PHASE SEPARATION AND SUPERCONDUCTIVITY IN THE $U = \infty$ LIMIT OF THE EXTENDED MULTIBAND HUBBARD MODEL

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Abstract

The three band Hubbard model with nearest neighbour repulsion is studied in the $U = \infty$ limit using the large $N$ expansion technique to order $1/N$. A charge transfer (CT) instability is found like in weak coupling theory. However at small doping a major role is played by the Brinkman-Rice point. The CT instability is always associated with a diverging compressibility leading to a phase separation. The evaluation to order $1/N$ of the effective scattering amplitude in the Cooper channel shows the presence of superconducting instabilities in the $s$ and $d$ wave channel near the phase separation.
1 INTRODUCTION

Since the discovery of high-temperature superconductivity, a large variety of mechanisms has been proposed; the origin of this phenomenon, however, is still unclear. A main theoretical effort has been devoted to model the CuO$_2$ layers, which are believed to contain the relevant physics of the new superconducting compounds.

Many analyses of the copper oxide phases begin with a two-dimensional extended Hubbard Hamiltonian containing a nearest neighbour repulsion $V$ in addition to the copper-oxygen hybridization $t_{ij}$ and the copper-oxygen site repulsion $U$ [2, 3]. The introduction of the nearest neighbour repulsion emphasizes the relevance of the charge degrees of freedom (excitation mode) with respect to the spin degrees of freedom which are more suitably studied in the context of the t-J model and related RVB theories (magnetic models) [4, 5]. Yasuo Suzuki and Abrahams [6] in particular suggested that for the special chemistry of Cu-O compounds where the effective copper and oxygen levels are close in energy the nearest neighbour repulsion can produce a wave superconductivity through charge transfer resonances.

This extended Hubbard model has been extensively analyzed in weak coupling[6, 7, 8] and near the two important features have been found: a) when the nearest neighbour copper-oxygen repulsion exceeds the copper-oxygen hybridization, the system undergoes a charge transfer (CT) instability characterized by the vanishing of the lowest excitation particle-hole excitation. The CT instability is reached by increasing the doping; b) near this instability the system undergoes a superconducting instability of $A_{1g}$ (extended s) or $B_{1g}$ (d$_{xy}$) character. However the extent of this attraction requires the order parameter average to extend over the complete Brillouin zone[9, 10].

In this paper we analyze the same model for the case in which the copper on site repulsion is much larger than all the other energy scales in the problem, using the large N expansion technique which is non-perturbative in the coupling constants. We shall study the model at the level of mean field theory ($N = \infty$) and of fluctuations ($\phi$ corrections).

There are several reasons for going beyond the weak coupling theory: a) from photoemission studies it is clear that the copper on site repulsion is the largest energy scale in the problem and filling the copper oxide bands is charge transfer instabilities. The proximity to an insulating state may be relevant to the physics and is entirely missed by the weak coupling theory.

It was in fact shown in a two band (p-d) t-J model that a phase separation takes place close and above the Brinkman and Rice transitions, where the kinetic term is non-frustrated, so the model is unable to stabilize the system [11]. A similar phase separation will be found here. In particular we shall show that there is never a pure CT instability. A divergence of the CT compressibility $\kappa$ is always accompanied by a divergence of the uniform charge susceptibility $\chi_0$. By Maxwell reconstruction phase separation always occurs before the electronic instability is reached.

We shall find that the pairing survives the large U limit. Near the boundary a phase separation of the phase diagram there is a superconducting instability in the s-wave channel. This instability can be seen by taking Fermi surface average of the scattering amplitudes in the Cooper channel. On the contrary the weak coupling analysis[6] suggests that the s-wave attraction rapidly disappears as U increases.

A short account of the present work has been reported elsewhere [12].

