Critical Properties of the Mott Transition in the Hubbard Model

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We introduce a systematic low-energy approach to strongly correlated electron systems in infinite dimensions, and apply it to the problem of the correlation-induced metal-insulator transition in the half-filled Hubbard model. We determine the low-energy scaling functions of the metallic state, including the single-particle Green function and dynamical spin susceptibility, as well as thermodynamic properties and relate them to experimental data in transition metal oxides.

PACS numbers: 71.27+a, 74.20Mn, 71.28+d, 71.10+x
The correlation driven metal-insulator transition is a fundamental problem in condensed matter physics which has attracted renewed theoretical and experimental interest. From a theoretical point of view, the problem is fascinating because of its non-perturbative nature, the absence of a small parameter and the emergence of new low energy scales. Early ideas of Mott [1], Hubbard [2], Brinkman and Rice [3] have recently been put on a more quantitative footing by the development of a mean-field approach to the strong correlation problem which becomes exact in the limit of large lattice coordination [4]. The work of several groups [5–7] has established the existence of a Mott transition in the paramagnetic phase of the half-filled Hubbard model on frustrated lattices, which is driven by the collapse of an energy scale, the renormalized Fermi energy. The presence of this small energy scale made it difficult to analyze the critical behavior near the transition.

In this letter, we introduce a novel projective self-consistent approach to solving correlated electron problems in large dimensions at low energies. We use the natural separation of energy scales to our advantage and are able to extract, for the first time, exact information about the critical behavior at the transition in infinite dimensions. We calculate the single particle spectral function near the Mott transition, which can in principle be measured in photoemission experiments. We establish that the coefficient of the $\omega^2$ term in the imaginary part of the self-energy diverges as the square of the coefficient of the linear term in the specific heat and, with few additional assumptions, relate it to the observed $T^2$ resistivity in the $LaSrTiO_3$ system. We show that the local spin susceptibility diverges in the same way as the linear term in the specific heat and calculate their ratio, a generalized Wilson number. Finally, we show that the linear coefficient of the imaginary part of the dynamical spin susceptibility, relevant to both NMR and neutron scattering experiments, diverges as the square of the linear coefficient of the specific heat.

Besides these results of theoretical and experimental interest, our method can be generalized to deal with other problems, in which the separation of energy scales typical of strongly correlated electron systems can be exploited [8]. Two examples are the breakdown of Fermi liquid theory in strongly correlated electron systems [9] and superconductivity
in models with repulsive interactions \[10,11\], which have been recently analyzed using the large-d techniques.

The Hamiltonian of the Hubbard model is given by

$$H = -\sum_{<ij>\sigma} (t_{ij} + \mu \delta_{ij}) f_{i\sigma}^+ f_{j\sigma} + U \sum_i (f_{i\uparrow}^+ f_{i\uparrow} - \frac{1}{2}) (f_{i\downarrow}^+ f_{i\downarrow} - \frac{1}{2})$$ \hspace{1cm} (1)

where the chemical potential $\mu$ is taken to be zero, and the hopping matrix $t_{ij}$ is scaled as $t_{ij} \to t/\sqrt{d}$. In the limit of infinite dimensions, all local correlation functions of the lattice model can be calculated in terms of a local action,

$$S_{\text{imp}}[G_o] = -\int_0^\beta d\tau d\tau' \sum_\sigma f_\sigma^+(\tau) G_o^{-1}(\tau - \tau') f_\sigma(\tau')$$
$$+ \int_0^\beta d\tau U(n_{f\uparrow}(\tau) - \frac{1}{2})(n_{f\downarrow}(\tau) - \frac{1}{2})$$ \hspace{1cm} (2)

provided that $G_o$ satisfies a self-consistency equation \[12\]. In order to make contact with physical systems in finite dimensions, for which the bandwidth is finite, we consider the case of a semi-circular bare density of states, $\rho_o(\epsilon) = \frac{2}{\pi D} \sqrt{1 - (\epsilon/D)^2}$ for which the self-consistency equation has the form

$$G_o^{-1}(i\omega_n) = i\omega_n + \mu - (D/2)^2 G(i\omega_n).$$ \hspace{1cm} (3)

