Effect of coulomb long range interactions on the Mott Transition

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We reconsider the Mott transition problem in the presence of long range Coulomb interactions. Using an extended DMFT, that sums an important class of diagrams absent in ordinary DMFT, we show that in the presence of Coulomb the Mott transition in two and three dimensions is discontinuous as envisioned by Mott.

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The study of Metal Insulator transitions [1] (MIT) seen in a host of interacting electronic systems, has been one of the most challenging problems in solid state physics. These transitions can result from simple band structure or from electronic correlations. The former occurs even in nearly non-interacting systems if the conduction and valence bands split as some parameter like composition is varied. The correlation driven transition i.e., Mott transition, is however, the most interesting. The nature of these transitions depend on the interplay of band structure, magnetism and electronic correlations. The simplest scenario for a MIT was first put forth by Mott [2]. Mott suggested that a crystalline array of hydrogenic atoms i.e., atoms with just one electron in their outermost shell, shows a zero temperature transition from a metal to an insulator as the density is decreased or effectively, as the distance between atoms increases [3]. Later, other possibilities for the MIT were put forth, namely, Slater’s band transition [4] where the system becomes insulating because of the doubling of the unit cell due to antiferromagnetism and the Brinkman-Rice scenario within the Hubbard model [5] which is characterised by a strong mass enhancement.

Mott’s original argument depended on the presence of coulomb long range interactions and pointed out that since the number of ”free” electrons could only vary discontinuously across the transition, the transition is necessarily first order. We recapitulate Mott’s ideas below: the main premise was that, due to the long range nature of the interactions, the electrons and the holes in the two Hubbard bands will always form bound states and not exist independently. The condition for the formation of at least one bound state, however, depends on the screening of the coulomb interaction. Using Thomas-Fermi estimates for screening by $N$ electrons per unit volume, Mott showed that no bound states exist provided

$$N^{1/3} a_H > 0.4$$

(1)

where $a_H$ is the Bohr radius. This implies that the system is metallic as long as the density satisfies (1). For densities where (1) is violated, the electrons and holes in the Hubbard bands always form bound pairs resulting in an insulating behavior. This implies that the number of carriers jumps at the transition. Since this results in a kink in the free energy, the transition is discontinuous and first order. For an illuminating discussion of these ideas see Ref. [6].

In contrast, various studies of the Hubbard model [6-10] indicate that the transition is continuous. The Hubbard model for interacting electrons has long been used as a prototype to describe various aspects of real systems [11]. This model contains a term which describes the hopping of electrons between different atomic sites and another describing the coulomb repulsion felt by two electrons on the same atom. In the past few years, the nature of the MIT in this model has been clearly elucidated using the Dynamical Mean Field theory (DMFT) in the limit of infinite lattice coordination $d$. It was shown that the MIT was characterised by a continuous vanishing of a Kondo like resonance at the Fermi level in the metal at the transition, leading to an insulator with a preformed gap. This led to the effective mass of the quasi-particles and hence the linear coefficient diverging from the metallic side at the transition [12]. Despite the discontinuous opening of the Mott Hubbard gap the destruction of the metal at zero temperature treated with DMFT, is a continuous one.

The purpose of this work is to incorporate some of the effects of the long range coulomb interactions and Mott’s ideas into the framework of Dynamical Mean Field Theory. For this purpose, we explore the effects of the long range interaction on the MIT seen in the single band Hubbard model [13], using a simple extension of DMFT [11,14]. It was shown, in a model of spinless fermions, that this approach captures important corrections [14]. This method was independently developed in Ref. [12] and it was applied to the problem of the breakdown of Fermi liquid theory. We first describe the approach by isolating a class of diagrams which can be formally controlled by scaling the interactions and the kinetic energy appropriately and which can be summed using impurity models. We then demonstrate that when this extended DMFT is applied directly to a 3 or 2 dimensional lattice with interactions having the coulomb form, it changes the Mott transition which was continuous in ordinary DMFT, to a discontinuous first order transition as envisioned by Mott.
The effective hamiltonian we use to describe our system is a generalization of the Hubbard hamiltonian
\[ H = \sum_{(ij)\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + \mu c_{i\sigma}^+ c_{i\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_{i \neq j, \sigma, \sigma'} V_{ij} : n_{i\sigma} n_{j\sigma'} : \]  

(2)
The first term is the hopping matrix element for an electron from site \( i \) (representing the ion at \( R_i \)) to its neighboring site \( j \), \( \mu \) is the chemical potential, \( U \) is the coulomb repulsion felt by the electrons when they are on the same atom \( (i = j) \) and the normal ordered last term is the coulomb interaction between electrons on different atoms. The coupling constants are given by overlap integrals involving a set of chosen basis vectors like the Wannier or Hartree basis. For example, the on-site interaction \( U \) is given by
\[ U = \int dr dr' |u(r)|^2 |u(r')|^2 \frac{e^2}{|r - r'|} \]  

(3)
\[ V_{ij} = \int dr dr' |u(r - R_i)|^2 |u(r' - R_j)|^2 \frac{e^2}{|r - r'|} \]
The hamiltonian (2) is now studied in the dynamical mean field approximation. The first step in the DMFT is to scale the parameters in the large \( d \) limit appropriately such that the corresponding energy terms remain finite. In addition, the scaling should be chosen such that the terms of interest remain relevant in the large \( d \) limit.