2 MEAN FIELD THEORY AT LARGE U

The model of interest is the three band extended Hubbard model

$$\mathcal{H} = \sum_{\nu \sigma} \epsilon_{\nu} c_{\nu \sigma}^\dagger c_{\nu \sigma} + U \sum_{\nu \sigma \sigma'} \langle c_{\nu \sigma}^\dagger c_{\nu \sigma'}^\dagger c_{\nu \sigma'} c_{\nu \sigma} \rangle +$$

$$+ V \sum_{\nu \sigma \sigma' \mu} \langle c_{\nu \sigma}^\dagger c_{\nu \sigma'}^\dagger c_{\nu \sigma'} c_{\nu \sigma} \rangle (\epsilon_{\nu} c_{\mu}^\dagger c_{\nu \sigma} + h.c.),$$

where $\nu$ is in the hole representation in which the vacuum state is the $3p^0$ configuration for the copper and the $3p^0$ for the oxygen. The $c_{\nu \sigma}^\dagger$ ($c_{\nu \sigma}$) operators are annihilation (creation) operators of holes in the $3dx_{2-y^2}$ orbitals of the Cu atoms, while $p_{\nu \sigma}$ and $p_{\nu \sigma}$ ($\sigma$ and $\sigma'$) are the corresponding operators for the $2p_x$ and $2p_y$ orbitals on the O sites and $\nu$ labels the spin. $c_{\nu \sigma}$ and $\nu$ are the basic atomic levels on O and Cu respectively. In the following we shall take the limit $U \to \infty$ and replace the $U$-term with the single occupancy requirement on copper [13].

The large N version of the model is then introduced by assuming that $\sigma$ runs from 1 to $N$ and suitably creating the coupling constants. Finally the model we shall consider reads

$$\mathcal{H} = \sum_{\nu \sigma} \epsilon_{\nu} c_{\nu \sigma}^\dagger c_{\nu \sigma} + V \sum_{\nu \sigma \mu} \langle c_{\nu \sigma}^\dagger c_{\nu \sigma}^\dagger c_{\nu \sigma'} c_{\nu \sigma} \rangle$$

$$+ \sum_{\nu \sigma \sigma'} \left[ \epsilon_{\nu} c_{\nu \sigma}^\dagger c_{\nu \sigma'}^\dagger c_{\nu \sigma'} c_{\nu \sigma} + h.c. \right]$$

$$+ V \sum_{\nu \sigma \sigma' \mu} \langle c_{\nu \sigma}^\dagger c_{\nu \sigma'}^\dagger c_{\nu \sigma'} c_{\nu \sigma} \rangle (\epsilon_{\nu} c_{\mu}^\dagger c_{\nu \sigma} + h.c.),$$

(1)
subject to the single occupancy constraint \( \sum d_{i}^{\sigma} = m_{i} \). The original system has \( m_{i} = 1 \) and \( N = 2 \). We carried out a controlled large-N expansion at \( \theta_{0} = 1 \), using the functional integral technique and the slave boson trick [14]. The physical copper hole boson operators \( \delta a_{i} = d_{i}^{\sigma} a_{i}^{\sigma} \) in the hybridization term in eq. 4 and, as usual, a Lagrange multiplier \( \lambda_{i} \) is introduced to enforce the single occupancy constraint.

We decouple the copper-oxygen repulsion introducing two Hubbard-Stratonovich real fields \( X \) and \( Y \). \( X \) is coupled to the difference in charge between a copper atom and its surrounding four oxygen orbitals and \( Y \) is coupled to the total charge of this cluster. The partition function of the model is then given by

\[
\mathcal{Z} = \int \mathcal{D}P \mathcal{D}e^{\sigma} \mathcal{D}a_{i} \mathcal{D}a_{i}^{\sigma} \mathcal{D}X \mathcal{D}Y \mathcal{D}X^{\prime} \mathcal{D}Y^{\prime} \exp \left( i \mathcal{S} \right)
\]

where

\[
\mathcal{S} = \sum_{i} \left[ \phi_{i} \left( \frac{\delta \phi_{i}}{\delta \phi_{i}^{\prime}} + \frac{\delta \phi_{i}^{\prime}}{\delta \phi_{i}} \right) + \frac{1}{2} \left( \frac{\delta \phi_{i}}{\delta \phi_{i}^{\prime}} + \frac{\delta \phi_{i}^{\prime}}{\delta \phi_{i}} \right)^{2} \right] + \frac{1}{2} \sum_{i} \left( \phi_{i}^{2} + \phi_{i}^{\prime 2} \right) + \frac{1}{2} \sum_{i} \left( \phi_{i}^{2} + \phi_{i}^{\prime 2} \right) + H_{1} + H_{2}.
\]

At mean field level we set \( X_{0} = \phi_{X} \), \( Y_{0} = \phi_{Y} \), \( m_{i} = \phi_{i} \), \( \lambda_{i} = \phi_{i}^{\prime} \), and \( r_{0} = \phi_{0} \).

