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DYNAMICAL MEAN FIELD THEORY OF STRONGLY CORRELATED FERMIONS: THE LIMIT OF LARGE DIMENSIONS

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Dynamical Mean Field Theory of Strongly Correlated Fermions: the limit of large dimensions

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We review the mean field theory of strongly correlated electrons systems which becomes exact in the limit of large lattice coordination. It is based on a mapping from lattice models onto quantum impurity models. We discuss the physical ideas underlying the mean field theory, its mathematical derivation and the techniques developed to study it. This method yields qualitative insights into the strong correlation problem and a quantitative description of the solution of model hamiltonians in the limit of large lattice coordination. Application of these techniques to the Mott metal-insulator transition is described in the attached reprints.

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References to be found in attached reprints

I. INTRODUCTION

The subject of these notes is a mean-field theory of strongly correlated fermion models, which freeses out spatial fluctuations but deals with *local quantum fluctuations* in an exact manner. This mean-field theory becomes exact in the limit of large lattice coordination, which insures the internal consistency of the approach. For this reason, it is analogous to the Weiss mean field theory in classical statistical mechanics. Suitably extended to take into account the specificity of the local density of states of realistic systems, the method can be applied to calculations on real materials.

The essential idea underlying this approach is to replace a quantum many body problem by a single site quantum impurity model in an effective medium which is determined self consistently. This self consistent quantum zero dimensional problem can be attacked with a variety of techniques. This method has already given new insights into fundamental problems such as the Mott transition, the superconductivity of strongly correlated electron systems, the interplay of magnetism and local moment formation in disordered systems, and the breakdown of Fermi liquid theory in metallic phases. Many other possible applications are currently being explored.

In these notes, a pedagogical introduction to the technical aspects of this mean-field approach will be given. Application to the Mott metal-insulator transition is described in the attached reprints, where references to the litterature is also to be found.

II. DYNAMICAL MEAN-FIELD EQUATIONS

To stress the analogy with the familiar mean-field theory of classical statistical mechanics, we shall describe in parallel the classical case and its quantum generalisation below. For the sake of clarity, we shall first summarize the mean-field equations without any proof, and then present various useful derivations.

A. Outlook

The goal of a mean field theory is to approximate a lattice problem with many degrees of freedom by a *single-site* effective problem with less degrees of freedom. The underlying physical idea is that the dynamics at a given site can be thought of as the interaction of the degrees of freedom at this site with an external bath created by all other degrees of freedom on other sites.

The simplest illustration of this idea is for the Ising model with ferromagnetic couplings $J_{ij} > 0$ between nearest-neighbour sites of a lattice with coordination z:

$$H = -\sum_{(ij)} J_{ij} S_i S_j - \sum_i h_i S_i \tag{1}$$

The 1907 Weiss mean-field theory views each given site (say, o) as governed by an effective hamiltonian:

$$H_{eff} = -h_{eff} S_o \tag{2}$$

All interactions with the other degrees of freedom are lumped into the Weiss effective field h_{eff}:

$$h_{eff} = h + \sum_i J_{oi} m_i = h + zJm \tag{3}$$

where $m_i = < S_i >$ is the magnetization at site i, and translation invariance has been used ($m_i = m$). Hence h_{eff} has been related to a local quantity which can in turn be computed from the single-site effective model H_{eff}. For the simple case at hand, this reads: $m = tanh(\beta h_{eff})$, which can be combined with (3) to yield the familiar mean-field equation for the magnetization:

$$m = tanh(\beta(h + zJm)) \tag{4}$$

These mean-field equations are, in general, an approximation to the true solution of the Ising model. They become *exact* however in the limit where the *coordination of the lattice becomes large*. It is quite intuitive indeed that the neighbours of a given site can be treated globally as an external bath when their number becomes large. As is clear from (3), the coupling J must be scaled as $J = J^*/z$ to yield a sensible limit $z \to \infty$ (this scaling is also required to keep the free energy per site finite).

These ideas can be directly extended to quantum many-body systems. This will be illustrated here on the example of the Hubbard model:

$$H = -\sum_{ij,\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + h.c + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{5}$$

It will be assumed in this section for simplicity that no symmetry breaking occurs, i.e that one deals with the translation-invariant paramagnetic phase. Phases with long-range order will be dealt with in section II.C.

Again, the mean-field description associates to this hamiltonian a single-site effective dynamics, which is conveniently described in terms of an imaginary-time action for the fermionic degrees of freedom $(c_{o,\sigma}, c^+_{o,\sigma})$ at that site:

$$S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c^+_{o\sigma}(\tau) G^{-1}_{eff}(\tau - \tau') c_{o\sigma}(\tau') + U \int_0^\beta d\tau\, n_{o\uparrow}(\tau) n_{o\downarrow}(\tau) \tag{6}$$

$G_{eff}(\tau - \tau')$ plays the role of the Weiss effective field above. Its physical content is that of an effective amplitude for a fermion to be created on the isolated site at time τ (coming from the "external bath") and being destroyed at time τ' (going back to the bath). The main difference with the classical case is that this generalised "Weiss field" is a *function of time* instead of a single number. This, of course, is required to take into account *local quantum fluctuations*. G_{eff} plays the role of a bare Green's function for the effective action S_{eff}, but it should not be confused with the non-interacting local Green's function of the original lattice model.

A closed set of mean-field equations is obtained by supplementing (6) with the expression relating G_{eff} to local quantities computable from S_{eff} itself, in complete analogy with eq.(3) above. As will be shown below, this expression reads:

$$1/G_{eff}(i\omega_n) = i\omega_n + \mu + 1/G(i\omega_n) - \tilde{D}^{-1}[G(i\omega_n)] \tag{7}$$

In this expression, $G(i\omega_n)$ stands for the on-site interacting Green's function calculated from the effective action S_{eff}:

$$G(\tau - \tau') \equiv - < T c(\tau) c^+(\tau') >_{S_{eff}} \tag{8}$$

and $\tilde{D}(\zeta)$ is the reciprocal function of the Hilbert transform of the density of states corresponding to the lattice at hand. Explicitly, given the d.o.s $D(\epsilon)$:

$$D(\epsilon) = \sum_k \delta(\epsilon - \epsilon_k) \ , \ \epsilon_k \equiv \sum_{ij} t_{ij} e^{ik.(R_i - R_j)} \tag{9}$$

$\tilde{D}^{-1}$ satisfies: $\tilde{D}^{-1}(\tilde{D}(\zeta) = \zeta$, where the Hilbert transform $\tilde{D}(\zeta)$ is defined by :

$$\tilde{D}(\zeta) \equiv \int d\epsilon \frac{D(\epsilon)}{\zeta - \epsilon} \tag{10}$$

Since G can in principle be computed as a functional of G_{eff} using the impurity action S_{eff} , equations (6,7,8) form a closed system of functional equations for the on-site Green's function G and the Weiss field G_{eff}. In practice, the main difficulty lies in the solution of S_{eff}.

It is instructive to check these equations in two simple limits. In the free limit $U = 0$, solving (6) yields $G(i\omega_n) = G_{eff}(i\omega_n)$ and hence from (7), $G(i\omega_n) = \tilde{D}(i\omega_n + \mu)$ reduces to the free on-site Green's function. In the 'atomic' limit $t_{ij} = 0$, one just has a collection of disconnected sites and $D(\epsilon)$ becomes a δ-function, with $\tilde{D}(\zeta) = 1/\zeta$. Then (7) implies $G_{eff}(i\omega_n)^{-1} = i\omega_n + \mu$ and the effective action S_{eff} becomes essentially local in time and

describes a four-state hamiltonian which yields: $G(i\omega_n)_{at} = (1-n/2)/(i\omega_n+\mu)+n/2(i\omega_n+\mu-U)$, with $n/2 = (e^{\beta\mu}+e^{\beta(2\mu-U)})/(1+2e^{\beta\mu}+e^{\beta(2\mu-U)})$.

Solving the coupled equations above not only yields *local quantities* but also allows us to reconstruct all the k-dependent correlation functions of the original lattice Hubbard model. For example, the Fourier transform of the one particle Green's function $G_{ij}(\tau-\tau') \equiv -<T c_{i,\sigma}(\tau)c^{\dagger}_{j,\sigma}(\tau')>$ can be shown to read:

$$G(k,i\omega_n) \equiv -<c_k(i\omega_n)c_k(i\omega_n)^{+}> = \frac{1}{i\omega_n+\mu-\epsilon_k-\Sigma(i\omega_n)} \tag{11}$$

where the self energy can be computed from the solution of the effective on-site problem as:

$$\Sigma(i\omega_n) = G^{-1}_{eff}(i\omega_n) - G^{-1}(i\omega_n) \tag{12}$$

It is therefore k-independent in this approach (i.e purely local in space: $\Sigma_{ij} = \delta_{ij}\Sigma$, a fact first noticed in. From this expression, one sees that the 'self-consistency condition', eq.(7) relating G and G_{eff} insures that the on-site component of the Green's function, given by $G_{ii}(i\omega_n) \equiv \sum_k G(k,i\omega_n)$ coincides with the Green's function $G(i\omega_n)$ calculated from the effective action S_{eff}. Indeed, summing (11) over k yields: $\tilde{D}(i\omega_n+\mu-\Sigma(i\omega_n))$. Identifying this expression with $G(i\omega_n)$ and using (12) leads to (7).

Thermodynamic quantities for the Hubbard model can all be simply related to their one-site model counterparts: the relevant expressions for the free energy and internal energy are given by eqs.() below. Higher order Green's functions, dynamical response functions and transport properties for the lattice model can also be related to vertex functions of the on-site action S_{eff}. Basically, when writing integral equations for the 2-particle Green's functions, the irreducible 2-particle vertex can be replaced by its momentum-independent (but frequency-dependent) impurity model counterpart.