The local action (2) can be rewritten in terms of an Anderson impurity model \[12\]

$$H_{\text{AM}} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} + \sum_{k\sigma} V_k (f_\sigma^+ c_{k\sigma} + \text{h.c.}) + U (n_{f\uparrow} - \frac{1}{2})(n_{f\downarrow} - \frac{1}{2}).$$ \hspace{1cm} (4)

The self-consistency equation (3) is satisfied provided that the bath dispersion $\epsilon_k$ and the hybridization coupling $V_k$ are determined through

$$\sum_k \frac{4V_k^2/D^2}{i\omega_n - \epsilon_k} = G(i\omega_n).$$ \hspace{1cm} (5)

where $G(i\omega_n) = -\int_0^\beta d\tau e^{i\omega_n\tau} < T_{\tau} f_\sigma(\tau) f_\sigma^+(0) >_{\text{AM}}$ is the impurity Green function.

For sufficiently strong interactions, a separation of energy scales occurs as demonstrated explicitly by previous numerical work on the Hubbard model \[3,7\]. It has been shown that the one particle spectral function can be decomposed into a sum of a low and a high energy...
part, \( \rho(\epsilon) = \rho^{\text{low}}(\epsilon) + \rho^{\text{high}}(\epsilon) \). \( \rho^{\text{low}}(\epsilon) \) 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 \( \Delta \)

\[
\Delta = \sum_k' 4V_k^2/D^2
\]

where the primed summation runs over the low energy states only. \( \rho^{\text{high}}(\epsilon) \) describes the upper and lower Hubbard bands, two atomic-like features at energy scales \( \pm U/2 \), and carries spectral weight \( 1 - \Delta \). When \( \Delta \) is small the presence of the low energy scale \( \Delta D \) makes the system of equations (4) and (5) numerically untractable.

The main idea of the projective self-consistent approach is to eliminate the high energy states to obtain a low energy effective problem involving \( \rho^{\text{low}} \) only and thus containing only one energy scale. To carry out this program we separate the impurity configurations of the impurity Hamiltonian (4) into a low energy sector \( f_\uparrow \sigma |E \rangle \), with eigenenergy \( -U/4 \), and a high energy sector \( |E \rangle \) and \( f_\uparrow \downarrow f_\uparrow \downarrow |E \rangle \), with eigenenergy \( U/4 \), where \( |E \rangle \) denotes the empty configuration. Furthermore, the self-consistency equation allows us to divide the conduction electron bath into three bands as illustrated in Fig. (1): a metallic band centered around the Fermi energy, and semiconducting 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 \cite{13}, with the corresponding atomic states created by \( \eta^\dagger_- \) and \( \eta^\dagger_+ \), respectively.

The low energy effective Hamiltonian can be derived through a canonical transformation. In addition to the high energy impurity configurations, which can be eliminated by the standard Schrieffer-Wolff \cite{14} transformation, the self-consistency requires the elimination of the valence and conduction bands of the electron bath. For this purpose we first separate out the atomic Hamiltonian

\[
H_{\text{atomic}} = U(n_{f\uparrow} - 1/2)(n_{f\downarrow} - 1/2)
+ \frac{U}{2}(\eta^\dagger_+\sigma\eta^\dagger_+\sigma - \eta^\dagger_-\sigma\eta^\dagger_-\sigma) + V \sum_{l=+,-} \sum_\sigma (f^\dagger_\sigma \eta^\dagger_\sigma + h.c.)
\]
where \(V\) is determined from the fact that both the upper and lower Hubbard bands have a spectral weight \((1 - \Delta)\), which together with the self-consistency equation (3) implies that \(V = (D/2)\sqrt{(1 - \Delta)/2}\). The lowest-energy eigenstates of this atomic Hamiltonian are a spin doublet \(|\sigma\rangle\) which correspond to the impurity spin doublet \(f_{\sigma}^\dagger|E\rangle\) dressed by the valence and conduction electrons. All other atomic configurations are located at energies higher by at least \(\sim U^2\).