These mean field parameters must be determined by solving the saddle point equations which are obtained by requiring the free energy per site and per spin

\[
F = \lambda_{i} \left( \phi_{i}^{2} - m_{i}^{2} \right) + \frac{1}{2} \left( \phi_{i}^{2} - \phi_{i}^{\prime 2} \right) - \frac{1}{H_{\text{sites}}} \sum_{i} \ln \left[ 1 + e^{-\phi_{i}^{2} / H_{\text{sites}}} \right]
\]

to be stationary with respect to variations of the mean field parameters. Here \( \beta_{\text{s}} \) are the three eigenvalues of the Hamiltonian (4) with saddle point values of the bosonic fields in it, \( \beta \) is the average number of particles per unit cell and per spin \( n \), \( \delta \) is the doping and gives the deviation with respect to half-filling.

It is instructive to examine in some detail the self-consistency equations and compare them with analysis of the three band model at \( \Delta = 0 \) by Kotliar, Lee and Read (KLR) [14]. In the absence of a direct oxygen-oxygen hopping integral the Hamiltonian in eq. 5 separates, at mean field level, into a two by two matrix connecting the \( d \) orbital with the \( 3d \) (bonding) \( 3d \) combination and a single unlinked \( a_{i} \) (non-bonding) \( 3d \) combination. For \( \beta_{\text{s}}(4) \) one gets

\[
\beta_{\text{s}}(4) = \left\{ \begin{array}{ll}
\frac{1}{2} \left( \lambda_{i} + \lambda_{i}^{\prime} + \sqrt{(\lambda_{i} - \lambda_{i}^{\prime})^{2} + 16 \phi_{0}^{2} \phi_{i}^{2}} \right), & \text{if } \lambda_{i} > 0 \\
\frac{1}{2} \left( \lambda_{i} + \lambda_{i}^{\prime} - \sqrt{(\lambda_{i} - \lambda_{i}^{\prime})^{2} + 16 \phi_{0}^{2} \phi_{i}^{2}} \right), & \text{if } \lambda_{i} < 0
\end{array} \right.
\]

where \( \phi_{0} \) is the solution of the equation \( \beta_{\text{s}}(4) = 0 \), which amounts to the solutions of eqs. (16) and (17) in terms of \( \lambda_{i} \).

The saddle point \( \beta_{\text{s}}(4) \) solution of eqs. (12), (13) and (15) at \( \Delta = 0 \) is shown in Fig. 1 for different values of \( \delta / \Delta \) as functions of the \( \Delta / \Delta \). The solutions of the full set of equations (12)-(16) is then given by the intersection of \( \beta_{\text{s}}(4) \) with the straight line in eq. (17).

For \( \Delta \) sufficiently large three intersections can appear corresponding to two local minima and a local maximum for \( \Delta \). At \( \Delta = 0 \) this happens for \( \Delta > \Delta_{c} \), \( \Delta < \Delta_{c} \). For \( \Delta > \Delta_{c} \), the Brakke-Brinkman transition occurs at \( \Delta_{c} = \Delta_{c} \approx 2 \Delta_{c} \). For \( \Delta < \Delta_{c} \), the Brakke-Brinkman transition occurs at \( \Delta_{c} = \Delta_{c} \approx 2 \Delta_{c} \). For \( \Delta_{c} = \Delta_{c} \approx 2 \Delta_{c} \), the Brakke-Brinkman transition occurs at \( \Delta_{c} = \Delta_{c} \approx 2 \Delta_{c} \).
3 CHARGE TRANSFER INSTABILITY AND PHASE SEPARATION

The CT instability is the only instability present at large $N$. It corresponds to diverging local charge fluctuations and is described by the CT susceptibility $\chi = \frac{\rho}{\mu}$, i.e., by the correlation function $\langle n_\alpha - n_\beta \rangle$ at zero frequency and momentum.

A straightforward inspection of the bubble diagrams shows that a divergent $\chi$ is always accompanied by a divergent $\frac{\rho}{\mu} \equiv \langle n_\alpha + n_\beta \rangle$. Because of this, one can localize the CT instability by simply looking at the behaviour of the mean field solution for the chemical potential $\mu = \mu(\delta)$ as a function of doping.