Table 1

Quantum Case	Classical Case	
$-\sum_{(ij)} t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$	$H = -\sum_{(ij)} J_{ij}S_iS_j - h\sum_i S_i$	Hamiltonian
$t_{ij} \sim \frac{1}{\sqrt{2}}^{\lvert i-j\rvert}$	$J_{ij} \sim \frac{1}{2}^{\lvert i-j\rvert}(ferromagnet)$	Scaling
$G(k,i\omega_n) = <c^{\dagger}_k(i\omega_n)c_k(i\omega_n)>$	$<S_iS_j>$	Correlation Function
$<c^{+}(i\omega_n)c(i\omega_n)>$	$m = <S_i>$	Local Observable
$-\int\int c^{\dagger}_{\sigma}(\tau)G^{-1}_{eff}(\tau-\tau')c_{\sigma}(\tau') + \int U n_{\uparrow}n_{\downarrow}$	$H_{eff} = h_{eff}S_o$	Single Site Hamiltonian
$H_{eff} = \sum_{l\sigma} E_l a^{\dagger}_{l\sigma}a_{l\sigma} + \sum_{l\sigma} V_l(a^{\dagger}_{l\sigma}c_{\sigma} + h.c)$		
$-\mu\sum_{\sigma} c^{\dagger}_{\sigma}c_{\sigma} + U n_{\uparrow}n_{\downarrow}$		
$G_{eff}(i\omega_n)$	h_{eff}	Weiss Field
$G^{-1}_{eff}(i\omega_n) =$	$h_{eff} = zJm$	Relation between Weiss
$i\omega_n+\mu+1/G(i\omega_n) - \tilde{D}^{-1}[G(i\omega_n)]$		Field and Local Observable

B. Connection with quantum impurity models

The structure of the mean field theory is that of a functional equation for the local Green's function $G(i\omega_n)$ and the 'Weiss field' $G_{eff}(i\omega_n)$. In contrast to mean-field theory for classical systems, the on-site effective action S_{eff} remains a *many-body problem*. This is because the present approach freezes *spatial fluctuations* but fully retains *local quantum fluctuations*. As a function of imaginary time, each site undergoes transitions between the four possible quantum states $|0>, |\uparrow>, |\downarrow>, |\uparrow,\downarrow>$ by exchanging electrons with the rest of the lattice described as an external bath. The dynamics of these processes is encoded in the Weiss field $G_{eff}(\tau-\tau')$.

For these reasons, no hamiltonian form involving *only* the on-site degrees of freedom $(c_{o\sigma}, c^{\dagger}_{o\sigma})$ can be found for the effective on-site model: once the bath has been eliminated, S_{eff} necessarily includes retardation effects. In order to gain physical intuition and also to make some practical calculations with S_{eff}, it is useful however to have such a hamiltonian formulation. This is possible upon reintroducing auxiliary degrees of freedom describing the 'bath'. For example, one can view $(c_{o\sigma}, c^{\dagger}_{o\sigma})$ as an 'impurity orbital', and the bath as a 'conduction band' described by operators $(a_{l\sigma}, a^{\dagger}_{l\sigma})$ and consider the hamiltonian:

$$H_{AM} = \sum_{l\sigma} E_l a^{\dagger}_{l\sigma}a_{l\sigma} + \sum_{l\sigma} V_l(a^{\dagger}_{l\sigma}c_{o\sigma} + c^{\dagger}_{o\sigma}a_{l\sigma}) - \mu\sum_{\sigma} c^{\dagger}_{o\sigma}c_{o\sigma} + U n_{o\uparrow}n_{o\downarrow} \tag{13}$$

This hamiltonian is quadratic in $a^{\dagger}_{l\sigma}a_{l\sigma}$: integrating these out give rise to an action of the form (6), with:

$$G^{-1}_{eff}(i\omega_n) = i\omega_n + \mu - \int_{-\infty}^{+\infty} dE \frac{\Delta(E)}{i\omega_n - E} \ , \ \Delta(E) \equiv \sum_{l\sigma} V_l^2 \delta(E - E_l) \tag{14}$$

Hence (13) can be viewed as a hamiltonian representation of S_{eff} provided $\Delta(E)$ (i.e the parameters V_l, E_l) is chosen such as to reproduce the actual solution G_{eff} of the mean-field equations. The spectral representation (14) is general enough to allow this in all cases. The hamiltonian (13) is the familiar Anderson model of a magnetic impurity coupled to a conduction bath. Here the isolated site o plays the role of the impurity orbital, and the conduction bath is built from all other lattice sites.

There is of course a degree of arbitrariness in the hamiltonian representation of the local action S_{eff}. Instead of viewing it in the Anderson model language, we can consider the Wolff model , in which the U-term acts only at a single-site of a conduction-electron lattice representing the bath:

$$H_{WM} = \sum_{l\sigma} E_l a^+_{l\sigma} a_{l\sigma} + U n_{o\uparrow} n_{o\downarrow} \tag{15}$$

If we adopt this point of view the Weiss field is given by

$$G^{WM}_{eff} = \int_{-\infty}^{+\infty} dE \frac{\Delta(E)}{i\omega_n - E} \ , \ \Delta(E) \equiv \sum_{l} \delta(E - E_l) \tag{16}$$

and it merely corresponds to a different spectral representation of G_{eff}.

Hence, the mean field theory of the Hubbard model reviewed here maps the lattice problem onto that of *an Anderson impurity embedded in a self consistent medium*. The solution of the mean-field equations involves the determination of G_{eff} such that, when inserted in the Anderson model, the resulting impurity Green's function obeys the self consistency condition (7).

The reduction of a lattice problem to a single-site problem with *effective* parameters is a common feature to both the classical and quantum mean-field constructions. The main difference is that the Weiss field is a number in the classical case, and a function in the quantum case. Physically, this reflects the existence of *many energy scales* in strongly correlated fermion models. (We note in passing that this also occurs in the mean-field theory of some classical problems with many energy scales such as spin glasses). This points out the limitations of other 'mean-field' approaches, such as the Hartree-Fock or slave bosons methods, where one attempts to parametrize the whole mean field function by a number (or a finite set of numbers). This in effect amounts to freeze local quantum fluctuations by replacing the problem with a purely classical one, and can only be reasonable when only one energy scale is important. One such example would be a Fermi liquid phase. of the Hubbard model. Even in such a case, parametrizing the Weiss field by a single number can

only be satisfactory at low energy, but misses the high energy incoherent features associated with the other energy scales in the problem. When no characteristic low-energy scale is present, a single number parametrisation fails completely: this is the case for example when correlation functions have power-law decays as a function of frequency (such as X-ray edge behaviour), as will be discussed in section .

Finally, the mapping onto impurity models, besides its intuitive appeal, has proven to be useful for practical calculations. These models have been studied intensively in the last 30 years by a variety of analytical and numerical techniques, and this knowledge can be employed to understand strongly correlated lattice models in large dimensions. The crucial step in this game is to use *reliable* tools to solve S_{eff}.

C. The limit of infinite dimensions

The above mean-field equations become exact in the limit of infinite coordination on various lattices. In this section, we discuss several such examples and in each case we give the relation (7) between the local Green's function and the Weiss field G_{eff} in explicit form. Notice that, in the paramagnetic phase, the mean-field equations depend *only on the free density of states* $D(\epsilon)$. Since many different lattices give rise to the same density of states in the limit of large coordination, one can construct models with the same single particle properties (*i.e* the same Green's function) in the paramagnetic phases but very different properties regarding magnetic responses and transitions to phases with long-range order.

The first example to be discussed is the d-dimensional cubic lattice with nearest-neighbour hopping (with coordination $2d$). In order that the kinetic and interaction energies remain of the same order of magnitude in the $d \to \infty$ limit, a scaling must be made on the hopping amplitude. The correct scaling is easily seen from the Fourier transform ϵ_k of t_{ij}, which for a 'generic' vector $\mathbf{k}$ involves $\sum_{n=1}^{d} cos(k_i)$, a sum of d numbers with essentially random signs. Hence t_{ij} must be scaled as $t_{ij} = \frac{t}{\sqrt{d}}$. More precisely, this insures that the d.o.s has a well-defined $d \to \infty$ limiting form, which reads (from the central-limit theorem):

$$D(\epsilon) = \frac{1}{t\sqrt{\pi}} \exp -(\frac{\epsilon^2}{t^2}) \tag{17}$$

This expression, and various useful properties of tight-binding electrons on a $d \to \infty$ cubic lattice is derived in Appendix A. The same density of states is obtained for the $d \to \infty$ cubic lattice with $t_{ij} = t_1/\sqrt{d}$ for nearest-neighbour hopping and $t_{ij} = t_2/d$ for next-nearest neighbor hopping. In this case, one should set $t = \sqrt{t_1^2 + t_2^2}$ in eq.(17). The Hilbert transform of (17) reads (for $t = 1$) $\tilde{D}(z) = -is\sqrt{\pi} \exp(-z^2) erfc(-isz)$, where $s = sign(Im(z))$ and $erfc$ denotes the complementary complex error function. There is no simple explicit form for

the reciprocal function $\tilde{D}^{-1}$ in this case and hence (7) must be used as an implicit relation between G_{eff} and G.

A second important example is the Bethe lattice (Cayley tree) with coordination $z \to \infty$ and nearest-neighbour hopping $t_{ij} = t/\sqrt{z}$. A semicircular d.o.s is obtained in this case:

$$D(\epsilon) = \frac{1}{2\pi t^2}\sqrt{4t^2 - \epsilon^2}\ ,\ |\epsilon| < 2t \tag{18}$$

The Hilbert transform reads (for $t = 1$): $\tilde{D}(\zeta) = (\zeta - s\sqrt{\zeta^2 - 4t^2})/2t^2$, and its reciprocal function takes a very simple form: $\tilde{D}^{-1}(\zeta) = t^2\zeta + 1/\zeta$, so that the self-consistency relation between the Weiss field and the local Green's function takes in this case the explicit form:

$$G_{eff}^{-1}(i\omega_n) = i\omega_n + \mu - t^2 G(i\omega_n) \tag{19}$$

The same d.o.s is also realised in a random Hubbard model on a fully connected lattice (all N sites pairwise connected) where the hoppings are independent random variables with variance $\overline{t_{ij}^2} = t^2/N$.