We have carried out the canonical transformation analytically to order \((D/U)^2\) \([3,15]\), resulting in a low-energy effective Hamiltonian \(H_{eff} = e^SHe^{-S}\) of the form

\[
H_{eff} = \sum_{kk'} J_{kk'} \vec{S} \cdot \vec{s}_{kk'} + \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma}
\]

where \(J_{kk'} = 8V_k V_{k'}(1 + \frac{D^2}{4 U^2} - \frac{D^2}{4 U^2} \Delta), \quad \vec{S} = \frac{1}{2} \sum_{\sigma\sigma'} X_{\sigma\sigma'} \bar{\sigma}_{\sigma\sigma'} \) and \(\vec{s}_{kk'} = \frac{1}{2} \sum_{\sigma\sigma'} c_{k\sigma}^\dagger \bar{\sigma}_{\sigma\sigma'} c_{k'\sigma'}\).

Here, \(X_{\alpha\beta} \equiv |\alpha\rangle \langle \beta|\), where \(|\alpha\rangle\) and \(|\beta\rangle\) 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 \(H_{eff}\),

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

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

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

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

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

The projective self-consistent method thus results in the closed set of equations \([8,11]\) which form the basis of our low energy analysis. The system contains only one energy scale, \(\Delta D\), which allows us to define rescaled variables, \(\tilde{V}_k = V_k/(\sqrt{\Delta D}), \tilde{\epsilon}_k = \epsilon_k/(\Delta D), \tilde{i\omega_n} = i\omega_n/(\Delta D), \) and \(\tilde{H}_{eff} = H_{eff}/(\Delta D)\).
In the following, we will focus on the critical properties of the Mott transition approached from the metallic side, for which it suffices to analyze Eqs. (8-11) to leading order in $\Delta$. Restricting to leading order in $\Delta$ implies that the requirement that the rescaled spectral weight is unity, $\int d\tilde{\omega} p^{\text{low}}(\tilde{\omega}) = 1$, can be satisfied together with the self-consistency equations (11) only for one particular value of $U$. This is precisely the critical interaction $U_c$.

The problem is now reduced to a self-consistent determination of the low-energy parameters $\tilde{\epsilon}_k$ and $\tilde{V}_k$, which is carried out iteratively using a recently introduced zero-temperature algorithm [16,17]. The functional equations (8) and (11) are truncated by representing the electron bath in terms of a finite set of free electron orbitals $c_i^\dagger$, $i = 1, ..., N - 1$, with the corresponding energy levels $\epsilon_i$ and hybridization matrix $V_i$. The ground state of the impurity problem, now defined on an $N$ site cluster, is obtained by the modified Lanczos technique [18]. The local Green function as well as correlation functions are calculated using a continued fraction expansion [19,16]. The projected self-consistency condition (11) can be implemented in terms of a $\chi^2$ fitting of the Matsubara Green function $\chi^2 = \sum_{\Omega_{\text{max}}} \Omega_{\text{min}} \frac{\tilde{V}_k^2}{\tilde{\omega}_n} - < F^\dagger F > \tilde{H}_\text{eff}(i\tilde{\omega}_n)^2$ where $\Omega_{\text{min}}$ and $\Omega_{\text{max}}$ are the low and high frequency cut-offs, respectively [17].