The instability has three equivalent manifestations:

1) The $2 \times 2$ matrix susceptibility $\chi_{\alpha\beta}$ diverges ($\alpha, \beta = n_\alpha + n_\beta, n_\alpha - n_\beta$). The eigenvector corresponding to the divergent eigenvalue determines the mixture between CT and density fluctuations in the soft mode;

2) The contribution to the free energy from the gap fluctuations diverges;

3) The condition $\frac{\rho}{\mu} = 0$ is verified. Since a divergent compressibility implies phase separa-
4 SUPERCONDUCTING PAIRING

Having established the region of the phase diagram which is free from instabilities, we turn to the study of the effective interaction between the quasiparticle. For \( U = \infty \) they are given by the eigenvalues of \( \alpha \) in eq.(6) which is diagonalised by \( \Phi_{\alpha} = \sum_{\alpha} \varphi_{\alpha} \Psi_{\alpha} \) where we introduced a three component notation for the orbitals \( \varphi_{\alpha} = (\varphi_{\alpha,1}, \varphi_{\alpha,2}, \varphi_{\alpha,3}) \) to get the quasiparticle operators \( \Phi_{\alpha} \). The unitary transformation \( \Theta \) is given by

\[
U(\theta) = \begin{pmatrix}
\cos \theta & -\sin \theta & 0 \\
\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

with \( \sin \theta \equiv \frac{\Delta_{0} \omega_{0}}{2} \). In the new basis \( H_{\text{P}} = \sum_{\alpha, \beta} \varphi_{\alpha}^{\dagger} \Psi_{\alpha}^{\dagger} H_{\varphi} \varphi_{\beta} \Psi_{\beta} \). The quasiparticles interact with the fluctuations of the four component field

\[
H_{\text{Int}} = \sum_{\mathbf{k}, \mathbf{q}} \varphi_{\mathbf{k}}^{\dagger} \varphi_{\mathbf{k}+\mathbf{q}}^{\dagger} \lambda^{\alpha}(\mathbf{k}, \mathbf{q}) \varphi_{\mathbf{k}+\mathbf{q}} \varphi_{\mathbf{k}}
\]

We work in the radial gauge [14] and define \( \varphi = \varphi_{r} + \varphi_{\theta} \). We confine ourselves to the static limit. The \((3 \times 3)\) vertices \( \lambda^{\alpha}(\mathbf{k}, \mathbf{q}) \) can be read off eq.(9).

\[
\lambda^{1} = -\frac{\omega_{0}}{2} \varphi_{r}^{\dagger} \varphi_{r}^{\dagger} \lambda^{2} = \lambda^{3} = 0
\]

\[
\lambda^{1} = \begin{pmatrix}
0 & 0 & \sin (\frac{\omega_{0}}{2} k_{x}) \\
\sin (\frac{\omega_{0}}{2} k_{x}) & 0 & \sin (\frac{\omega_{0}}{2} k_{y}) \\
0 & \sin (\frac{\omega_{0}}{2} k_{y}) & 0
\end{pmatrix}
\]

while the quasiparticle vertices \( \lambda^{\alpha}(\mathbf{k}, \mathbf{q}) \) are defined as \( \lambda^{\alpha}(\mathbf{k}, \mathbf{q}) = \varphi_{\alpha}^{\dagger}(\mathbf{k}+\mathbf{q}) \lambda^{\alpha}(\mathbf{k}, \mathbf{q}) \lambda^{\alpha}(\mathbf{k}) \).

The propagators of the \( A \) field are given by

\[
W^{\alpha}(\mathbf{q}) = \varphi_{\alpha}^{\dagger}(\mathbf{k}+\mathbf{q}) \varphi_{\alpha}(\mathbf{k}) \lambda^{\alpha}(\mathbf{k}, \mathbf{q})
\]

with

\[
W^{\alpha}(\mathbf{q}) = -\sum_{\mathbf{k}, \mathbf{q}} \frac{\varphi_{\alpha}^{\dagger}(\mathbf{k}+\mathbf{q}) - \varphi_{\alpha}(\mathbf{k}) - \frac{1}{2} \lambda^{\alpha}(\mathbf{k}, \mathbf{q}) \lambda^{\alpha}(\mathbf{k}, \mathbf{q})}{D^{\alpha}(\mathbf{k}+\mathbf{q}) - D^{\alpha}(\mathbf{k})}
\]