Finally, the Lorentzian density of states

$$D(\epsilon) = \frac{t}{\pi(\epsilon^2 + t^2)} \tag{20}$$

can be realized with a t_{ij} matrix involving long-range hopping. One possibility is to take for the Fourier transform of $t_{i,j}$: $\epsilon_k = \frac{t}{d}\sum_{i=1}^{d} tan(k_i) * sign(k_i)$ on a cubic lattice as $d \to \infty$. Because of the power-law tails of the d.o.s, this model needs a regularization to be properly defined. If one introduces a cutoff in the tails, which is like a bottom of the fermi sea, then a $1/d$ expansion becomes well defined. Some quantities like the total energy are infinite if one removes the cutoff. Other, low energy quantities, like the difference between the energy at finite temperatures and at zero temperature, the specific heat, and the magnetic susceptibility have a finite limit when the cutoff is removed. The Hilbert transform of (20) reads: $\tilde{D}(\zeta) = 1/(\zeta + it sign(Im(\zeta)))$. Using this into (7), one sees that a drastic simplification arises in this model: the Weiss field no longer depends on G, and reads explicitly:

$$G_{eff}(i\omega_n)^{-1} = i\omega_n + \mu + it\, sign\omega_n \tag{21}$$

Hence the mean-field equations are no longer coupled, and the problem reduces to solving S_{eff} with (21). It turns out that (21) is precisely the form for which S_{eff} becomes solvable by Bethe-Ansatz, and thus many properties of this $d \to \infty$ lattice model with long-range hopping can be solved for analytically. Some of its physical properties are non-generic however (such as the absence of a Mott transition), as will be discussed below.

III. DERIVATION OF THE MEAN-FIELD EQUATIONS

A. The cavity method

The purpose of this section is to derive the mean-field equations introduced above, using a method which is both simple and easily generalised to several models. This method is borrowed from classical statistical mechanics, where it is known under the name of 'cavity method'. The underlying idea is to focus on a given site of the lattice, say $i = o$, and to explicitly integrate out the degrees of freedom on all other lattice sites in order to define an effective dynamics for the selected site.

Let us first illustrate this on the Ising model. The effective hamiltonian H_{eff} for site o is defined from the partial trace over all other spins:

$$\sum_{S_i, i\neq o} e^{-\beta H} \equiv e^{-\beta H_{eff}[S_o]} \tag{22}$$

The hamiltonian H in eq.(1) can be splitted into three terms: $H = -h_o S_o - \sum_i J_{io} S_o S_i + H^{(o)}$. $H^{(o)}$ is the Ising hamiltonain for the lattice in which site o has been removed together with all the bonds connecting o to other sites, i.e a 'cavity' surrounding o has been created. The first term acts at site o only, while the second term connects o to other sites. In this term, $J_{io}S_o \equiv \eta_i$ plays the role of a field acting on site i. Hence summing over S_i's produces the generating functional of the connected correlation functions of the cavity hamiltonian $H^{(o)}$ and a formal expression for H_{eff} can be obtained as: $H_{eff} = const + \sum_{n=1}^{\infty}\sum_{i_1\ldots i_n}\frac{1}{n!}\eta_{i_1}\ldots\eta_{i_n} < S_{i_1}\ldots S_{i_n} >_c^{(o)}$. For a ferromagnetic system, with $J_{ij} > 0$ scaled as $1/d^{|i-j|}$ ($|i-j|$ is the Manhattan distance between i and j), only the first ($n = 1$) term survives in this expression in the $d \to \infty$ limit. Hence H_{eff} reduces to $H_{eff} = h_{eff}S_o$, where the effective field reads:

$$h_{eff} = h + \sum_i J_{oi} < S_i >^{(o)} \tag{23}$$

$< S_i >^{(o)}$ is the magnetization at site i once site o has been removed. The limit of large coordination brings in a further simplification to this expression: because each site has of the order of d neighbours, removing a single site produces an effect of order $1/d$ in local quantities, which can be neglected. Hence the magnetisation $< S_i >^{(o)}$ calculated for the cavity hamiltonian equals the magnetization $< S_i >$ for the full hamiltonian. Furthermore, translation invariance implies $< S_i >=< S_o >\equiv m$. Since this quantity can be computed using the effective hamiltonian H_{eff}, the Weiss field h_{eff} can be related to local quantities only, which leads to a closed set of mean-field equations.

Let us mention that the relation between the cavity and full lattice magnetizations is more involved for Ising models with non-uniform signs of J_{ij}. For spin-glass models with $J_{ij} = +1, -1$ at random, one is forced to scale the couplings as $1/\sqrt{d}$ so that a correction term must be retained in the difference $< S_i > - < S_i >^{(o)}$. This correction term, first discovered by Onsager in his studies on dielectrics, accounts for local-field effects created by the removal of one site ('reaction terms').

This derivation extends in a straightforward manner to quantum many-body models. It is convenient to write the partition function of the Hubbard model (??) as a functional integral over Grassman variables:

$$Z = \int \prod_i Dc^+_{i\sigma} Dc_{i\sigma} e^{-S} \tag{24}$$

$$S = \int_o^\beta d\tau (\sum_{i\sigma} c^+_{i\sigma} \partial_\tau c_{i\sigma} - \sum_{ij,\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} c^+_{i\sigma} c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}) \tag{25}$$

We follow closely the Ising analogy: all fermions are traced out except for site o in order to obtain an effective action:

$$\frac{1}{Z_{eff}} e^{-S_{eff}[c^+_{o\sigma} c_{o\sigma}]} \equiv \frac{1}{Z} \int \prod_{i \neq o,\sigma} Dc^+_{i\sigma} Dc_{i\sigma} e^{-S} \tag{26}$$

Note that the knowledge of S_{eff} allows us to calculate *all the local* correlation functions of the original Hubbard model, since we can couple sources to degrees of freedom at site o. This observation is valid in any number of dimensions. In order to obtain a formal expression for S_{eff}, the original action is again splitted into three parts: $S = S^{(o)} + S_o + \Delta S$, where $S^{(o)}$ is the lattice action in the presence of the 'cavity', and:

$$S_o = \int_0^\beta d\tau \sum_\sigma c^+_{o\sigma} (\partial_\tau - \mu) c_{o\sigma} + U n_{o\uparrow} n_{o\downarrow} \tag{27}$$

$$\Delta S = - \int_0^\beta d\tau \sum_{i\sigma} t_{io} (c^+_{i\sigma} c_{o\sigma} + c^+_{o\sigma} c_{i\sigma}) \tag{28}$$

Again, $\eta_i \equiv t_{io} c_{o\sigma}$ plays the role of a source, and the integration over fermions for $i \neq o$ brings in the generating functional of the connected Green's functions of the cavity Hamiltonian, $G^{(o)}$:

$$S_{eff} = \sum_{n=1}^{\infty} \sum_{i_1 \ldots j_n} \int \eta^+_{i_1}(\tau_{i_1}) \ldots \eta^+_{i_n}(\tau_{i_n}) \eta_{j_1}(\tau_{j_1}) \ldots \eta_{j_n}(\tau_{j_n}) G^{(o)}_{i_1 \ldots j_n}(\tau_{i_1} \ldots \tau_{i_n} \tau_{j_1} \ldots \tau_{j_n}) + S_o \tag{29}$$

As before, the large d limit (with a scaling $1/\sqrt{d}^{|i-j|}$ of the hopping t_{ij}) brings in a crucial simplification: the nth order term is of order $\frac{1}{d}^{n-2}$ so only $n = 2$ survives the $d \to \infty$ limit.

This is easily seen by means of a few examples. The scaling of t_{ij} insures that $G^{(o)}_{ij} \sim (\frac{1}{\sqrt{d}})^{|i-j|}$ so the first term is of order 1. The second order term involves a ***connected*** 4 point function $G^{(o)}_{ijkl}$ with falls off as $(\frac{1}{\sqrt{d}})^{|i-j|}(\frac{1}{\sqrt{d}})^{|i-k|}(\frac{1}{\sqrt{d}})^{|i-l|}$. While there are four sums which give d^4, and four factors of t giving $\frac{1}{d^2}$. The net result is, since $|i-j|$ is at least 2, of order $\frac{1}{d}$. The effective action therefore reduces to eq.(6) as $d \to \infty$, with:

$$G^{-1}_{eff} = -\partial_\tau + \mu - \sum_{ij} t_{oi} t_{oj} G^{(o)}_{ij} \tag{30}$$

Expression (30) is important because it relates the Weiss field G_{eff} to the Green's function $G^{(o)}_{ij}$ of a Hubbard model with one site removed. In order to obtain a closed set of equations, one still needs to relate the latter to the Green's function of the original lattice. Again, the $d \to \infty$ limit makes this possible here, but this relation takes in general a slightly more complicated form than for the classical case discussed above. On the Bethe lattice however, it remains very simple. In this case, the summation in (30) can be restricted to $i = j$ (since neighbours of o are completely disconnected on this lattice once the cavity has been introduced), and again, in the limit of infinite connectivity, removing one site does not change the Green's function so that $G^{(o)}_{ii} = G_{ii}$. Using translation invariance, one finally obtains expression (19) for the Weiss field on this lattice: $G^{-1}_{eff} = i\omega_n + \mu - t^2 G(i\omega_n)$.

For a general lattice, the relation between the cavity and full Green's functions reads:

$$G^{(o)}_{ij} = G_{ij} - \frac{G_{io} G_{oj}}{G_{oo}} \tag{31}$$

This equation can be proven by expanding both sides in powers of t_{ij}: the substracted term corresponds to paths connecting i and j through site o, which do not exist when the cavity is present. Interestingly, this equation, which is essential to the whole formalism, already appears in early works of Hubbard himself.

Inserting (31) into (30) we have to compute: $\sum_{ij} t_{io} t_{jo} G_{ij} - (\sum_i t_{io} G_{io})^2 / G_{oo}$. To proceed, let use Fourier transforms and insert the form (11) of the lattice Green's function, assuming a local self-energy (this has to be justified independently by power-counting in $1/d$). The above expression reads: $\int d\epsilon D(\epsilon) \frac{\epsilon^2}{\zeta - \epsilon} - (\int d\epsilon D(\epsilon) \frac{\epsilon}{\zeta - \epsilon})^2 / \int d\epsilon D(\epsilon) \frac{1}{\zeta - \epsilon}$ with $\zeta \equiv i\omega_n + \mu - \Sigma(i\omega_n)$. This can be simplified further, using the following relations:

$$\int \frac{D(\epsilon)\epsilon^2}{\zeta - \epsilon} = \zeta \int \frac{D(\epsilon)\epsilon}{\zeta - \epsilon} \ , \ \int \frac{D(\epsilon)}{\zeta - \epsilon} \epsilon = -1 + \zeta \int \frac{D(\epsilon)}{\zeta - \epsilon} \tag{32}$$

We have used $t_{oo} = \sum_k t_k = \int D(\epsilon)\epsilon = 0$. Finally, inserting (31) into (30) yields: $G^{-1}_{eff} = \Sigma + 1/\tilde{D}(i\omega_n + \mu - \Sigma)$, which coincides with (7,12).

