Superconductivity in the two-band Hubbard model in infinite dimensions

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Abstract. We study a two-band Hubbard model in the limit of infinite dimensions, using a combination of analytical methods and Monte-Carlo techniques. The normal state is found to display various metal to insulators transitions as a function of doping and interaction strength. We derive self-consistent equations for the local Green’s functions in the presence of superconducting long-range order, and extend previous algorithms to this limit. We present direct numerical evidence that in a finite range of parameter space, the normal state is unstable against a superconducting state characterized by a strongly frequency dependent order parameter.

Introduction

The discovery of high temperature superconductivity in copper-based transition metal oxides has revised the view in superconductivity of strongly correlated electronic systems. Mechanisms of high temperature superconductivity which are not phonon-mediated have been around for a long time, and their existence has remained controversial subject. This old problem cannot be solved perturbatively [1].

The large-dimensionality limit of the strong correlation problem has received much recent attention [2-11] especially in the context of the Hubbard model. This is a non-trivial limit of the strong correlation problem which can be solved non-perturbatively.

In this paper we define a model with two degrees of freedom per unit cell which also has a well defined limit when the coordination number gets large. On the atomic level the interactions in this model are purely repulsive.

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We show that the normal phase is stable against phase separation and displays interesting metal-insulator transitions as a function of doping, and of the interaction strength.

For the first time we give in this paper a derivation of the self consistent equations for the local Green’s functions in the presence of off-diagonal superconducting long range order that become exact in the limit of infinite dimensions. We then solve these equations by extending the Hirsch-Fye Quantum Monte Carlo algorithm [12].

We present evidence that in a well defined region of parameters of the two-band model the normal state is unstable against a superconducting state, characterized by a strongly frequency dependent superconducting order parameter. We observe that superconductivity in this model is promoted in regions of parameters where two different atomic configurations are close in energy, that is, in the mixed valence regime.

II. The model

We consider the following Hamiltonian:

\[ H = - \sum_{\mathbf{i}, \mathbf{j}, \alpha, \beta} t_{\mathbf{i}, \mathbf{j}} \delta_{\alpha, \beta} n_{\mathbf{i}, \alpha} + \hbar c \]

\[ + \epsilon_p \sum_{\mathbf{j} \in \mathbf{B}, \alpha} n_{\mathbf{j}, \alpha} p_{\mathbf{j}, \alpha} + \epsilon_d \sum_{\mathbf{i} \in \mathbf{A}, \alpha} \delta_{\alpha, \beta} d_{\mathbf{i}, \alpha} d_{\mathbf{i}, \beta} + U_d \sum_{\mathbf{i} \in \mathbf{A}} n_{\mathbf{i}, \alpha}^2 n_{\mathbf{i}, \beta}^2 \]

(\(d_{\mathbf{i}, \alpha}, p_{\mathbf{j}, \alpha}\)) represent two atomic orbitals on different sublattices \((A, B)\) of a bipartite lattice. The ‘copper’ orbital \(p_{\mathbf{j}, \alpha}\) is strongly correlated, while the ‘oxygen’ orbital \(d_{\mathbf{i}, \alpha}\) is uncorrelated. Each site has identical connectivity \(z\), so that the model describes a ‘CuO2’-type system. A two-dimensional three-band model has been proposed by Emery [17] and by Varma et al. [18] as a minimal model of the copper-oxide \(\text{CuO}_2\) planes. The model we consider is similar in spirit, while having a non-trivial large \(d\) limit (as opposed to other possible generalizations of multiband
models which have somewhat degenerate large $d$ limits [6, 19]). Multiband models have been investigated intensively, but no clear numerical evidence for superconductivity in two dimensions has so far been obtained [20, 23]. In infinite dimensions several circumstances facilitate the numerical work: the model reduces to an effective single-site model, in which the thermodynamic limit is taken exactly, without the need for finite-size extrapolations, and the Monte Carlo algorithm is free from minus-sign problems, allowing us to reach lower temperatures than in previous works [20, 23].