We adopt the following scaling: \( t_{ij} \) is scaled as \( \sqrt{d}^{-|i-j|} \), \( U \rightarrow U \) and \( V_{ij} \) is scaled by \( \sqrt{d}^{-|i-j|} \). The leading diagrams can then be summed up using the cavity method described in Ref. [3]. This scaling is a prescription for choosing a set of diagrams that contribute to the self energy and hence the Green’s function. DMFT prescribes a scheme for choosing different sets of diagrams that contribute to the different Green’s functions. In the case of the Hubbard model \( (V = 0) \), this corresponds to retaining only skeleton diagrams constructed from \( U \) and the local Green’s functions \( G_{ii} \) in the self energy, resulting in the self energy \( \Sigma_{ij} \) being local.

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at it. In effect, this corresponds to replacing the \( U \) by an \( U_{eff} \) in the local self energy evaluated for a Hubbard model. An example of the diagrams retained is shown in Fig. We mention that the Hartree term (arising only from \( U \)) is generated in the cavity method. Depending on the basis chosen to derive the effective model parameters [3] care should be exerted to see that the Hartree term is not double counted. We neglect the Fock term in the ensuing calculations, since the Fock term is of higher order in \( 1/d \) than the Hartree term.

Using the cavity method and integrating out all sites save a chosen site or cavity \( a \), we obtain the following local effective impurity action with retarded interactions
\[ S_{eff} = \int d\tau d\tau' \sum_\sigma c_{0\sigma}^{-1}(\tau - \tau')c_{0\sigma}(\tau') + U n_{0\uparrow}(\tau) - \sum_{\sigma, \sigma'} n_{0\sigma}(\tau) \Pi_{0}^{-1}(\tau - \tau') n_{0\sigma'}(\tau') \]  

(4)
where
\[ \Pi_{0}^{-1}(\tau - \tau') = \sum_{ij} V_{0i} V_{0j} \Pi_{ij}^{(0)}(\tau - \tau') \]
and the retarded interaction
\[ \Pi_{ij}^{(0)}(\tau - \tau') = \sum_q V(q) \Pi_{ij}^{(0)}(q, \tau - \tau') \]  

(6)
with \( G_{ij}^{(0)} \) denoting the single particle Green’s function and \( \Pi_{ij}^{(0)} = (\sum_{\sigma, \sigma'} n_{i\sigma}(\tau)n_{j\sigma'}(\tau'))_0 \). The superscript \( (0) \) implies that the quantities have been evaluated in the system from which the site 0 and all the links to this site have been removed. These in turn are related to quantities evaluated on the entire lattice. Summing over the sites leads to \( G_0 \) and \( \Pi_0 \) being determined by self-consistent equations involving local quantities evaluated on the full lattice. Note that the effect of all non-local quartic interactions is to dynamically screen the on-site repulsion, with the screening potential given by [6]. These equations depend on the nature of the lattice used. For example, on the Bethe lattice, \( G_{ij}^{(0)} = G_{ij} \) and \( \Pi_{ij}^{(0)} = \Pi_{ij} \). Retaining only the on site and nearest neighbor interactions, the self-consistency condition that should be satisfied by the retarded interaction on the Bethe lattice takes the simple form \( \Pi_{0}^{-1} = V^2 \Pi_{loc} \), where \( \Pi_{loc} \) is the local density density correlator. For arbitrary lattices and interactions (i.e. general \( t_{ij} \) and \( V_{ij} \)) the (extended) dynamical mean field equations can be derived by generalizing the discussion presented here, to the case where the hoppings \( t_{ij} \) are scaled by \( \sqrt{d}^{-|i-j|} \).