We have solved the equations for clusters of 4, 6, 8 and 10 sites. The critical interaction $U_c$ is found to be essentially unchanged as the number of sites is increased from 4 to 10, varying from 3.03 to 3.04 [20]. In the inset of Fig. (2) we show the single particle spectral function for $N = 10$. The large number of poles clearly demonstrates the power of the projection onto the low energy sectors. The Matsubara Green functions as functions of the rescaled Matsubara frequency for $N = 6, 8$ and 10 are shown in Fig. (2). The low frequency part of the Green function improves systematically as $N$ increases, and remains essentially unchanged for $N = 8$ and 10. Also shown in Fig. (2) is the Green function for the non-interacting problem. The value of the scaled Green function at zero frequency is determined by the low energy self-consistency equation and is the same as that of the Green function of the non-interacting problem, consistent with the pinning of the density of states expected from Fermi liquid theory [21]. The solution for the Green function also allows us to determine
the scaled self-energy $\Sigma_{\text{low}}(i\tilde{\omega}_n)$ by extracting from $\Sigma(i\omega_n) = i\omega_n - (D/2)^2 G(i\omega_n) - G^{-1}(i\omega_n)$ the terms with a singular dependence on $\Delta$. Both $G_{\text{low}}(i\tilde{\omega}_n)$ and $\Sigma_{\text{low}}(i\tilde{\omega}_n)$ can be fitted by quadratic polynomials at low frequencies with the expressions

$$G_{\text{low}}(i\tilde{\omega}_n) = -i2.0 + 3.3(i\tilde{\omega}_n) + i3.9(i\tilde{\omega}_n)^2,$$

$$\Sigma_{\text{low}}(i\tilde{\omega}_n) = -1.7i\tilde{\omega}_n - i1.1(i\tilde{\omega}_n)^2. \quad (12)$$

The term of the self-energy linear in $i\tilde{\omega}_n$ implies a quasi-particle residue $z \equiv (1 - \partial\Sigma/\partial i\omega_n)^{-1} = \Delta/1.7$ which vanishes as the critical point is approached. The momentum-independence of the self-energy in turn leads to a quasi-particle mass $m^*/m = 1/z = 1.7/\Delta$, and a linear coefficient of the specific heat,

$$\gamma = \frac{4\pi k_b^2}{3} \frac{1.7}{D\Delta} \quad (13)$$

which diverge at the critical point. This divergence is consistent with the Brinkman-Rice scenario of the Mott transition \[3\], as well as the previous result in the Hubbard model at half-filling within second order perturbation theory \[22,23\]. The term of the self-energy quadratic in $(i\tilde{\omega}_n)^2$ gives rise to an imaginary part of the analytically-continued self-energy

$$\text{Im}\Sigma(\omega + i0^+) = -\frac{1.1\omega^2}{\Delta^2 D} \quad (14)$$

which also diverges at the critical point.

The local dynamical spin susceptibility $\chi_s(i\omega_n) = (g\mu_B/2)^2 \int_0^\beta d\tau e^{i\omega_n\tau} < T\tau S_z(\tau)S_z(0) >_{\text{eff}}$, where $S_z = \frac{1}{2} e^S(f_{\uparrow}^\dagger f_{\uparrow} - f_{\downarrow}^\dagger f_{\downarrow})e^{-S} = (X_{\uparrow\uparrow} - X_{\downarrow\downarrow})/2$, can also be calculated from a continued fraction expansion. The result in terms of rescaled frequency, $\chi_s(i\tilde{\omega}_n)$, is shown in Fig. (3). At low frequencies, $\chi_s(i\tilde{\omega}_n)$ can be fitted by

$$\chi_{\text{low}}^s(i\tilde{\omega}_n) = (g\mu_B/2)^2 (9 - 47|\tilde{\omega}_n|)/\Delta D \quad (15)$$