B. Local nature of perturbation theory in infinite dimensions

From a historical perspective, the notion that in infinite dimensions the local Green's function obeys a closed functional equation was derived by various authors from considerations on perturbation theory in the interaction strength U.

Indeed, remarkable simplifications in the many-body diagrammatics occur in this limit, as first noticed by Metsner and Vollhardt. Consider a given diagram, in which the interaction term $Un_{i\uparrow}n_{i\downarrow}$ is depicted as a 4-leg vertex at site i, and in which each line stands for a free-fermion propagator between two sites (it is easier to proceed in real-space). The crucial observation made by Metsner and Vollhardt is that, whenever two *internal* vertices (i,j) can be connected by *at least three* paths, they must correspond to identical sites: $i=j$. This property is of course only true for $d=\infty$, and can be shown by simple power-counting. Since the hopping has been scaled by $1/\sqrt{d}$, each path made of fermion propagators connecting i to j will involve at least a factor $(1/\sqrt{d})^{|i-j|}$. On the other hand, i being held fixed, the eventual summation to be performed on the internal vertex j will bring in a factor of order d^R, the number of sites j located at a (Manhattan) distance $|i-j|\equiv R$ from i (R can be summed over afterwards). Hence an overall factor of $d^R(1/\sqrt{d})^{R\mathcal{P}_{ij}}$ where $\mathcal{P}ij$ is the number of (independant) paths joining i to j in the diagram. Thus, if $\mathcal{P}_{ij}>2$, only those contributions with $i=j$ ($R=0$) will survive the $d\rightarrow\infty$ limit. Alternatively, in the perhaps more familiar reciprocal-space formulation of perturbation theory, this property means that whenever two vertices can be 'collapsed' according to the rule above, the fermion propagators $G^{(0)}(k,i\omega_n)$ connecting them can be replaced by their local, k-independent counterpart $\sum_k G^{(0)}(k,i\omega_n)$, ignoring momentum conservation at the vertices. Frequency conservation is retained however as $d\rightarrow\infty$. Fig. illustrates these considerations on two diagrams contributing to the self-energy at second and fourth orders.

This simplification of weak-coupling expansions is of course very useful in practice, since evaluating momentum sums is the main practical obstacle in going to high orders. In fact, discarding momentum conservation at some vertices has sometimes been used in many-body physics as a 'local approximation'. The $d=\infty$ limit provides a framework in which this approximation can be controlled. This has been used recently by various groups.

Besides this practical use, these properties of perturbation theory in $d=\infty$ can also be used to formally derive the mean-field equations. Consider the self-energy $\Sigma_{ij}(i\omega_n)$. It is clear that not all diagrams of a standard weak-coupling expansion for this quantity can be fully collapsed to a local form. An example of a diagram which cannot be collapsed is provided by fig.. We can consider however making a 'skeleton' expansion of Σ rather than a direct expansion: this amounts to group together all corrections to internal propagators, so that all lines of a skeleton diagram stand for the full *interacting* fermion propagator G_{ij}. The

diagram in fig is a skeleton diagram, but the one in fig. is not . In this way, the self-energy can be viewed as a functional of the interacting Green's functions: $\Sigma_{ij}=\Sigma_{ij}^{skel}[\{G_{kl}\}]$. It is easily seen that two internal vertices of a *skeleton* diagram can always be connected by more than two paths, so that all diagrams contributing to Σ in a skeleton perturbation expansion can be fully collapsed to a single-site. More generally, this is true of the Luttinger-Ward free-energy functional $\Phi[G_{ij}]$, which is the sum of all vacuum to vacuum skeleton graphs, such that:

$$\Sigma_{ij}(i\omega_n)=\frac{\delta\Phi}{\delta G_{ij}(i\omega_n)} \tag{33}$$

Hence, as $d\rightarrow\infty$, Φ and Σ_{ij}^{skel} depend *only on the local (site-diagonal) Green's function* G_{ii}. An obvious consequence is that the self-energy is site-diagonal: $\Sigma_{ij}(i\omega_n)=\delta_{ij}\Sigma(i\omega_n)$. Futhermore, it must be possible to generate the functionals $\Phi[G]$ and $\Sigma^{skel}[G]$ from a purely local theory. A simple inspection of Feynman rules shows that the effective action $\mathcal{S}_{eff}$ precisely achieves this goal. From this point of view, the Weiss field G_{eff} just plays the role of a dummy variable which never enters the final forms of Φ,Σ^{skel}. Once these functionals are known, the actual *value* of Σ is found by writing that the local lattice Green's function is given by $\sum_k G(k,i\omega_n)$, namely:

$$G(i\omega_n)=\int d\epsilon\frac{D(\epsilon)}{i\omega_n-\epsilon-\Sigma^{skel}[G(i\omega_n)]} \tag{34}$$

This should be viewed as a functional equation for $G(i\omega_n)$, which is of course eqivalent to the self-consistency condition (7). This point of view is formally useful to prove reduction to a single- site problem, but is not practical because of the difficulty in handling skeleton functionals. In fact, it has been so far impossible to obtain exact or approximate expressions of Σ^{skel} for the Hubbard model which would give reasonable results when inserted in (34), except for very small U. An exception is the Falicov-Kimball model (section.) for which $\Sigma^{skel}[G]$ can be obtained exactly. For most models, it is much more useful in practice to think of all quantities as functionals of the Weiss field G_{eff} and to promote the latter at the rank of a fundamental object.

This formalism is also useful to establish the relation between the lattice and the impurity model free-energies, Ω and Ω_{imp} Indeed, Ω is related to the Luttinger-Ward functional Φ by

:

$$\frac{\Omega}{N}=\Phi[G]+\frac{T}{N}\sum_{n,k,\sigma}[lnG_\sigma(k,i\omega_n)-\Sigma_\sigma(i\omega_n)G_\sigma(k,i\omega_n)] \tag{35}$$

while, for the impurity model (6):

$$\Omega_{imp}=\Phi[G]+T\sum_{n\sigma}[lnG_\sigma(i\omega_n)-\Sigma_\sigma(i\omega_n)G_\sigma(i\omega_n)] \tag{36}$$

Eliminating the functional Φ, one obtains the following relation:

$$\frac{\Omega}{N} = \Omega_{imp} - T\sum_{n\sigma}[\int_{-\infty}^{+\infty} d\epsilon D(\epsilon) ln(i\omega_n + \mu - \Sigma_\sigma(i\omega_n) - \epsilon) + lnG_\sigma(i\omega_n)] \quad (37)$$

Note that also the internal energy can be expressed in terms of local quantities only:

$$\frac{E}{N} = T\sum_{n,\sigma}\int_{-\infty}^{+\infty} d\epsilon \frac{\epsilon D(\epsilon)}{i\omega_n + \mu + h\sigma - \Sigma_\sigma(i\omega_n) - \epsilon} + \frac{1}{2}T\sum_{n,\sigma}\Sigma_\sigma(i\omega_n)G_\sigma(i\omega_n) \quad (38)$$

IV. PHASES WITH LONG-RANGE ORDER

For simplicity, the mean-field equations have been derived in the previous sections under the condition that no long-range order is present. This section consider the possibility of phases with some symmetry breaking and establish the mapping onto an impurity model for these cases.

A. Ferromagnetic LRO

In the presence of a magnetic field h coupl;ed to S_z, or if there is a spontaneous uniform magnetization the Green's functions for up and down electrons are not equivalent. Then one has to retain the spin-dependence of the local Greens functions and of the Weiss field in the derivations of section. The local effective action associated with the Hubbard model in a ferromagnetic phase reads:

$$S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\sigma^+(\tau)G^{-1}_{eff,\sigma}(\tau - \tau')c_\sigma(\tau') + U\int_0^\beta d\tau\, n_\uparrow(\tau)n_\downarrow(\tau) \quad (39)$$

The self consistent equations for the two functions $G_\uparrow, G_\downarrow$ and their corresponding Weiss fields are straightforward generalizations of (7) to this spin-dependent case. They read:

$$G_\sigma(i\omega_n) = \int d\epsilon \frac{D(\epsilon)}{i\omega_n + \mu + h\sigma - \Sigma_\sigma(i\omega_n) - \epsilon} \quad (40)$$

where:

$$G_\sigma(i\omega_n) \equiv < c_\sigma^+(i\omega_n)c_\sigma(i\omega_n) >_{S_{eff}}\ ,\ \Sigma_\sigma(i\omega_n) = G^{-1}_{eff,\sigma} - G^{-1}_\sigma \quad (41)$$

From the solution of (39,40), one can reconstruct the lattice Green's functions:

$$G_\sigma(k, i\omega_n) = \frac{1}{i\omega_n + \mu + h\sigma - \epsilon_k - \Sigma_\sigma(i\omega_n)} \quad (42)$$

The spontaneous magnetization in the ferromagnetic phase is given by:

$$m = lim_{h\to o}\sum_n e^{i\omega_n o^+}[G_\uparrow(i\omega_n) - G_\downarrow(i\omega_n)] \quad (43)$$

B. Antiferromagnetic and incommensurate LRO

Similar considerations can be used to study commensurate antiferromagnetic long range order in the Hubbard model. Note that the $1/\sqrt{d}$ scaling of the hopping amplitude is such that the exchange coupling obtained For simplicity we will again concentrate on the Hubbard model and we will add to the Hamiltonian a staggered magnetic field to the hamiltonian

$$H_s = h_s\sum_{i\sigma} e^{iQ\cdot r_i}C^+_{\sigma i}C_{\sigma i} \quad (44)$$

and to restrict ourselves to the simple cubic lattice. In this case there are two inequivalent sublattices, say A and B and a simple relation between the local Green's functions on each sublattice: $G_{ii,\sigma} = G_{A,\sigma}, G_{B,\sigma}$ for $i \in A, B$ with:

$$G_{A\sigma}(i\omega_n) = G_{B\sigma}(i\omega_n) \quad (45)$$

In $d = \infty$, the skeleton functional Φ now depends on both local Green's functions: $\Phi = \Phi[G_{A\sigma}, G_{B\sigma}]$. The self-energy is purely local and can take two values with $\Sigma_{A\sigma}(i\omega_n) = \Sigma_{B\sigma}(i\omega_n)$. It is convenient to write the hamiltonian in terms of two sublattice operators:

$$\begin{aligned} H_0 = &\sum_{\sigma K\epsilon RBZ}\epsilon_K(C^+_{AK\sigma}C_{BK\sigma} + C^+_{BK\sigma}C_{AK\sigma}) \\ &+ \sum_{\sigma K\epsilon RBZ}\sigma h_s(C^+_{AK\sigma}C_{AK\sigma} - C^+_{BK\sigma}C_{BK\sigma} \end{aligned} \quad (46)$$

The Greens functions are obtained by inverting the matrix

$$\begin{pmatrix} \zeta_{A\sigma} & -\epsilon_k \\ -\epsilon_k & \zeta_{B\sigma} \end{pmatrix}$$

Here $\zeta_{A\sigma} = i\omega_n + \mu - \sigma h_s - \Sigma_{A\sigma}, \zeta_{B\sigma} = i\omega_n + \mu + \sigma h_s - \Sigma_{B\sigma}$. The impurity model to be considered is still (??), but the self consistency conditions now read:

$$G_{\alpha\sigma} = \zeta_{\alpha\sigma}\int_{-\infty}^{\infty} d\epsilon \frac{D(\epsilon)}{\zeta_{A\sigma}\zeta_{B\sigma} - \epsilon^2} \quad (47)$$

with $\alpha = A, B$. The staggered magnetization and the free energy of the antiferromagnetic phase are given by similar equations as above.