In the absence of correlations ($U_d = 0$), diagonalization of $\mathcal{H}$ yields two bands (bonding and antibonding):

$$E^\pm_k = \epsilon_p \pm \sqrt{(\epsilon_p - \epsilon_d)^2 + 4\epsilon_k^2}/2,$$

where $\epsilon_k$ is the Fourier transform of $t_{ij}$. These bands are separated by a gap $\Delta_0 = \epsilon_p - \epsilon_d$. (Having in mind the copper-oxides in the hole representation, we choose throughout this paper $\epsilon_d < \epsilon_p$.) For a total hole density $n = \sum \langle n_{\sigma}\rangle$ smaller than 2, the $U_d = 0$ ground-state is a partially filled copper band and an empty oxygen band. For $2 < n < 4$, the $U_d = 0$ ground-state is a full $d$-band and a partially filled $p$-band. The $T = 0$ chemical potential is discontinuous as a function of density at $n = 2$, with $\mu (n = 2^-) = \epsilon_d$, $\mu (n = 2^+) = \epsilon_p$. Hence, for $U_d = 0$, this model describes a metal for all densities except $n = 2$, where one has a band insulator. The copper and oxygen density of states have simple expressions for $U_d = 0$:

$$N_d(\epsilon) = \sqrt{\frac{s - \epsilon}{\Delta_0}} N(\sqrt{(\epsilon - \epsilon_p)(\epsilon - \epsilon_d)})$$

$$N_p(\epsilon) = \sqrt{\frac{s - \epsilon}{\Delta_0}} N(\sqrt{(\epsilon - \epsilon_p)(\epsilon - \epsilon_d)})$$

where $N(\epsilon) = \sum \delta (\epsilon - \epsilon_k)$.

The limit of infinite connectivity $z \to \infty$ requires a scaling of the hybridization $t_{ij}$ as $t_{ij} = t_{ij}/\sqrt{z}$, so that the density of states $N(\epsilon)$ has a proper limit [2]. 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 $z \to \infty$. We shall establish the general equations for an arbitrary $N(\epsilon)$ but, for the sake of simplicity, will perform all numerical simulations for the Bethe lattice.

It is by now well-established that, in the limit $z \to \infty$, the problem reduces to a single-site 'impurity' model supplemented by a self-consistency condition. Standard methods [6] that will not be reviewed here allow us to derive the corresponding equations for the one-particle Green's functions. In this section, we assume no long-range order of any kind (magnetic or superconducting) and display equations valid in the paramagnetic normal state.

Since only the 'copper' sites are correlated, all the local quantities can be derived from an impurity model for those sites only. The effective action of the impurity model is given by:

$$\mathcal{S} = U_d \int_0^\beta d\tau n_{\sigma\uparrow}(\tau) n_{\sigma\uparrow}(\tau)$$

$$+ \frac{i}{\beta} \int_0^\beta d\tau' \sum_{\sigma \sigma'} \langle D_{\sigma}\rangle (\tau) D_{\sigma'}^{-1}(\tau - \tau') d_{\sigma'}^{\dagger}(\tau').$$

We denote by $D(\tau - \tau') = \langle -TD(\tau) D^{\dagger}(\tau') \rangle$ the interacting Green's function calculated with this action and by $\Sigma_d$ the impurity self-energy (seen as a functional of $D_0$), $\Sigma_d(\omega_n) = D_{\sigma}^{-1}(\omega_n) - D_{\sigma}^{-1}(\omega_n)$. The self-consistency equation for $D_0$ then reads, $(\omega_n = (2n + 1)\pi/\beta)$:

$$D(\omega_n) = \zeta_p(\omega_n) \int d\epsilon N(\epsilon)$$

$$\zeta_p(\omega_n) \zeta_d(\omega_n - \epsilon) - \epsilon^2,$$

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

Once (4), (3) are solved for $D_0$, the impurity self-energy evaluated at the self-consistent value of $D_0$ gives the electron lattice self energy in the $(k_{\sigma}, p_{\sigma})$ basis, it reads in matrix form:

$$\begin{pmatrix} 1 & \zeta_p(\omega_n) \\ \zeta_p(\omega_n) & \zeta_d(\omega_n - \epsilon) - \epsilon^2 \end{pmatrix}.$$