To obtain the Green’s functions of [6], we now define certain irreducible quantities. The lattice Green’s functions, can be expressed in terms of a self energy \( \Sigma \) which

In the presence of the longer range interaction, the above scaling retains all skeleton diagrams constructed using the local Greens function \( G_{ii} \) and the interaction vertices \( U \) and \( V_{ij} \), such that every point \( i \) which has a vertex \( V_{ij} \) originating from it has another vertex \( V_{ki} \) terminating in it.
is two particle irreducible and which becomes local in the limit of infinite dimensions.

\[ G(i\omega_n, q) = \frac{1}{i\omega_n - \epsilon_q - \Sigma(i\omega_n)} \quad (7) \]

where \( \epsilon_q \) is the dispersion on the lattice and \( i\omega_n \) are the Matsubara frequencies. Similarly, the density density correlator \( \Pi(q, i\omega_n) \) on the lattice defines an irreducible part \( \tilde{\Pi} \) via the Dyson equation

\[ \Pi(q, i\omega_n) = \frac{\tilde{\Pi}}{1 + V(q)\Pi} \quad (8) \]

where \( \tilde{\Pi} \) is the sum over all polarization diagrams constructed with the full \( G \) and interaction vertices \( V(q) \) such that all the diagrams are irreducible with respect to \( V(q) \). Within the infinite \( d \) approximation, since all vertex functions become independent of momenta, \( \tilde{\Pi} \) also becomes independent of momenta. The impurity model allows us to compute all local quantities, in particular \( \Sigma \) and \( \tilde{\Pi} \) and hence, the local density density correlator \( \Pi_{\text{loc}} \) as functionals of the Weiss fields \( \mathcal{G}_0 \) and \( \Pi_0 \).

\[ \Pi_{\text{loc}}^{-1}(\Pi_0, \mathcal{G}_0)(i\omega_n) = \Pi_0^{-1}(\Pi_0, \mathcal{G}_0)(i\omega_n) - \Pi_0^{-1}(i\omega_n) \quad (9) \]

and

\[ \Sigma(\Pi_0, \mathcal{G}_0)(i\omega_n) = \mathcal{G}_0^{-1}(i\omega_n) - \Pi_{\text{loc}}(\Pi_0, \mathcal{G}_0)(i\omega_n) \quad (10) \]

Using (8) and (9), we can eliminate \( \tilde{\Pi} \) to obtain a self-consistent equation for \( \Pi_{\text{loc}} = \sum_q \Pi(q, i\omega_n) \)

\[ \Pi_{\text{loc}}(\Pi_0, \mathcal{G}_0) = \sum_q \frac{1}{\Pi_{\text{loc}}^{-1}(\Pi_0, \mathcal{G}_0) - \Pi_0^{-1} + V(q)} \quad (11) \]

Similarly, we obtain an equation for \( G_{\text{loc}} \)

\[ G_{\text{loc}}(\Pi_0, \mathcal{G}_0) = \sum_q \frac{1}{i\omega_n - \epsilon_q - \Sigma(\Pi_0, \mathcal{G}_0)} \quad (12) \]

These equations where derived by an appropriate scaling of the interactions and the hopping elements in the original model so as to obtain a well defined limit of large coordination. In the spirit of DMFT, we can, however, regard these equations as defined on a finite dimensional lattice by replacing \( V \) by the usual coulomb interaction on the lattice. We use these equations to make qualitative predictions of the effect of the coulomb long range interaction in finite dimensions, on the order of the Mott transition seen.

In earlier DMFT studies of the Hubbard model the continuous Mott transition was found to occur at a critical \( U_c = U_c^2 \) and was signaled by the vanishing of a Kondo like resonance at \( \omega = 0 \) at \( U_c^2 \). The continuous character of that transition was established using the projective self consistent method. We briefly review the projective method below. Then, using the results of Ref. we study how long range Coulomb interactions treated within the extended DMFT, modify the previous discussion. The projective method uses the separation of two energy scales that exists in the metallic phase close to the MIT i.e., \( wD \) where \( w \) is the weight of the Kondo resonance seen in the metal and scale of the Hubbard bands \( U \). \( D \) is the half bandwidth. The high energy scales are then eliminated to obtain an effective theory governed by one low energy scale which is \( w \), which goes to zero at the MIT. Using this effective low energy model, which is a Kondo model of an impurity spin interacting with a bath of electrons, we can obtain the free energy or the ground state energy of the lattice problem close to the transition point. This free energy correctly describes the low energy and coherent part of the spectra. To order \( w \), the low energy Kondo problem has been derived in Ref. and is given by

\[ \mathcal{H} = w\Gamma \mathbf{S} \cdot \mathbf{s}_L + \mathcal{H}_b \quad (13) \]

Here \( \mathcal{H}_b \) describes a band of low energy conduction electrons and \( \mathbf{s}_L \) represents the local spin operator of these electrons. \( \mathbf{S} \) is the impurity spin and the Kondo coupling \( \Gamma \) is determined by matrix elements in the high energy sector (comprising the two Hubbard bands). The self-consistency conditions translate to conditions on the expectation value \( \langle \mathbf{S} \cdot \mathbf{s}_L \rangle \). The high energy sector is an insulator and has a spin doublet ground state which is separated from the excited states by a large gap. Using the results of Ref., the simplest approximation to the high energy sector of the Hubbard model yields \( \Gamma = \frac{2D^2}{U} \).