It is instructive to notice that the simplest approximation to the self energies: $\Sigma_{A\sigma} = (U/2)(n_{A\sigma} - n_{B\sigma})$, reproduces the usual Hartree Fock results for the staggered magnetization. Also as soon as Neel order is established and $\Sigma_{A\sigma} \neq \Sigma_{B\sigma}$ it is possible to open a gap in the single particle spectrum i.e. $ImG(\omega + i0^+) = 0$ if $|\omega + \mu + \frac{\Sigma_B - \Sigma_A}{2}| \leq \frac{(\Sigma_A + \Sigma_B)}{2}$ This should be contrasted with the results obtained in the unbroken symmetry phase. Notice that to study the phase transition between different magnetic phases we have to investigate a free energy functional in the space of all possible magnetic states. Alternatively one can calculate directly the relevant divergent susceptibility.

C. Superconductivity and pairing in infinite dimensions

Superconducting long-range order can be studied in the present dynamical mean-field framework. We shall illustrate this on the example of the 2-band 'copper-oxyde' model described below, in section. Local 'anomalous' Green's functions are introduced:

$$F_d(\tau-\tau') \equiv -T < d_{i,\downarrow}(\tau) d_{i,\uparrow}(\tau') > \quad F_p(\tau-\tau') \equiv -T < p_{i,\downarrow}(\tau) p_{i,\uparrow}(\tau') > \tag{48}$$

Singlet pairing corresponds to F even: $F(\tau) = F(-\tau) = -F(\beta-\tau)$, while $S_z = 0$ triplet pairing corresponds to F odd: $F(\tau) = -F(-\tau) = F(\beta-\tau)$ Allowing for a non-trivial time-dependence of F is crucial. The underlying physical idea is that on-site *equal-time* pairing is likely to be strongly suppressed in the presence of a strong on-site repulsion but that pairing involving a 'time-lag' between the paired holes may occur. This idea dates back to Berezinskii's proposal for triplet pairing in ^3He, a generalization of which has been recently considered for cuprates superconductors by Balatsky and Abrahams.

In the preence of a non-zero F it is convenient to work with Nambu spinors $\Psi_d^+ \equiv (d_\uparrow^+, d_\downarrow)$ (similarly Ψ_p) and with the matrix formulation of one-particle Green's functions:

$$D(\tau-\tau') \equiv -T < \Psi(\tau)\Psi^+(\tau') > = \begin{pmatrix} G_d(\tau-\tau') & F_d(\tau-\tau') \\ F_d(\tau-\tau') & -G_d(\tau'-\tau) \end{pmatrix} \tag{49}$$

With these notations, the kinetic term of the hamiltonian $\mathcal{H}$ reads: $-t_{ij}\Psi_{d,i}\sigma_3\Psi_{p,j}$ where σ_3 denotes the Pauli matrix. We will illustrate the derivation of the mean field equations in the superconducting state using the coper oxide model of the previous section as an example.

We integrate out fermionic variables on all sites except on a single copper site. The 'impurity' action obtained in this way now reads:

$$S_{eff} = U_d \int_0^\beta d\tau\, n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) - \int_0^\beta d\tau \int_0^\beta d\tau' \Psi_d^+(\tau) D_0^{-1}(\tau-\tau')\Psi_d(\tau') \tag{50}$$

where D_0 is given in terms of D and P by the self-consistency equations:

$$\begin{aligned} D_0^{-1}(i\omega_n) &= i\omega_n + (\mu-\epsilon_d)\sigma_3 - t_{pd}^2\sigma_3 P(i\omega_n)\sigma_3 \\ P^{-1}(i\omega_n) &= i\omega_n + (\mu-\epsilon_p)\sigma_3 - t_{pd}^2\sigma_3 D(i\omega_n)\sigma_3 \end{aligned} \tag{51}$$

We can account for an externally applied dynamic pairing field $\Delta_d(i\omega_n)$ on all copper sites in the original lattice problem by adding a forcing term

$$\begin{pmatrix} 0 & \Delta_d(i\omega_n) \\ \Delta_d(i\omega_n) & 0 \end{pmatrix} \tag{52}$$

to the r. h. s. of eq. (51).

The impurity action [50] describes an Anderson impurity in a superconducting medium. Since this problem, even with static pairing turns out to be highly non trivial, we can expect that the self consistent solution of eqs (51) will allow for very intricate densities of states. The equivalent of the Weiss mean field hamiltonian for a strongly correlated superconductor in the same spirit that the Anderson impurity model action is the quantum equivalent of a Weiss mean field hamiltonian for a strongly correlated metallic state.

V. MEAN-FIELD EQUATIONS FOR VARIOUS MODELS

A. Copper Oxide lattice in large dimensions

A two-orbital model closely related to the structure of copper-oxygen layers can be built, which has a well defined limit when the coordination number gets large.

The hamiltonian reads:

$$\mathcal{H} = -\sum_{i\in A, j\in B,\sigma} t_{ij} d_{i\sigma}^+ p_{j\sigma} + h.c. + \epsilon_p \sum_{j\in B,\sigma} p_{j\sigma}^+ p_{j\sigma} + \epsilon_d \sum_{i\in A,\sigma} d_{i\sigma}^+ d_{i\sigma} + U_d \sum_{i\in A} n_{i\uparrow}^d n_{i\downarrow}^d \tag{53}$$

(d_σ, p_σ) represent two atomic orbitals on different sublattices (A, B) of a bipartite lattice. The ('copper') orbital d_σ is strongly correlated, while the ('oxygen') orbital p_σ is uncorrelated. Each site has identical connectivity z, so that the model describes a 'CuO'-type system. This model is a large d realization of the three-band model proposed by Emery and by Varma *et al* as a minimal model of the copper-oxide planes.

In the absence of correlations ($U_d = 0$), diagonalization of $\mathcal{H}$ yields two bands (bonding and antibonding): $E_k^\pm = \{\epsilon_p + \epsilon_d \pm \sqrt{(\epsilon_p-\epsilon_d)^2 + 4\epsilon_k^2}\}/2$, where ϵ_k is the Fourier transform of t_{ij}. These bands are separated by a gap $\Delta_0 \equiv \epsilon_p - \epsilon_d$. The copper and oxygen density of states have simple expressions for $U_d = 0$:

$$N_d(\epsilon) = \sqrt{\frac{\epsilon-\epsilon_p}{\epsilon-\epsilon_d}}\, N(\sqrt{(\epsilon-\epsilon_p)(\epsilon-\epsilon_d)}) \quad N_p(\epsilon) = \sqrt{\frac{\epsilon-\epsilon_d}{\epsilon-\epsilon_p}}\, N(\sqrt{(\epsilon-\epsilon_p)(\epsilon-\epsilon_d)}) \tag{54}$$

where $N(\epsilon) \equiv \sum_k \delta(\epsilon-\epsilon_k)$.

The limit of infinite connectivity $z \to \infty$ requires a scaling of the hybridization t_{ij} as: $t_{ij} = t_{pd}/\sqrt{z}$, so that the density of states $N(\epsilon)$ has a proper limit. In practice, one may consider the d-dimensional hypercubic lattice ($z = 2d$), for which: $N(\epsilon) = 1/\sqrt{2\pi}t_{pd}\, e^{-\epsilon^2/2t_{pd}^2}$ as $d \to \infty$ or the Bethe lattice with connectivity z for which $N(\epsilon) = \sqrt{4-(\epsilon/t_{pd})^2}2\pi t_{pd}$ as $z \to \infty$.

The associated impurity model describing the local physics at the 'copper' sites is given by:

$$S = U_d \int_0^\beta d\tau\, n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d_\sigma(\tau) D_0^{-1}(\tau - \tau')\, d_\sigma^+(\tau') \qquad (55)$$

Denoting by $D(\tau - \tau') \equiv - < T d(\tau) d^+(\tau') >_S$ the *interacting* Green's function calculated with this action and Σ_d the impurity self-energy as a functional of D_0, $\Sigma_d(i\omega_n) \equiv D_0^{-1}(i\omega_n) - D^{-1}(i\omega_n)$.

we can set the self-consistency equation for D_0, ($\omega_n = (2n+1)\pi/\beta$):

$$D(i\omega_n) = \zeta_p(i\omega_n) \int d\epsilon \frac{N(\epsilon)}{\zeta_p(i\omega_n)\zeta_d(i\omega_n) - \epsilon^2} \qquad (56)$$

where we have set set $\zeta_p(i\omega_n) \equiv i\omega_n + \mu - \epsilon_p$, $\zeta_d(i\omega_n) \equiv i\omega_n + \mu - \epsilon_d - \Sigma_d(i\omega_n)$.