In the $z \to \infty$ limit, self-energies become purely diagonal, so that $\Sigma_d$ depends only on frequency and $\Sigma_p$ component is absent. The absence of the diagonal component $\Sigma_p$ in (5) comes from the simplifying assumption of an uncorrelated $p$-orbital. From (5), 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: $D(\omega_n) = \sum_k D(k, \omega_n)$. Also, the $p$-orbital on-site Green's function is simply given by:

$$P(\omega_n) = \zeta_d(\omega_n) \int d\epsilon N(\epsilon)$$

$$\zeta_p(\omega_n) \zeta_d(\omega_n - \epsilon) - \epsilon^2.$$

It is straightforward to extend these equations to a model involving a Hubbard repulsion on oxygen orbitals also. One then has to solve simultaneously two separate impurity models, one for each orbital, and both $\Sigma_d$ and $\Sigma_p$ enter the self-consistency equations (4, 6). It is also possible to include a direct oxygen-oxygen hopping $t_{pd}$ (with a $1/z$ scaling as $z \to \infty$). For the sake of simplicity, these additional terms will not be considered in this paper.

Throughout the rest of this paper, we shall work with the $z = \infty$ Bethe lattice with the semi-circular d.o.s. given above. This is motivated by the very simple form taken by the self-consistency equations in this case:

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

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

A direct way to derive these equations for the Bethe lattice is to integrate out fermionic degrees of freedom on all lattice sites except a single one. Because of the $z = \infty$ limit, only one-particle processes (involving the full Green's function) yield precisely $\gamma$.

In order to (7), we use in detail the procedure solved (g = L = $\beta/\Delta_1$, and the Monte-Carlo algorithm, which, of course, in order to iterated u...
functions $D, P$ are generated in this partial summation, yielding the effective action equation (3), with $D_0$ explicitly given in terms of $D$ by (7).

In order to solve the coupled problem defined by (3), (7), we use a numerical method that has been described in detail elsewhere [7, 9–11]. It is based on an iterative procedure: for a given $D_0(\tau)$, the impurity model (3) is solved (given a discretization of the interval $[0, \beta]$, $= \beta/\Delta \tau$ time slices) using the Hirsch-Fye quantum Monte-Carlo algorithm. This produces a discretized $D(\tau)$ which, after Fourier transformation, is inserted into (7) in order to produce a 'new' function $D_0$. This process is iterated until convergence is reached.

III. Metal-insulator transitions

A. The metal-insulator transition at $n = 1$

For a density $n = 1$ this model displays a transition from metallic to an insulating state following a scenario outlined by Zaanan et al. [13].

For very large $U_0/\Delta_0$ and $t_{pd} \ll \Delta_0 = \varepsilon_p - \varepsilon_d$, the $n = 1$ ground state has all copper sites nearly singly occupied and all oxygen sites nearly empty. Hybridization between the two orbitals costs an energy $\approx \Delta_0$, while the kinetic energy gain is only $\approx t_{pd}^2/\Delta_0$. Hence, for $t_{pd} \ll \Delta_0$, we have a charge-transfer insulator at $n = 1$, with a jump in the chemical potential $\mu (n = 1^-) - \mu (n = 1^+) \equiv 0$. The numerical data for $n_\sigma, n$, and the total density $n$ as a function of the chemical potential $\bar{\mu} = \mu - \varepsilon_d$ confirms these expectations. In Fig. 1, we show data at $\beta = 30$, $U_0 = 8$, and $\Delta_0 = 4$.

In the opposite limit ($t_{pd} \gg \Delta_0$) the delocalization energy wins, and we have a strongly correlated metal with a strong hybridization of 'copper' and 'oxygen' orbitals. A metal to charge-transfer insulator transition separates these two regimes, at $(\Delta_0/t_{pd})_c = O(1)$ for large $U_0$.