The matrix \( D^{\alpha} \) has zero everywhere except for the elements \( D^{11} = \gamma_{0}, D^{22} = \gamma_{0}, D^{33} = \gamma_{0} \). With this notation one can write the effective interaction among the quasiparticles in the Cooper channel as

\[
\gamma^{\alpha}(\mathbf{k}, \mathbf{q}) = -\sum_{\mathbf{k}, \mathbf{q}} \left( \frac{\varphi_{\alpha}^{\dagger}(\mathbf{k}+\mathbf{q}) - \varphi_{\alpha}(\mathbf{k}) - \frac{1}{2} \lambda^{\alpha}(\mathbf{k}, \mathbf{q}) \lambda^{\alpha}(\mathbf{k}, \mathbf{q})}{D^{\alpha}(\mathbf{k}+\mathbf{q}) - D^{\alpha}(\mathbf{k})} \right)
\]
\[
\begin{align*}
\Delta_{\text{eff}} & = 0.1 \quad 0.15 \quad 0.2 \quad 0.25 \quad 0.3 \quad 0.35 \quad 0.4 \quad 0.45 \quad 0.7 \\
\begin{array}{|c|c|c|c|c|c|c|c|c|}
\hline
\Delta_{\text{eff}} & 1.5 & 0.5015 & 0.5726 & 0.6410 & 0.7058 & 0.7216 & 0.1299 & 0.24 \\
1.75 & 1.05 & 0.3697 & 0.4056 & 0.4315 & 0.4574 & 0.5058 & 0.5216 & 0.2412 & 0.082 \\
2.5 & 3.5 & 0.739 & -1.1226 & -0.2412 & -0.082 & -0.1299 & -0.1574 & -0.24 & 0.2412 & 0.082 \\
\end{array}
\end{align*}
\]

Table 1: a-wave coupling constants (\(\Delta_{a}\)) and d-wave coupling constants (\(\Delta_{d}\)) for \(V_{U=\infty} \text{Villars model}\) and various values of \(\Delta_{\text{eff}}\) and \(\delta\).

\[
\Delta_{\text{eff}} = \left( \frac{\Delta_{a} + \Delta_{d}}{2} \right) + \Delta_{a} \left( 1 + e^{-\frac{\Delta_{d}}{2}} \right) \Delta_{d} \left( 1 + e^{-\frac{\Delta_{a}}{2}} \right)
\]

A typical shape of the effective interaction among the quasiparticles on the Fermi surface is shown as a function of the momentum transfer in Fig. 4. Notice that the interaction is attractive for a wide region of \(q\). The superconducting coupling constants are calculated as Fermi surface averages.

\[
\lambda_{a} = \frac{\int \int \sigma_{a}(k,k')\rho_{a}(k')\rho_{a}(k)\rho(k'k')d\Omega d\Omega'}{\int \int \rho_{a}(k')\rho_{a}(k')d\Omega d\Omega'}
\]

We studied Fermi surface averages with \(\rho_{a}(k) = \cos(k_{x})\) and \(\rho_{a}(k') = \cos(k_{x'})\).

The \(\lambda_{a}\) and \(\lambda_{d}\) couplings are found to be generally attractive near the phase separation region. They are tabulated in Table 1 for the parameter \(V_{U=\infty} \text{Villars}\).

Both a and d wave scattering amplitudes are found to be attractive near the boundary of the phase separation region. The superconducting instability in the a wave channel can be understood by observing that near a phase separation boundary \(\delta_{c}\) is large. Within a Fermi liquid picture \(\delta_{c}\) is proportional to \(1 - \lambda_{a}\). Therefore, since in the present case the effective mass ratio \(\delta_{c}\) is not strongly enhanced, a large \(\delta_{c}\) indicates a large negative value of the symmetric Landau amplitude \(\Delta_{a}\). This signals the presence of attractive forces in the particle-hole channel, which can reasonably lead to a negative scattering amplitude in the
particle-particle channel. Note that all previous studies [16, 18] using simple boson techniques have so far failed to give a wave superconductivity because they did not include the parameter V.