Once Eqs.(56, 55) are solved for D_0 , the impurity self energy evaluated at the self consistent value of D_0 gives the d electron lattice self energy which determines completely the lattice one-particle Green's function. In the $(d_{k\sigma}, p_{k\sigma})$ basis, it reads in matrix form:

$$\frac{1}{\zeta_p\zeta_d - \epsilon_k^2} \begin{pmatrix} \zeta_p & \epsilon_k \\ \epsilon_k & \zeta_d \end{pmatrix} \qquad (57)$$

In the $z \to \infty$ limit, self-energies become purely site-diagonal, so that Σ_d depends only on frequency and the Σ_{pd} component is absent. The absence of the diagonal component Σ_p in eq.(57) comes from the simplifying assumption of an uncorrelated p-orbital. From eq.(57), one sees that the self-consistency equation simply means that the impurity model Green's function must coincide with the on-site d-orbital Green's function: $D(i\omega_n) = \sum_k D(k, i\omega_n)$. Also, the p-orbital on-site Green's function is simply given by:

$$P(i\omega_n) = \zeta_d(i\omega_n) \int d\epsilon \frac{N(\epsilon)}{\zeta_p(i\omega_n)\zeta_d(i\omega_n) - \epsilon^2} \qquad (58)$$

Notice that on the Bethe lattice the self consistency conditions have the simpler form:

$$D_0^{-1} = i\omega_n + \mu - \epsilon_d - t_{pd}^2 P(i\omega_n) \qquad P^{-1} = i\omega_n + \mu - \epsilon_p - t_{pd}^2 D(i\omega_n) \qquad (59)$$

B. The Periodic Anderson Model

The periodic Anderson hamiltonian is defined by:

$$H = \sum_K C_{K\sigma}^+ C_{K\sigma} + V \sum_{i\sigma} (C_{i\sigma}^+ f_{i\sigma} + f_{i\sigma}^+ C_{i\sigma}) + \epsilon_f \sum_i f_{i\sigma}^+ f_{i\sigma} + U \sum_i n_{f_i\uparrow} n_{f_i\downarrow} \qquad (60)$$

It describes the interaction of localised f moments with delocalised conduction electrons with dispersion ϵ_k. This is the starting point of many theoretical investigations of the heavy fermion problem.

The Green's functions read:

$$G_c(i\omega_n, K)^{-1} = i\omega_n - \epsilon_K - \frac{V^2}{[i\omega_n - \epsilon_f - \Sigma(i\omega_n)]} = - < C(i\omega_n) C^+(i\omega_n) >^{-1} \qquad (61)$$

$$G_f(i\omega_n, K)^{-1} = i\omega_n - \epsilon_f - \Sigma(i\omega_n) - \frac{V^2}{(i\omega_n - \epsilon_K)} = - < f(i\omega_n) f^+(i\omega_n) >^{-1} \qquad (62)$$

$$G_{cf}(i\omega_n, K)^{-1} = \frac{V}{(i\omega_n - \epsilon_K)} \frac{1}{i\omega_n - \epsilon_f - \Sigma(i\omega_n) - \frac{V^2}{(i\omega_n - \epsilon_K)}} = - < f(i\omega_n) C^+(i\omega_n) >^{-1} \qquad (63)$$

Here $\Sigma(i\omega_n)$ is the self energy part of the f-electrons (irreducible with respect to G_c G_f and G_{fc}). Consider the skeleton expansion of Σ. In infinite dimensions it is a functional of the local f electron Green function only, $\Sigma[G_{f,ii}, i\omega_n]$. Using the logic of section II we view the f electron self energy as an impurity self energy

$$\Sigma_{imp}(G_0, i\omega_n) = G_0^{-1} - < f(i\omega_n) f^+(i\omega_n) >_{S_{imp}(G_0)}^{-1} \qquad (64)$$

The average <> is calculated with the impurity action

$$S_{imp}(G_0) = \sum_n f_\sigma^+(i\omega_n) G_o^{-1}(i\omega_n) f_\sigma(i\omega_n) + U \int_o^\beta d\tau f_\uparrow^+(\tau) f_\uparrow(\tau) f_\downarrow^+(\tau) f_\downarrow(\tau) \qquad (65)$$

The self consistency condition requires that the local f Green's function of the original problem obtained 62 coincides with the local Greens function of the impurity problem i.e.

$$\int_{-\infty}^{\infty} \frac{d\epsilon D(\epsilon)}{i\omega_n - \epsilon_f - \Sigma_{imp}[i\omega_n, G_0^*] - \frac{V^2}{i\omega_n - \epsilon}} = < f^+(i\omega_n) f(i\omega_n) >_{S_{imp}(G_0^*)} \qquad (66)$$

Here $D(\epsilon)$ refers to the density of states of the conduction electrons in infinite dimensions.

Impurity models for the ferromagnetic and antiferromagnetic phases of this model can be easily constructed following the lines of section III.

C. The N channel spin 1/2 Kondo Lattice

The hamiltonian

$$\sum_{K\sigma a} \epsilon_K C^+_{K\sigma a} C_{K\sigma a} + J \sum_{ia\sigma\sigma' a} S^a_i C^+_{ia\sigma} \sigma^a_{\sigma\sigma'} C_{ia\sigma'} \tag{67}$$

describes N "flavours" or "channels" of conduction electrons interacting with a lattice of localised 'spin 1/2 moments described by spin operators S^a_i where i is a lattice and a an $Su(2)$ index .

The *conduction electron* Green function defines a self energy

$$G_c(i\omega_n, K) = \frac{1}{i\omega_n - \epsilon_K - \Sigma(i\omega_n)} \tag{68}$$

Using the tehcniques of section () we derive the local impurity action by integrating out all the degrees of freedom except for those at a selected site to obtain:

$$S_{imp} = -\sum_n C^+_\sigma(i\omega_n) G^{-1}_o(i\omega_n) C_\sigma(i\omega_n) + J \sum_a \int_o^\beta d\tau S^a \hat{\sigma}^a + L_s[S] \tag{69}$$

where $L_s[S]$ is a spin $\frac{1}{2}$ Lagragian which can be expressed in any of the standard representations used to construct a spin lagrangian such as the Popov representation , the slave fermion or the Schwinger boson representation, the Abrikosov pseudo fermion or alternatively if the spin is treated in the coherent path integral formulateion then L_s is the spin Berry phase . In eq. 69

$$\hat{\sigma} = \sum_{\sigma\sigma' a} C^+_{\sigma a} \sigma_{\sigma\sigma'} C_{\sigma' a} \tag{70}$$

and the second term describes the interaction of a spin with conduction electrons at the origin. This is the single impurity (N channel) Kondo problem. An impurity model which gives rise to the local action 69 is the Multichannel Kondo impurity

$$\sum_{K\sigma a} \epsilon_K C^+_{K\sigma a} C_{K\sigma a} + J \sum_{a\sigma\sigma' a} S^a_i C^+_{0a\sigma} \sigma^a_{\sigma\sigma'} C_{0a\sigma'} \tag{71}$$

S_{imp} allow us to calculate the conduction electron self energy

$$\Sigma(i\omega_n)(G^o) = < C^+_\sigma C_\sigma >^{-1} - S_{imp}(G^o_o) - (G^o)^{-1} \tag{72}$$

To express the self consistency condition as

$$< C^+_\sigma C_\sigma >_{S_{imp}(G^o_o)} = \int_{-\infty}^{\infty} \frac{D(\epsilon) d\epsilon}{[i\omega_n - \epsilon - \Sigma_(G^o_o)]} \tag{73}$$

In the last few years there has been an intensive search of lattice models exhibiting a non Fermi liquid fixed point at low temperatures. Model (71) with $N > 1$ is a very interesting candidate for this behavior since in the absence of the self consistency condition (73) the local action (70) is known since Blandin and Nozieres to be driven to a non Fermi liquid fixed point. This implies that the lattice model () with the Lorentzian density of states is not a Fermi liquid. The same is likely to be true for other lattices in $d = \infty$.

D. The Falicov Kimball Model

We now turn to the Falicov Kimball model, the first model to have been solved exactly in infinite dimensions in the pioneering work of Brandt and Mielsch. This is briefly explained here.

This model is defined by the following Hamiltonian:

$$H = \sum_{ij} t_{ij} d^+_i d_j + \sum_i E^o_f f^+_i f_i - \mu \sum_i (d^+_i d_i + f^+_i f_i) + U \sum_i d^+_i d_i f^+_i f_i \tag{74}$$

It includes spinless conduction d electrons with hopping parameters t_{ij}, localized f electrons which have an energy level E^o_f with respect to the center of the d electron band. The on-site interaction between d and f electrons is given by U. When $E^o_f = 0$, the model corresponds to the spin-$\frac{1}{2}$ Hubbard model with only one of the spin components allowed to hop. Integrating out all the electrons except for those at the central site we obtain the impurity action:

$$S_{site}(G_o) = -\int_0^\beta d\tau \int_0^\beta d\tau' c^+(\tau) G^{-1}_o(\tau - \tau') c(\tau') + \int_0^\beta d\tau (U c^+ c d^+ d + f^\dagger (\frac{\partial}{\partial\tau} + E_f 0) f \tag{75}$$

The local Green's function is easily obtained from the impurity action

$$G(i\omega_n) = - < dd^+ >_{S(G_o)} = \frac{w_o}{G^{-1}_o(i\omega_n)} + \frac{w_1}{G^{-1}_o(i\omega_n) - U} \tag{76}$$

where $w_o = 1 - w_1$ and

$$w_1 = [1 + exp(\beta(E^o_f - \mu) + \sum_n [ln(G^{-1}_o(i\omega_n)) - ln(G^{-1}_o(i\omega_n) - U)] e^{i\omega_n 0^+})]^{-1} \tag{77}$$

Differentiating the partition function with respect to E^o_f, we see that w_1 is the f particle number per site.

The local self energy is defined through

$$G(i\omega_n) = (G^{-1}_o(i\omega_n) - \Sigma_n)^{-1} \tag{78}$$

When combined with the explicit form of the Green's function Eq. (76), this leads to the functional form of the self-energy in terms of the local Green's function:

$$\Sigma_n(G_n) = U/2 - 1/2G_n + \sqrt{(U/2 - 1/2G_n)^2 + w_1 U/G_n} \tag{79}$$

Furthermore, a self-consistent equation is provided by the Dyson equation:

$$G_n = \int_{-\infty}^{\infty} d\epsilon \frac{N_o(\epsilon)}{i\omega_n + \mu - \epsilon - \Sigma_n(G_n)} \tag{80}$$

where $N_o(\epsilon)$ is the d-particle bare density of states. the Gaussian density of states.