In the opposite regime of weak correlations ($U_0 \ll \Delta_0$), the metal-insulator transition at $n = 1$ has the character of a Mott transition within the copper band. Assuming $t_{pd} \ll \Delta_0$, most of the $d$-orbital density of states is, for $U_0 = 0$, concentrated around $\varepsilon_d$, with a small band of order $t_{pd}^2/\Delta_0$ (see (2)) and the hybridization with the oxygen orbital is weak. As $U_0$ is increased, the lower copper-band is gradually split by the interactions, and a Mott transition occurs when $U_0$ becomes comparable to the band with $t_{pd}^2/\Delta_0$, i.e. $(\Delta_0/t_{pd})_c = t_{pd}/U_0$ for small $U_0$.

In Fig. 2 we show data at $\beta = 30$, $U_0 = 1.5$, and $\Delta_0 = 4$ displaying this behavior.

Based on these arguments, the phase boundary separating the metallic and insulating regimes at $n = 1$ is expected to have the schematic shape [13] described in Fig. 3.

When $U \sim \Delta_0$, there is a crossover regime which to our knowledge has not been investigated previously. Data in this region is shown in Fig. 4. The detailed investigation of these phase transitions is left for future work.

B. The metal to band insulator transition at $n = 2$

Interactions can also induce a transition from insulating to metallic behavior at a density $n = 2$. At $U_0 = 0$ the system is a band insulator with a band gap $\Delta_0 = \varepsilon_p - \varepsilon_d$. Turning on the interactions has the effect of reducing the band gap. Whenever the gap is less than the temperature, we expect metallic behavior.

This change from insulating to metallic behavior at $n = 2$ is clear in the $n$ vs $\mu$ curves in Figs. 1, 2, and 4. In

![Fig. 2](image-url)
Fig. 3. Schematic phase diagram (cf. [13]). The special point occurs when \( U_d - \Delta_0 \).

Fig. 4. \( n_e \) (full line) \( n^o \) (dotted line) and \( n \) (dashed line) vs \( \mu - \varepsilon_d \) at \( \Delta_0 = 4 \), \( U_d = 4.5 \), and \( \beta = 30 \).

Fig. 5. \( \text{Im}(G(i\omega_n)) \) (full line) and \( \text{Re}(\Sigma,(i\omega_n)) \) (dotted line) at \( U_d = 1.5, \mu - \varepsilon_d = 4, \Delta_0 = 4 \), and \( \beta = 45 \) (\( L = 128 \)).

Fig. 6. \( \text{Im}(G(i\omega_n)) \) (full line) and \( \text{Re}(\Sigma,(i\omega_n)) \) (dotted line) at \( U_d = 2.5, \mu - \varepsilon_d = 4, \Delta_0 = 4 \), and \( \beta = 45 \) (\( L = 128 \)).

Fig. 7. \( \text{Im}(\Sigma) \) at \( U_d = 4.5, \mu - \varepsilon_d = 4 \), \( \Delta_0 = 4 \), and \( \beta = 45 \) (\( L = 128 \)).

Fig. 8. \( D(0 + i0^+) = e_p - e_d \). The low-frequency constrained solutions: 1)

Fig. 2 the case \( U_d < \Delta_0 \) is realized, for which the atomic ground-state [14] at \( n = 2 \) has nearly all copper sites doubly occupied and all oxygen sites empty. We see gaps at \( n = 1 \) and \( n = 2 \) with \( \mu (n = 1^+) - \mu (n = 1^-) \approx U_d, \mu (n = 2^+) - \mu (n = 2^-) \approx \Delta_0 - U_d \). In Fig. 1 the case \( U_d > \Delta_0 \) is realized and the corresponding atomic ground-state at \( n = 2 \) [14] has all copper and oxygen sites singly occupied. Here, gaps exist at \( n = 1 \) and \( n = 3 \), with \( \mu (n = 1^+) - \mu (n = 1^-) \approx \Delta_0, \mu (n = 3^+) - \mu (n = 3^-) \approx U_d - \Delta_0 \).

Hence an insulator to metal transition occurs at \( n = 2 \) at a critical value of the ratio \( U_d/\Delta_0 \approx 1 \), which can be interpreted as the upper Hubbard band hitting the \( p \) level. In Fig. 4 such an intermediate situation is realized. Below, we find that very interesting physics arises in the mixed valence regime \( (U_d \approx \Delta_0) \), where the strongly correlated copper level lies close to the uncorrelated oxygen level.

