustrated situations.

Stated in a different language the large d picture is one where $\epsilon_{\rm F} = Zt$, the renormalized Fermi energy, is larger than J_{ij}, the magnetic superexchange between a pair of spins. Clearly this is justified in the formal infinite d limit because $J_{ij} = t_{ij}^2/U \propto \frac{1}{d}$ is vanishingly small no matter how small $\epsilon_{\rm F}$ is. That situation changes immediately once J_{ij} is finite. Clearly new physics is expected when J_{ij} is larger than $\epsilon_{\rm F}$.

Within DMFT the influence of magnetic correlations on the Mott transition has been recently studied recently [39] by approaching the metal insulator transition from an ordered state. In this case, one can quantitatively study how the magnetic correlations dramatically modify the behavior near the metal insulator transition point. In the absence of magnetic long range order, the task is more difficult. We have to do it without the guidance of the infinite d limit, because all those effects disappear in that case. These effects appear next order in $1/d$, but a complete treatment of those corrections, is still missing [40].

We believe that the basic idea of this paper, *i.e.* that different types of Mott transition should be viewed as different types of bifurcations, of a system of functional equations for a metallic order parameter closely related to the one particle Green's function, will also be useful beyond the limit of large lattice coordination.

Note added in proof

After this paper was completed, two numerical studies of the problem discussed in this note have appeared. In an algorithmic tour de force, Bulla [23] obtained a value of $U_{\rm c2}$ in excellent agreement with earlier results [16]. Using a different numerical method Gebhard and Noack [21], obtained a value of $U_{\rm c1}$ which is in excellent agreement with earlier work [15,14]. Their value for $U_{\rm c2}$ however, is much smaller than all previous estimates.

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Appendix A

To illustrate the main features of the Landau Functional we discuss in this Appendix a toy free energy which has a structure similar to equation (13) but which is much easier to analyze. This free energy is a function of two variables: j (which should be thought of as one of the ${V_k}^2$ of the previous sections) and t which should be thought of as a single ϵ_k. It is given by:

$$F[t,j] = \frac{j^2}{t} + \left(t - \sqrt{j^2 {J_s}^2 + t^2} \right) - \frac{10\, j\, J_s}{{\rm e}^{\frac{t}{j}}} \cdot \qquad \text{(A.1)}$$

The analogy with the discussion in previous sections should be apparent, the first term is the cost of making the Weiss field, the second term is the energy that the impurity gains once the Weiss field is formed. We have mimicked the non analytic dependence of the free energy on the coupling strength in weak coupling by the exponential term which does not have a Taylor series in j, around $j = 0$ The analysis leading to the determination of $U_{\rm c1}$ consists of simply evaluating whether there is an energy gain by increasing j away from zero, in weak coupling, that is for a fixed value of t and for an infinitesimal value of j. This stability analysis is equivalent to checking whether the second derivative of the free energy with respect to j, at fixed t is positive or negative at the origin From equation (A.1) we conclude that the $U_{\rm c1}$ like instability occurs at the value of U (J_s is a function of U) such that

$$\frac{2}{t} - \frac{J_s^2}{\sqrt{t^2}} = 0. \qquad \text{(A.2)}$$

We now perform the determination of the critical value which parallels $U_{\rm c2}$, *i.e.* we perform a minimization of the free energy without assuming whether the minimum occurs at weak or strong coupling. In other words, we focus on the functional which tells us if energy is gained or lost by increasing w, the weight at the origin, for fixed value of the inverse coupling strength a which we define as $a = \frac{t}{j}$. $U_{\rm c2}$ is determined by then optimizing with respect to the coupling strength a.

$$f[j = w, t = w.a] = g[w,a] = \frac{w}{a} + a\, w - \frac{10\, J_s\, w}{{\rm e}^a} - \sqrt{a^2\, w^2 + J_s^2\, w^2}. \qquad \text{(A.3)}$$

Now we notice that since in this toy model the free energy is linear in w, the instability occurs when this term is negative (w by definition is always positive). The calculation

that parallels U_{c2} requires us to minimize with respect to a and search for instability. Terms non linear in w could be added to the toy free energy so as to obtain well defined solutions to the full non linear problem, but will not be considered here.

It is clear that at U_{c2}, the system prefers to be metallic and favors a strong coupling state.

Appendix B

To derive equation (44) we need the asymptotic behavior of the real part of the Green's function in the Anderson impurity model in the regime $ZD \ll \omega \ll \Delta_g$, (*i.e.* for energies much less than the Mott Hubbard gap but greater than the resonance width). From the asymptotic behavior

$$\delta\Delta_L(i\omega_n) \approx \frac{D^2 Z}{4i\omega_n} \tag{B.1}$$

it follows that $\int_\infty^\infty \phi_1(x)dx = \frac{1}{4}$ The low energy part of the f electron operator is given in equation (23). Using the definition of the local electron spin (38) and the identity

$$\frac{1}{2}\sum_\sigma \langle\{(\mathbf{S}c^\dagger{}_L\boldsymbol{\sigma})_\sigma, (\mathbf{S}\boldsymbol{\sigma}c_L)_\sigma\}\rangle = 2\left(\frac{3}{8} - \langle\mathbf{S}\cdot\mathbf{S}_L\rangle\right) \tag{B.2}$$

we obtain

$$\int \rho_L(\epsilon)d\epsilon = \frac{1}{2}\sum_\sigma \langle\{F_\sigma F^\dagger{}_\sigma\}\rangle \approx \frac{Z}{2}(DJ_s)^2\left(\frac{3}{8} - \langle\mathbf{S}\cdot\mathbf{S}_L\rangle\right). \tag{B.3}$$

It follows that $\int_\infty^\infty \phi(x)dx = \frac{1}{2}(DJ_s)^2\left(\frac{3}{8} - \langle\mathbf{S}\cdot\mathbf{S}_L\rangle\right)$ which is then used in equation (44) in the text.

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