The effective hamiltonian corresponding to the impurity action 75 is the xray hamiltonian

$$H = \sum_{ij} t_{ij} d_i^\dagger d_j + E_f^o f^+ f + U d_0^\dagger d_0 f^+ f \tag{81}$$

VI. METHODS OF SOLUTION

The mean field equations are coupled functional equations to be solved for the Weiss field and the local Greens function. The most difficult aspect of the mean field theory is the solution of the Anderson impurity model in an arbitrary bath. This class of problems has been studied intensively in the last 30 years and we will draw on this knowledge to make exact and approximate statements on the solution lattice models in large dimensions. The essential insight is to use *reliable* approximations to calculate $G\{G_0\}$. This step captures the local aspects of the problem. The self consistency condition [7] then brings back the lattice aspect of the problem.

Several techniques that have been used in the analysis of the mean field equations, they range from qualitative arguments and analytic perturbative schemes to numerical methods based on Quantum Montecarlo and exact diagonalization. All the insights obtained on the Mott transition problem rely on a combination of these techniques.

A. Quantum Montecarlo

Numerical schemes introduce a *discrete* parametrization of the Greens functions, and the Weiss field , involving a finite number N_p of parameters and reduce the system of functional equations (26)(7)(??) to a system of N_p non linear equations in N_p unknowns. The hope is that as N_P increases physical quatities converge relatively fast to their physical values so that this converged value can be inferred by extrapolating results obtained from a finite (and usually small) number of parameters N_p. The application of Quantum Montecarlo methods to impurity models was carried out by Hirsch and Fye. Here we present an alternative derivation of this class of algorithms.

To apply the quantum montecarlo method to our problem one parametrizes $G(\tau)$ in $[0,\beta]$ by a discrete set of points $G(\tau_i)$ $\tau_i = \frac{i\beta}{N_p}$ $i = 0 \ldots N_p - 1$, Then one introduces a discrete Hubbard Stratonovich field to linearize the interaction term and reduce the action [26] to a quadratic form. Then one traces over the fermion field and the partition function then becomes a sum over Ising variables $\sigma_i, i = 0, ..., N_p - 1$.

$$Z = \sum_{\sigma_l} det[A_\uparrow(\sigma_l)][A_\downarrow(\sigma_l)] \tag{82}$$

Here A is the discretized version of the effective action after the U term is linearised by an Ising Hubbard Stratonvic transformation.

The discretised Greens function are also expressed as a sum over Ising variables.

$$G(\tau_l - \tau_{l'}) = \frac{\sum_{\sigma_l} det[A_\uparrow(\sigma_l)][A_\downarrow(\sigma_l)] A^{-1}_{l,l'}}{Z} \tag{83}$$

Most of the work was carried out with the Fye Hirsch algorithm which corresponds to a specific discretization of the functional integral

$$A^\mu_{ll'} = \delta_{ll'} + e^{V_l^\mu} e^{-\Delta\tau\mu} \delta_{ll'+1} + e^{V_l^\mu} \Delta_{l,l'} \tag{84}$$

Here $\mu = \uparrow, \downarrow$, $\Delta_{ll'}$ is a discretized version of the Hybridisation function in eq.[??] and the antiperiodic delta function is defined by $\delta_{ll'+1} = 1$ if $l = l' + 1, l = 2, \ldots N-1$,$\delta_{ll'+1} = -1$ if $l = ll' = N$ and is zero otherwise. The quantities V_l^μ are proportional to the Ising variables σ_l

$$V_l^\mu = \sigma_l \mu \text{arccosh}(e^{\epsilon\Delta\tau U}) \tag{85}$$

All the sums are evaluated by importance sampling. To decide wether a Montecarlo move from σ to σ' is accepted or rejected one needs the ratio of two determinants. This ratio is evaluated in terms of the local Greens function

$$R \equiv \frac{det[A(\sigma_l')]}{det[A(\sigma_l)]} = 1 + (1 - G(l,l))(e^{V_l' - V_l} - 1) \tag{86}$$

When the move is accepted the new greens function G' is given by

$$G'(l'',l') = G(l'',l') + (G(l'',l) - \delta_{l''l})(e^{V_l' - V_l} - 1)\frac{G(l,l')}{R} \tag{87}$$

Other discretizations of the effective action such as

$$A^\mu_{ll} = \delta_{ll} + e^{V_l^\mu} e^{-\Delta\tau\mu} \delta_{ll+1} + \Delta_{l,l'} \tag{88}$$

have been investigated and they give comparable results. Therefore we concluded that a major improvement of the algorithm requires a discretization which is accurate to order $\Delta\tau^2$

Typical values of L are 64 and 128 and 254. Typical values of $\delta\tau$ is .25 which in practice restricts the simulations to inverse temperatures less than β of 64 .

We stress that there are two approximations in this scheme, the first has to do with the finite discretization of the greens function while the second has to do with the subsequent discretization of the functional integral. Both this approximations get better as $\delta\tau$ goes to zero. In addition there is a source of error in the evaluation of the sum by importance sampling. This statistical error can be reduced by increasing the length of Montecarlo run.

B. Exact diagonalisation

The results of section I paves the way for the application of exact diagonalization techniques to large d problem. To use exact diagonalization methods one needs to produce: a) a correspondence between the exact G_0 and an Anderson hamiltonian involving a finite number of conduction electron orbitals and b) a correspondence between the exact local Green's function $G(i\omega_n)$ and G_0 or the parameters of the Anderson impurity hamiltonian.

Once the correspondence a is defined, one can carry out the operation illustrated on the upper box in figure ??. Given G_0 ,the correspondence a assigns to it a unique Anderson impurity with a finite number of orbitals, i.e. a finite dimensional matrix whose green function G can be computed by standard exact diagonalization algorithms.

Once the correspondence b) is established we can carry out the operation illustrated on the lower box in figure ??. The G obtained by the methods described in the previous paragraph contains a large number of poles. The correspondence b) assigns to any Greens function G a G_0 containing a finite (small) number of poles, i.e. an Anderson impurity model with a finite number of conduction electron orbitals.

Combining these two steps we obtain a discretized version of the mean field equations that converges to the exact answer as the number of orbitals is increased. There is a large amount of flexibility in tbe application of this method.

In the first application of exact diagonalisation techniques to the $d = \infty$ Hubbard model Krauth and Caffarel associated to $G0$ an Anderson model with N_c bloch orbitals.

$$H_{AM} = \sum_{kl,N_b} \epsilon_k a^+_{k\sigma} a_{k\sigma} + U f^+_\uparrow f_\uparrow f^+_\downarrow f_\downarrow + \sum_{k=1,N_b} V_k (a^+_{k\sigma} f_\sigma + f^+_\sigma a_{k\sigma}) + \epsilon_f f^+_\sigma f_\sigma \qquad (89)$$

For the purposes of the exact diagonalization it can be visualized as a star geometry, (see fig ??). To carry out step b, one represents the greens function $G(i\omega_n)$ obtained form the exact diagonalisation by a rational approximant descibed by $2N_b$ parameters which are obtained by minimaising the L_2norm of the difference between $G(i\omega_n)$ and its rational approximant:

$$\chi^2 = \sum_{\omega_n=\Omega_{min}}^{\Omega_{max}} |\sum_k \frac{\tilde{V}_k^2}{i\tilde{\omega}_n - \tilde{\epsilon}_k} - G(i\omega_n)|^2 \qquad (90)$$

here Ω_{min} and Ω_{max} are low and high frequency cut-offs, respectively.

G_0 is parametrised by an Anderson model :

$$\begin{aligned} H = & \sum_\sigma \sum_{p=>,<} \Big(\sum_{a=1}^{N_C-1} a^p_a c^{p\dagger}_{a\sigma} c^p_{a\sigma} + b^p_0 (c^{p\dagger}_\sigma f_\sigma + h.c.) \\ & + \sum_{a=1}^{N_C-2} (b^p_a c^{p\dagger}_{a\sigma} c^p_{a+1\sigma} + h.c.)) + U(n_{f\uparrow} - \frac{1}{2})(n_{f\downarrow} - \frac{1}{2}) \\ & + \sum_\sigma b_0 (f^\dagger_\sigma c_{0\sigma} + h.c.). \end{aligned} \qquad (91)$$

It contains two chains of conduction electrons and an extra orbital having zero energy.

The correspondence b is obtained by: decomposing the Green function $G(z)$ into "particle" and "hole" contributions as $G(z) = G^>(z) + G^<(z)$ with $G^>(z) =< 0|c\frac{1}{z-(H-E_0)}c^\dagger|0 >$ and $G^<(z) =< 0|c^\dagger\frac{1}{z+(H-E_0)}c|0 >$. and expanding the respective contributions in a continued fraction expansion:

$$< f_0^{>/<}|\frac{1}{\omega \mp (H - E_0)}|f_0^{>/<} >= \cfrac{< f_0^{>/<}|f_0^{>/<} >}{z - a_0^{>/<} - \cfrac{b_1^{>/<}}{z-a_1^{>/<} - \cfrac{b_2^{>/<}}{z-a_2^{>/<} - \dots}}} \qquad (92)$$

where $|f_0^> >= f^\dagger|gs >$, $|f_0^< >= f|gs >$ and $|f_{n+1} >= H|f_n > -a_n|f_n > -b_n^2|f_{n-1} >$, $a_n =< f_n|H|f_n >$, $b_n^2 = \frac{<f_n|f_n>}{<f_{n-1}|f_{n-1}>}$, $b_0 = 0$. This implies that $G^>$ and $G^<$ can be regarded as resulting from a Hamiltonian describing an impurity coupled to two chains with site energies $a_n^{>/<}$ and hopping amplitudes $b_n^{>/<}$ and an extra site at zero energy. Since the number of poles in the Green function is in general larger than then number of sites of the hamiltonian and the continued fraction is truncated to a given finite depth.

The approximation in this scheme relies on the fact that the continued fraction representation captures exactly the moments of the energy of the hamiltonian, up to the order retained in the continued fraction. It can thus be thought of as the best rational approximation in a norm that measures the difference between the first $2N_c$ moments of the exact greens function and its rational approximant. The approximate momenta moment by moment fitting. The extra site at the Fermi energy is introduced in order to better represent the low frequency region and, more importantly, to allow a feed-back of a metallic bath.