Additional insights on this transition can be gained by looking at the self-consistency equation (7) for the special point \( \mu = \varepsilon_p \), which reads for low-frequency \((i\omega_n \rightarrow \omega + i0^+, \omega \rightarrow 0)\):
Fig. 7. Im($G(i\omega_d)$) (full line) and Re($\Sigma_d(i\omega_d)$) (dotted line) for $U_d=4.5$, $\mu-\varepsilon_d=4$, $\Delta_0=4$, and $\beta=45$ ($L=128$)

Fig. 8. Im($G(i\omega_d)$) (full line) and Re($\Sigma_d(i\omega_d)$) (dotted line) for $U_p=6.5$, $\mu-\varepsilon_d=4$, $\Delta_0=4$, and $\beta=45$ ($L=128$)

Fig. 9. Hubbard III approximation for the one-particle density of states $\rho_d(\omega)$ vs $\omega-\mu-\Sigma_d$ for $\Delta_0=4$, and $U_d=0.25, 3, 4.5, 8$

i) is obviously realized for small $U_d$, while case ii) can be interpreted as the effective d level $\Sigma(i\varepsilon^+_d)+\varepsilon_d$ becoming degenerate with the p level. Although we cannot obtain the numerical solution at zero temperature we find numerical evidence that one goes from i) to ii) as $U_d$ is increased. This is readily seen in the data of Figs. 5–8 for four different values of the interaction strength. From these curves, it is apparent that $\Sigma_d(i\varepsilon^+_d)$ remains close to $\varepsilon_p-\varepsilon_d$ for all values of $U_p$ larger than a critical value. These figures display in fact the results of two subsequent iterations of the self-consistency loop, which we display in order to highlight the remarkable accuracy of the Monte Carlo algorithm.

The qualitative behavior of n vs $\mu$ can also be understood from a Hubbard III-type solution of the coupled equations (7), which takes into account the physics of high-energy processes in a qualitatively correct manner [9]. The appropriate generalization of the Hubbard III approach to the two-band model inserts the following expression for $D(i\omega_n)$

$$D(i\omega_n) \approx \frac{1}{2} \left\{ D_0 + \frac{1}{D_0 - U_d} \right\}$$

(9)

into the self-consistency equation (7), to obtain the following closed equation for $D(i\omega_n)$:

$$i\varepsilon_{pd}(x_p^2-U_p^2/4)D^3$$

$$+i\varepsilon_{pd}(x_p U_p^2/2 - 2x_p x_d^2 + \varepsilon_{pd} x_d)D^2$$

$$+(x^2-U_d^2 x_d^2/4 + \varepsilon_{pd} x_d x_d + \varepsilon_{pd}^2) D - x x_p = 0$$

(10)
where \( x_d = i \omega_n + \mu - \varepsilon_d - U_d/2 \), \( x_p = i \omega_n + \mu - \varepsilon_p \), and \( x = x_p x_d - \frac{t^2}{2} \).

This simple approximation gives a rather satisfactory account of the various metal-insulator transitions described above (except as \( U_d \to \infty \)): zero-temperature spectral densities are displayed in Fig. 9 for various values of the parameters. It is unable however to account for the low-energy quasiparticle excitations in the metallic regimes, since it just ignores the Kondo effect in the impurity model equation (3).

IV. Superconducting properties

A. Dynamical pairing in infinite dimensions

In this section we extend the \( d = \infty \) formalism to incorporate the possibility of superconducting long-range order. The equation that we will establish here allow the investigation of the model within the broken symmetry phase (cf. [6, 11] where the Hubbard model was studied within magnetically ordered states). Let us define 'anomalous' Green's functions:

\[
\begin{align*}
F_d(\tau - \tau') &
= - T \langle d_{i, \uparrow}(\tau) d_{i, \uparrow}(\tau') \rangle \\
F_p(\tau - \tau') &
= - T \langle p_{i, \uparrow}(\tau) p_{i, \uparrow}(\tau') \rangle
\end{align*}
\]

(11)

This describing the formation of on-site pairs. Singlet pairing corresponds to \( F \) even: \( F(\tau) = F(-\tau) = F(\beta - \tau) \), while \( S = 0 \) 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 \textit{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 [21] for triplet pairing in \( ^3 \text{He} \), a generalization of which has been recently considered for cuprate superconductors by Balatsky and Abrahams [22] in the singlet case.