The analysis above indicates the existence of a wave pairing in specific regions of model (1) in the limit of large N near phase separation. To obtain a substantial attraction for realistic values of V (several studies maintain V ≪ V_{c}) the system has to operate close to the BnNk-Mott transition. This feature is certainly present in the copper-oxides system and absent in the usual coupling approach.

The Coulomb interaction will rule out the phase separation and disfavour the JT instability, as far as this mode is coupled to density fluctuations. However, the short range physics discussed above will be affected only at small momenta and frequencies. On the other hand, the intermediate g's behaviour will lead to stable pairing within the static limit, a full analysis of the long range case requires the introduction of a dynamical screening and a subsequent solution of the Eliashberg equations. It is clear, however, from this and earlier work [5, 6, 7] that the three band model with Ga-O repulsion, in the parameter range near the metal-insulator transition, has physics, in the metallic state, which is different from the one band repulsive Hubbard model.

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References
[13] We have not included the on site oxygen repulsion U_{o}. For not too large values of U_{o} this repulsion can be treated within an Hartree-Fock scheme, leading to minor renormalization effects in the small doping region.
[15] The paths for λ and Y in the functional integral have to be deformed away from the real axis to meet the saddle point values.
[17] The spin density wave instability appears in higher order. A J coupling is in fact generated at order p_{F}.
where we sum over frequencies \( \omega_n = (2n + 1)\pi T \) with small fictitious temperature \( T^{*} = 0.01 \) and large cutoff \( N_{C} \Delta \omega = 2U \), to obtain the new set of parameters \( V_n \) and \( \epsilon_n \). Note that this Hamiltonian effectively describes an impurity surrounded by a "star" of both electrons.

An alternative route was introduced in the context of an extended Hubbard model.11 This procedure takes advantage of the fact that the Green function \( G(x) \) can be decomposed into "particle" and "hole" contributions as \( G(x) = G_{p}(x) + G_{h}(x) \) with \( G_{p}(x) = \langle 0 | e^{ix[(H - E_{F})]} | 0 \rangle \) and \( G_{h}(x) = \langle 0 | e^{-ix[(H - E_{F})]} | 0 \rangle \).

The respective contributions can be obtained from a continued fraction expansion as

\[
\langle \phi^{\dagger} \phi \rangle = \frac{1}{1 + \frac{1}{1 + \frac{1}{z - a^{2}\langle \phi^{\dagger} \phi \rangle}}} = \frac{1}{1 - \frac{a^{2}\langle \phi^{\dagger} \phi \rangle}{z - a^{2}\langle \phi^{\dagger} \phi \rangle}},
\]

where \( | \phi^{\dagger} \phi \rangle = \hat{f}_{\alpha} \hat{f}_{\alpha}^{\dagger} \) and \( | \phi^{\dagger} \phi \rangle = \hat{f}_{\alpha} \hat{f}_{\alpha}^{\dagger} \) and \( \hat{f}_{\alpha} \hat{f}_{\alpha}^{\dagger} = H_{\alpha} - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} = \langle \alpha | \alpha \rangle / \langle \alpha | \alpha \rangle - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} \rangle \), \( b_{\alpha} = \langle \alpha | \alpha \rangle / \langle \alpha | \alpha \rangle - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} angle \), and \( b_{3} = 0 \). This implies that \( G_{p} \) and \( G_{h} \) can be regarded as resulting from a Hamiltonian describing an impurity coupled to two chains with site energies \( \epsilon \) and hopping amplitudes \( \epsilon^{2} \).

Again the number of poles in the Green function is, in general, larger than the number of sites of the Hamiltonian and, in order to close the self-consistency, the continued fraction expansion has to be truncated. 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 a moment by moment fitting. This scheme has the numerical advantage that it avoids the multi-dimensional fit of the Green function, but the disadvantage that it can be implemented practically only in the case of a semiconducting state. In the metallic case an explicit site at the Fermi energy is introduced in order to better represent the low frequency region and, more importantly, to allow us to feedback a metallic bath. The hopping parameter to this extra site is calculated by a single parameter minimization of the expression

\[
\chi^{2}(\alpha) = \sum_{\omega_{n}} \left| G_{\alpha}(\omega_{n}) \right|^{2} - \langle \phi^{\dagger} \phi \rangle^{2},
\]

where now \( G_{\alpha}(\omega_{n}) \) is \( \langle \alpha | \omega_{n} \rangle \) and \( \langle \phi^{\dagger} \phi \rangle \) is the truncated Green function of length \( N_{C} = \text{length} / 2 \), and \( \omega_{n} \) and \( \omega_{n} \) are low and high energy cutoffs defined by the lowest pole of \( G \) and \( G_{\alpha} \), respectively. In this case the moments will be modified by a small lattice \( \alpha \) which decreases as the system size is increased.