The local static susceptibility is given by the constant term of Eq. (15),

$$\chi_s = (g\mu_B/2)^2 9/2 \quad (16)$$
from which we derive a generalized Wilson ratio at the critical point,

$$R \equiv \frac{\chi_s/\chi_{s,loc}}{\gamma/\gamma_{free}} = 3.2$$

(17)

where $\chi_{s,loc}^{free} = 16/(3\pi D)\left(\frac{g\mu_B}{2}\right)^2$ and $\gamma_{free} = \frac{4\pi}{3D} k_B$, are the static local spin susceptibility and the linear coefficient of the specific heat for the free electron gas with a semicircular density of states, respectively. Compared to the universal value for the infinite bandwidth Anderson impurity model, $R_{AM} = 2$, the critical value $R$ is enhanced as a result of the finite bandwidth of the electron bath. In large dimensions the susceptibility at a generic $q$ is not affected by the antiferromagnetic exchange interaction and, hence, has the typical value $\chi_{loc}$. The enhancement of $R$ is consistent with the ferromagnetic tendencies found in the Gutzwiller approximation [25] where the magnetic exchange is ignored as well. We note that the usual definition of the Wilson ratio in a lattice model is given in terms of the $q = 0$ component of the static susceptibility, $\chi_s(q = 0)$. The antiferromagnetic exchange interaction does affect $\chi_s(q = 0)$ (as well as $\chi_s(q)$ for special $q$ points in the Brillouin zone), leading to a vanishing ratio $\chi_s(q = 0)/\gamma$ at the transition point. [26]

Finally, the term of the imaginary part of the dynamical spin susceptibility linear in $|\tilde{\omega}_n|$ implies that $\lim_{\omega \to 0} \frac{\chi_\omega^{\prime\prime}(\omega + i0^+)}{\omega} = 4\gamma/(D\Delta)^2(\frac{g\mu_B}{2})^2$. If we use $\chi_{loc}$ for the static spin susceptibility this implies a finite generalized Korringa ratio at the critical point, which is again modified from the universal value for the infinite bandwidth Anderson model [27].

Our results have direct implications for the Mott-Hubbard systems. The conductivity can be estimated by converting the $\omega^2$ at zero temperature to $(\pi T)^2$ at finite temperature and assuming that the self-energy we derived at the critical point also applies to the case of a hypercubic lattice in $d$ dimensions [28]. Using the Kubo formula, we find a resistivity

$$\rho(T) = A T^2$$

where $A = -\frac{\pi^2}{6} \hbar c \frac{\partial^2 \Sigma(i\omega_n)}{\partial(i\omega_n)^2}$ giving rise to a finite ratio

$$\frac{A}{\gamma^2} = 8.2 \times 10^3 a (\Omega m)$$

(18)

where $a$ is the hypercubic lattice spacing in units of meter. For $Sr_{1-x}La_xTiO_3$ with $x = 0.9$, which is close to the Mott transition, Eq. (18) yields $A/\gamma^2 = 4.4 \times 10^{-6} \Omega m$ when we
use $a = 8.3 \times 10^{-10} m$ [29]. This result is in good agreement with the measured value $A/\gamma^2 = 8 \times 10^{-6} \Omega m$ [30].

In summary, we have introduced a projective self-consistent approach to strongly correlated electron systems, which allows us to determine the critical properties at the Mott transition in the half-filled Hubbard model. We find low energy scaling functions that can be quantitatively related to experimental results in transition metal oxides.

We thank V. Dobrosavljević, A.E. Ruckenstein, and X.Y. Zhang for useful discussions. This work was supported by the NSF under grant #DMR 9224000.
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FIGURES

FIG. 1. Schematic plot of the spectral functions of the conduction electrons and the impurity configurations, illustrating the low and high energy parts.

FIG. 2. Imaginary part of the Matsubara Green function versus the rescaled frequency $\tilde{\omega}_n$ for system size $N = 6, 8, 10$ and non-interacting (semi-circular) density of states. The inset shows the single particle spectral function as function of the rescaled frequency $\tilde{\omega}$ with a broadening $\delta = .01$ for $N = 10$.

FIG. 3. Real part of the Matsubara spin susceptibility as a function of the rescaled frequency $\tilde{\omega}_n$ for $N = 10$. 