In the presence of a non-zero \( F \) it is convenient to work with Nambu spinors \( \Psi_d^\dagger \equiv (d_{i, \uparrow}, d_{i, \downarrow}) \) (similarly \( \Psi_p^\dagger \)) and with the matrix formulation of one-particle Green's functions:

\[
D(\tau - \tau') = - T \langle \Psi_d(\tau) \Psi_d^\dagger(\tau') \rangle
\]

\[
= \begin{pmatrix} G_d(\tau - \tau') & F_d(\tau - \tau') \\ F_d(\tau - \tau') & -G_d(\tau - \tau') \end{pmatrix}.
\]

(12)

With these notations, the kinetic term of the hamiltonian \( \mathcal{H} \) reads: \(-t_{ij} \Psi_{d, \sigma}(\tau) \sigma_3 \Psi_{p, \sigma}(\tau) \) where \( \sigma_3 \) denotes the Pauli matrix. Following the usual method, we integrate out fermionic variables on all sites except on a single copper site. The 'impurity' action obtained in this way now reads:

\[
\mathcal{S}_{\text{sup}} = U_d \sum_{\downarrow} \int_0^\beta d\tau n_{d, \downarrow}(\tau) n_{d, \downarrow}(\tau)
\]

\[
- \sum_{\downarrow} \int_0^\beta \int_0^\beta d\tau d\tau' \Psi_d^\dagger(\tau) D_0^{-1}(\tau - \tau') \Psi_d(\tau')
\]

(13)

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

\[
D_0^{-1}(i \omega_n) = i \omega_n + (\mu - \varepsilon_d) \sigma_3 - i \frac{\sigma_3}{\tau} D(i \omega_n) \sigma_3
\]

\[
P^{-1}(i \omega_n) = i \omega_n + (\mu - \varepsilon_p) \sigma_3 - i \frac{\sigma_3}{\tau} D(i \omega_n) \sigma_3.
\]

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

\[
\left( \begin{array}{cc} 0 & \Delta_d(i \omega_n) \\ \Delta_d(i \omega_n) & 0 \end{array} \right)
\]

(15)

to the r.h.s. of (14).

The impurity action (13) describes an Anderson impurity in a superconducting medium. Since this problem even with static pairing [24] turns out to be highly non-trivial, we can expect that the self consistent solution of (14) will display very rich behaviour.

B. Algorithm in the presence of pairing [16]

In the present paragraph we show how the Hirsch-Fye algorithm [12] can be generalized in the presence of off-diagonal terms (in the spin indices) in the Green's function (12) which, after the usual Trotter breakup, become a \( 2 \times 2 \) matrix.

The quartic term in the action is decoupled, as usual, by the introduction of Ising variables.

\[
\exp[-\Delta \tau Un' n^2 - (n^2 + n'^2)/2]
\]

\[
= \text{Tr}_\sigma \exp[\lambda \sigma(l) [n^2 - n'^2]]
\]

(16)

According to the prescription given by Soper [15], all terms in the action have to be normal-ordered (here, \( \Psi^+, \Psi \) with \( \Psi^+(\tau) = (\Psi_1^+(\tau), \Psi_2^+(\tau))(c_1^\dagger, c_1) \)), before performing the discretization. Consequently, (16) written as

\[
\text{Tr}_\sigma \exp[\lambda \sigma(\Psi_1^+ \Psi_1 + \Psi_2^+ \Psi_2)] \exp[-\lambda \sigma(l)]
\]

(12)

The Green's functions for different spin configurations are related by the following Dyson equation:

\[
D_\sigma(\tau, \tau') = D_\sigma + (D_\sigma - 1)(\exp(W' - W) - 1) D_\sigma
\]