The effective Anderson model therefore reads

\[
H = \sum_{\alpha} \sum_{\omega_{n} \in \text{sites}} \left[ \begin{array}{l}
\epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} + U_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} \hat{f}_{\alpha} + h.c. \\
\end{array} \right] + \sum_{\alpha} U_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} \hat{f}_{\alpha} + h.c. \\
\sum_{\alpha} U_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} \hat{f}_{\alpha} + h.c.
\]

(7)

In both schemes, ground state wave function and ground state energy of the Anderson Hamiltonian are determined by exact diagonalization (up to ten sites) and the modified Lanczos technique.12 Systems of up to ten sites can be handled on a workstation. The zero temperature Green function of the local site is finally obtained from a continued fraction expansion using the recursion method discussed above.

As mentioned in the introduction, a further advantage of the formulation of the problem in terms of an Anderson impurity model is the fact that the energy of the Hubbard model can be obtained directly without frequency summations using Anderson model relations. The kinetic energy per site of the Hubbard model is given as

\[
\mathcal{T} = \langle \mathcal{T} \rangle = \sum_{\alpha} \langle \alpha | \alpha \rangle / \langle \alpha | \alpha \rangle - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} angle \rangle = \sum_{\alpha} V_{\alpha} \| \alpha \| / \langle \alpha | \alpha \rangle - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} angle \rangle
\]

Taking the limit of infinite coordination number this reduces to

\[
\mathcal{T} = \langle \mathcal{T} \rangle = \sum_{\alpha} \langle \alpha | \alpha \rangle / \langle \alpha | \alpha \rangle - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} angle \rangle
\]

Using the self-consistency condition as well as the fact that in the Anderson model \( \langle \mathcal{T} \rangle = \sum_{\alpha} \langle \alpha | \alpha \rangle / \langle \alpha | \alpha \rangle - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} angle \rangle = \sum_{\alpha} V_{\alpha} \| \alpha \| / \langle \alpha | \alpha \rangle - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} angle \rangle
\]

we obtain

\[
\mathcal{T} = \sum_{\alpha} V_{\alpha} \| \alpha \| / \langle \alpha | \alpha \rangle - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} angle \rangle, \quad \langle \alpha | \alpha \rangle - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} angle \rangle = \sum_{\alpha} \langle \alpha | \alpha \rangle / \langle \alpha | \alpha \rangle - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} angle \rangle
\]

(8)

where \( \alpha \) labels the sites neighboring the impurity. The potential energy of the Hubbard model is obtained as

\[
V = \langle \mathcal{V} \rangle = \langle \mathcal{V} \rangle = \sum_{\alpha} \langle \alpha | \alpha \rangle / \langle \alpha | \alpha \rangle - \epsilon_{\alpha} \hat{f}_{\alpha}^{\dagger} \hat{f}_{\alpha} angle \rangle
\]

(9)

3. Results

In our analysis we have focused on two major aspects: the determination of a region where two solutions are allowed, and the resolution of controversy regarding the lowest energy solution. The two approaches considered yield a consistent picture of the transition. We are able to obtain converged metallic and insulating solutions for a finite range of the interaction \( U \) within both schemes. We further demonstrate that the metallic solution is lower in energy in the whole coexistence region. The energy difference between the solutions goes to zero as \( U_{C} \) is approached, implying that the transition can be classified as second order. This should be contrasted with the results from second-order perturbation theory, where the two solutions
were found to cross in energy at an intermediate value of the interaction $U$. A point worth noticing (as was already observed within the perturbative approach) is that the energy difference between the solutions is much smaller than any energy scale of the problem. This is due to an almost perfect compensation of the gain in delocalization (kinetic) energy by the loss of energy through double occupancy (potential energy) in the metallic state compared to the insulator.