The chain geometry is reminiscent of the Wanier represenation. It naturally captures the high frequency parts of the spectral function. The star geometry is much more suitable for describing the low energy features of the spectral function. Rational approximations using norms which are convex combinations of the ones would correspond to more complicated geometries and are probably worth exploring.

The hopping parameter $\alpha = \frac{b_0}{t'}$ is calculated by a single parameter minimization of the expression

$$\chi^2(\alpha) = \sum_{i\omega_n L}^{i\omega_n H} |G_A(i\omega_n, \alpha) - G(i\omega)|^2 \qquad (93)$$

where now $G_A(i\omega_n, \alpha) = \frac{\alpha}{i\omega_n} + (1 - \alpha) G_{N_C}(i\omega_n)$. G_{N_C} is the truncated Green function to length $N_C = N_{Site}/2$ and ω_L and ω_H are low and high energy cut-offs defined by the lowest poles of G and G_{N_C}, respectively. The coefficients a and b in eq. 91 are obtained from the coefficients of the partial fraction expansion in eq 92.

C. Iterated Perturbation Theory

One of the advantages of dealing with a well studied impurity model, is that one can rely on a host of reliable approximate methods which have been specifically designed for treating this problem. At half filling Yamada and Yoshida demonstrated that *for the Anderson impurity model* second order perturbation theory in U converged extremely well up to values of $\frac{U}{D}$ of order 6. Georges and Kotliar implemented this scheme to study the large d Hubbard model at half-filling.

It was later shown that this approach to the Hubbard model gives results in very good agreement with the quantum Montecarlo results at finite temperatures. Furthermore they showed that this scheme gives the atomic limit results for large U and therefore it is an interpolating scheme valid for small and large U. The important insight is that the Anderson impurity problem is *analytic in* U irrespectively of the nature of the bath, so it can be treated perturbatively. The non analyticies, describing the lattice aspects of the problem, are brought in by the self consistency condition which is treated exactly by this method.

The results obtained with this method are useful because they provide a concrete analytic realization of the functional $\Sigma_{imp}[G_0]$ and exhibits the functional form of $G[G_0] \approx [G_0 - \Sigma_{imp}[G_0]]^{-1}$ defined in section II, and illustrates in a simple example the important role played by the self consistency condition. The perturbative calculation is very fast and allows us to scan the paramter space at low temperature. This task would be prohibitively expensive for current QMC or exact diagonalization algorithms.

To second order in perturbation theory impurity self energy is given by:

$$\Sigma_{imp}[G_0](\tau) = -U^2 G_0^3(\tau). \tag{94}$$

We can understand the success of this approximation for the following reasons: 1) It is good for weak couplings ($U << t$) by construction, since the expansion is around $U = 0$. As shown by Yamada and Yosida (YY), it is able to produce not only the Abrikosov-Suhl resonance, but also the upper and lower incoherent bands as well. YY showed that the 4^{th} order correction is two orders of magnitude smaller that the 2^{nd} order contribution for the range of the interaction where the MIT occurs. 2) The atomic limit is exactly captured. When U is very large, and the system is deep in insulating side, ${G_0}^{-1} \approx i\omega_n$, the non-magnetic Hartree-Fock solution of the Green's function becomes exact,

$$G_L(i\omega) = \frac{1/2}{G_0^{-1}(i\omega_n) - U/2} + \frac{1/2}{G_0^{-1}(i\omega_n) + U/2} \tag{95}$$

therefore, the self energy reads,

$$\Sigma = (\frac{U}{2})^2 G_0(i\omega_n) \tag{96}$$

which is identical to the self energy that results from inserting G_0 in Eq. (94) and Fourier transforming. Thus, the second order approximation is at least an interpolation scheme which becomes exact for both the $U \to 0$ and $U \to \infty$ limits.

D. The self consistent projective method

The self consistent impurity model near U_{c2} has two energy scales U and Δ. The collapse of the scale Δ causes unsurmountable numerical difficulties. To handle this problem the projective self consistent technique was introduced in reference The idea is to eliminate the high energy configurations having scale U and simultaneously the high energy states of the bath of conduction electrons to obtain a problem containing a single energy scale Δ which can then be easily handled with the methods of the previous subsections. This method is quite general, and is applicable to a large class of models of strongly correlated electrons where separation of scales takes place.

The one particle spectral function is decomposed into a sum of a low and a high energy part, $\rho(\epsilon) = \rho^{low}(\epsilon) + \rho^{high}(\epsilon)$. $\rho^{low}(\epsilon)$ contains all states up to a cut-off that we take to be the Kondo temperature or renormalized Fermi energy of the half-filled Hubbard model and carries spectral weight Δ.

$$\Delta = \sum_k{}' 4V_k^2/D^2 \tag{97}$$

where the primed summation runs over the low energy states only. $\rho^{high}(\epsilon)$ describes the upper and lower Hubbard bands, two atomic-like features at energy scales $\pm\frac{U}{2}$, and carries spectral weight $1 - \Delta$.

We can solve for $\rho^{high}(\epsilon)$ using the techniques of the previous section. The main idea of the projective self-consistent approach is to eliminate the high energy states to obtain a low energy effective problem involving ρ^{low} only and thus containing only one energy scale. To carry out this program we separate the impurity configurations of the impurity Hamiltonian (89) into a low energy sector $f_\sigma^\dagger|E>$, with eigenenergy $-U/4$, and a high energy sector $|E>$ and $f_\uparrow^\dagger f_\downarrow^\dagger|E>$, with eigenenergy $U/4$, where $|E>$ denotes the empty configuration. Furthermore, as a result of the self consistency condition the conduction electron bath is divided into three bands (see fig (??)) : a metallic band centered around the Fermi energy, and semiconducing valence and conduction bands centered around energies $\pm U/2$. For the analysis of low energy properties, the valence and conduction bands can be taken as dispersionless, with the corresponding atomic states created by $\eta_-^\dagger$ and $\eta_+^\dagger$, respectively.

We now eliminate the high energy impurity configurations and the high energy orbitals of the conduction electron bath, to obtain a low energy hamiltonian wich we can use to

calculate ρ_{low}. This is done using a canonical transformation which results in:

$$H_{eff} = \sum_{kk'}{}' J_{kk'} \vec{S} \cdot \vec{s}_{kk'} + \sum_{k\sigma}{}' \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} \tag{98}$$

where $J_{kk'} = 8\frac{V_k V_{k'}}{U}(1 + \frac{7}{4}\frac{D^2}{U^2} - \frac{7}{4}\frac{D^2}{U^2}\Delta)$, $\vec{S} = \frac{1}{2}\sum_{\sigma\sigma'} X_{\sigma,\sigma'}\vec{\sigma}_{\sigma\sigma'}$ and $\vec{s}_{kk'} = \frac{1}{2}\sum_{\sigma\sigma'} c^\dagger_{k,\sigma}\vec{\sigma}_{\sigma\sigma'}c_{k',\sigma'}$. Here, $X_{\alpha\beta} \equiv |\alpha><\beta|$, where $|\alpha>$ and $|\beta>$ are the eigenstates of the atomic Hamiltonian, are projection operators.

H_{eff} corresponds to a Kondo problem coupling the atomic spin doublet to the low energy conduction electron bath.

The low energy part of the Green function can now be calculated directly from H_{eff},

$$G^{low}(i\omega_n) = -\int d\tau e^{i\omega_n\tau} < T_\tau F(\tau)F^\dagger(0) >_{H_{eff}} \tag{99}$$

where $F_\sigma = e^S f_\sigma e^{-S}$ is the canonically transformed single particle operator and has the form

$$F_\sigma = \sum_k{}' \alpha_k[(X_{\sigma\sigma} - X_{-\sigma-\sigma})c_{k\sigma} + 2X_{\sigma-\sigma}c_{k-\sigma}] \tag{100}$$

with $\alpha_k = \frac{2V_k}{U}(1 + \frac{7}{4}\frac{D^2}{U^2} - \frac{7}{4}\frac{D^2}{U^2}\Delta)$. The self-consistency equation for the low energy Green function then becomes

$$\sum_k{}' \frac{4V_k^2/D^2}{i\omega_n - \epsilon_k} = G^{low}(i\omega_n). \tag{101}$$

The projective self-consistent method thus results in the closed set of equations (98-101) which form the basis of our low energy analysis. The system contains only *one* energy scale, ΔD and is therefore numerically tractable.

VII. THE MOTT METAL-INSULATOR TRANSITION

The Mott transition, that is the metal insulator transition induced by the electron electron interactions in a periodic system, has been investigated theoretically and experimentally for many years. Experimentally it is realized in three dimensional transition metal oxides such as V_2O_3 and NiI_2 and can be driven by varying pressure temperature and composition.

From a theoretical point of view, several ideas have been put forward and various approximation schemes have been used to understand this transition. Hubbard first dealt with the problem using a single-particle (rigid-band) approach and introduced the notion of Hubbard bands. These describe propagating empty and doubly occupied sites in a half full lattice. For large U these bands are separated by a gap of order $U - 2D$. As U is reduced there is a critical value of U where the two bands merge again. This is the Hubbard

picture of the metal insulation transition. This kind of approach emphasises the *incoherent*, high-energy parts of the spectrum but fails to provide a suitable Fermi-liquid description of the quasiparticles in the metal.

Brinkman and Rice, building on the work of Gutswiller, started from the metallic phase which they described as a strongly renormalised Fermi liquid with a characteristic Fermi energy scale the fermi energy. As the interaction strenght incrases this energy vanishes at a critical value of the interaction U. In this framework the metal insulator transition is driven by the disappearance of the Fermi liquid quasiparticles. Incoherent parts of the spectrum (associated with charge fluctuations) are neglected in this approach, leading to a very crude description of the insulator.

Slater pointed out that the metal insulator transition is always accompanied by long range antiferromagnetic order, and viewed the doubling of the unit cell which makes the band structure of the system that of a band-insulator, as the driving force behind the metal insulator transition.

The limit of large dimensions provides a unique framework in which these various aspects can be studied *simultaneously*, i.e in which quasiparticles and incoherent features are treated on the same footing, and in which the competition between a Mott paramagnetic insulator and a Slater insulator can be quantitatively studied. This is reviewed in the attached reprints.