Since we are interested only in the qualitative features of the transition, we replace the bath of electrons by a single electron. Therefore, using this toy model, the energy of the Kondo model is

\[ E_K = -\frac{3}{4} w\Gamma \quad (14) \]

Using the results of Ref., and taking into account the kinetic energy of the lattice which is positive and of order \( w \), the ground state energy of the lattice model has the following expansion in terms of \( w \)

\[ E_0 = (\alpha - \beta \frac{2D^2}{U})w + \gamma w^2 + \text{corrections} \quad (15) \]

Here \( \alpha, \beta, \gamma \) are all positive. The transition is determined by the \( U \) at which the coefficient of the term linear in \( w \) vanishes. Since the energy minimum still occurs at \( w = 0 \), this transition is continuous.

Though the DMFT and the self-consistent projective method are both formulated in infinite dimensions, it is nonetheless known that they capture some aspects of the physics of systems in finite dimensions rather well. We therefore, use the projective method to make
some predictions about the transition in three dimensions. First, in the presence of the long range coulomb interaction, there are corrections to (15), because of the screening of the on-site coulomb interaction given by (13). This implies that $U$ in (13) has to replaced by an $U_{eff}$. For the free energy (15), it is sufficient to consider the effective static on-site repulsion. Taking $\Pi^{(0)} = \Pi + \text{sub-leading corrections in (13)}$ and using the fact that at zero frequency, $\Pi$ in (8) is by definition the compressibility $\kappa$ of the system, one obtains from (3)

$$U_{eff} = U - \sum_q V^2(q) \frac{\kappa}{1 + \kappa V(q)}$$  \hspace{1cm} (16)$$

Note that $V(q)$ is the Fourier transform of the coulomb potential in $d$ dimensions. Since the effective interaction remains finite at the transition, the leading critical behavior of the compressibility $\kappa$ is the same as that found in the Hubbard model and $\kappa$ is given by its value in the Hubbard model (17)

$$\kappa \propto \frac{w}{D}$$  \hspace{1cm} (17)$$

Note that $\kappa$ is finite in the metal and goes to zero smoothly at the transition. This implies that the effective repulsion seen by the electrons in the metallic phase is not screened at all. This is physically correct because one does expect the itinerant electrons in the metallic phase to better screen the coulomb repulsion. Using (17) in (16), and performing the $q$ sum in $d = 3$ we find that the effective repulsion felt on-site is

$$U_{eff} = U - aw^{1/2}$$  \hspace{1cm} (18)$$

where $a$ is some positive constant. The screening is proportional to $\log w$ in two dimensions. Substituting (18) in (13), we see that the expansion of the energy in terms of the low energy scale $w$ has non-analytic terms i.e.,

$$E_0 = (\alpha - \beta \frac{2D^2}{U})w - a\beta \frac{2D^2}{U^2}w^2 + \gamma w^2 + \text{correction}$$  \hspace{1cm} (19)$$

Notice that the parameter $w$ in the projective self consistent method, neatly embodies the notion of "number of free carriers" in Mott’s original number. The non-analyticity in (19) arises purely from the self-consistency conditions (13) when coulomb interactions are taken into account. We now see that at the transition, though the linear term still vanishes, the minimum of the energy which formerly was at $w = 0$ is now shifted to a non-zero value because of this non-analytic term. This is a feature of a first order transition! Hence, we see that taking into account the long-range nature of the coulomb interaction does make the Mott transition first order in $d = 3$. Regarding the effects of coulomb interactions in two dimensions, we find that the screening results in a term proportional to $w \log w$ in the free energy (15), again making the Mott transition discontinuous. Even though the DMFT is too crude an approximation in $d = 2$ where spatial fluctuations are large, we argue that it still captures some of the essential physics of strongly correlated systems.

To conclude, we have studied the effects of long range coulomb interactions on the Mott transition using an extended DMFT. We find that the coulomb interactions dynamically screen the effective on site interaction. We find that to lowest order, the screening is determined by the low energy scale $w$ which is related to the width of the Kondo resonance at the Fermi level. Consequently, the screening is zero in the insulator. Extending our analysis to three dimensions, we find that the screening term is non-analytic in $w$ resulting in non-analytic terms in the free energy. As a result the Mott transition which was continuous in the absence of these dynamical screening terms, now becomes a first order transition vindicating Mott’s ideas.