![Graph](image1.png)

**Fig. 1.** Comparison of the metallic and insulating Matsubara Green functions for $U = 2.7$, as obtained from the two variations of the algorithm. Full line "star geometry" and dotted line "two-chain geometry" (10 sites for the metallic case and 8 sites for the insulating).

Metallic and insulating solutions for $U = 2.7$ inside the coexistence region are, respectively, shown in Figs. 1 and 2 (the half-bandwidth $2t$ is set equal to unity). In the first figure the Green function displays a narrow resonance at low frequency (note that the pinning condition at $\omega = 0$ is fulfilled), while the insulator in the second case merely consists of high energy features (upper and lower Hubbard bands). The figures also illustrate the consistency of the two schemes considered here. In both (the metallic and insulating) cases the agreement is very good. We also find that the results of both methods for the single particle Green function on the imaginary axis compare very well with the second-order perturbative calculation and QMC5,7 (the latter is discussed in Ref. 10).

![Graph](image2.png)

**Fig. 2.** Kinetic, potential, and total energy of the metallic and insulating solutions in the coexistence region. Differences between the metallic and the insulating solution are shown in the inset (from the "two-chain geometry").

The kinetic, potential and total energies for the two solutions in the coexistence region are displayed in Fig. 2. An interesting feature is the already mentioned almost perfect cancellation of delocalization and double occupancy energy. Another important observation is that while a finite size effect is apparent in the results for the kinetic and potential energy, the convergence of the total energy is much faster. A few runs for a ten-site system show almost no differences to the results for eight sites.

The energy difference of the two solutions is shown in the inset of Fig. 2. As the critical point $U_c$ is approached from below, the finite size effects become relevant for $U \approx 2.8$. This limitation of the scheme is due to the fact that at a low energy
scale associated with the quasiparticle peak goes to zero close to the transition, the discrete nature of the approximation starts playing an important role and the Kondo resonance is represented by only a single pole.

The smallest of the differences in energy between the metallic and the insulator can be understood from the picture of a second-order critical point where the metallic and insulating solutions merge with a vanishing scale $\Delta = U_{\text{cr}} - U$. The problem can be formulated from a variational point of view, with the free energy $F$ becoming an extremum at the metallic and insulating solutions, i.e., $\delta F / \delta G_M = (\delta F / \delta G_I) = 0$. Since the two solutions merge at the point $U_{\text{cr}}$, $F$ can be expanded in power series of $G_M - G_I$ as

$$F_M - F_I = \frac{\delta^2 F}{\delta G^2} (G_M - G_I)^2.$$  \hspace{1cm} (10)

As the difference between the metallic and the insulating solution is parameterized by $\Delta$, and the second derivative vanishes at the critical point as $\Delta$, it follows that the energy difference goes to zero as $\Delta^2$. The critical region cannot be accessed by the present method. In order to capture the vanishing energy scale, a higher resolution (i.e., an effective bath with more sites) is needed.

Finally, we would like to comment on the disappearance of the insulating solution at $U_{\text{cr}}$. From the "two-chain" scheme, the insulating solution is found to persist all the way down until the gap closes. This differs from the results of the perturbation theory and resembles the Hubbard III scenario for the destruction of the insulating state.\footnote{In a recent preprint, Gros et al. [9] performed a finite-size study and obtained similar results on the nature of the disappearance of the insulator.} In the case of the "star configuration," while a converged insulating solution can be obtained as values of the interaction $U$ well below $U_{\text{cr}}$, the question of the closing of the gap cannot be answered conclusively.

4. Conclusions

We have resolved the standing questions regarding the metal-to-insulator transition in the Hubbard model in infinite dimensions, using a powerful algorithm to obtain Green functions at zero temperature.\footnote{Note that this can also be useful to obtain the dynamical correlation functions like the spin-spin correlation function.} We were able to demonstrate the existence of a region in which metallic and insulating solutions coexist, which is in agreement with previous results, and showed that the metallic solution is always lower in energy. This implies that while at finite temperature the transition is first order, it becomes second order at $T = 0$, similar to the work of Brinkman and Rice in the context of the Gutzwiller approximation.\footnote{Both the Hubbard and the Anderson models are strongly correlated electron systems.} Since the method presented is very general as well as simple, especially when compared to Monte Carlo simulations, it is an appealing approach to the study of strongly correlated electron systems.

References