(18)

where \( D_\sigma(\tau, \tau') \) is the full \( 2 \times 2 \) matrix Green's function of \( \Psi \) for a given spin configuration \( \sigma(l) \), and \( W_k = \Psi_{k+L} \equiv \lambda \sigma(k) \). Equation (18) is derived in the same way as the one in [12], and differs from that expression only in a sign for the down-spin sector. The Green's function of the model is given by

\[
D(\tau, \tau') = \sum_\sigma D_\sigma(\tau, \tau') \text{Det}(D_\sigma^{-1}) \exp(-\lambda \sum_l \sigma(l))
\]

(19)
The statistical weight of a configuration is thus given by the product of the usual fermion determinant, and of a scalar factor, which arises from the commutator in (16).

As in the Hirsch-Fye algorithm [12], we can use the Dyson equation to calculate the ratio \( R \) of statistical weights for flipping a spin \( \sigma (k) \rightarrow \sigma' (k) = - \sigma (k) \),

\[
R = R_s, R_c, \exp ( - 2 \lambda \sigma [k] )
\]

\[
R_s = 1 + [1 - D (k, k)] f
\]

\[
R_c = 1 + [1 - D (k + L, k + L) - D (k + L, k) \times D (k, k + L) f / (1 + (1 - D (k, k)) f)] f
\]

with \( f = [\exp ( - 2 \lambda \sigma (k) ) - 1] \). Once a flip of spin \( \sigma (k) \) is accepted, all the elements of the \( 2L \times 2L \) Green’s function are updated in a 2-step procedure, corresponding to the flip of \( W_k \) and \( W_{k + L} \).

\[
D^* (l, l') = D (l, l') + D (l, k) - \delta (l, k) f / (1 + (1 - D (k, k)) f) D (k, l')
\]

\[
D^* (l, l') = D^* (l', l) + D (l, k + L) - \delta (l, k + L) f / (1 + (1 - D') \times (k + L, k + L)) f) D' (k + L, l').
\]

We have extensively compared the algorithm with exact diagonalization results for an impurity interacting with a few conduction electrons in the presence of explicit pairing terms \( d^*_\sigma d^+_{\sigma'} \), and conclude that the algorithm is correct, and practical. In Fig. 10 we show data of one such realization of the superconducting Anderson model for \( \Delta = 1, 0.5, 0.25, 0.125, \) and 0 (exact diagonalization). Notice the quadratic convergence.

### C. Numerical results

To investigate the transition into the superconducting state at finite temperature we define a pairing susceptibility \( \chi_p (i \omega_n, i \omega_m) \)

\[
F_d (i \omega_n) = \sum_m \chi_p (i \omega_n, i \omega_m) \Delta_d (i \omega_m)^* \quad \text{for} \quad \Delta_d (i \omega_m) \rightarrow 0.
\]

This susceptibility is a well defined symmetric matrix and is finite in the normal state. The divergence of its largest eigenvalue signals the transitions into the superconducting state. In our approach it is natural to express \( \chi_p \) in terms of two operators, \( \lambda \) and \( \alpha \). \( \lambda (i \alpha, i \omega_m) \) describe the pairing response of the impurity model equation (13)

\[
F_d (i \omega_n) = \sum_m \lambda (i \omega_n, i \omega_m) [G_{od}^{-1}]_{12} (i \omega_m),
\]

\[
\quad \text{for} \quad [G_{od}^{-1}]_{12} \rightarrow 0
\]

while the diagonal operator \( \alpha \) describes the response of the self consistent medium to the impurity site and can be obtained from (14) as \( \alpha (n, m) = \delta (n, m) \chi_{od} (i \omega_n) / \chi_{od} (i \omega_n) \).

Clearly, \( \lambda, \alpha \), and \( \chi_p \) are related by the following equation

\[
\chi_p = [I - \lambda \alpha]^{-1} \lambda.
\]

When the largest eigenvalue of \( \lambda = \lambda \alpha \) approaches one, the susceptibility diverges. It is clearly more accurate to study the behavior of the largest eigenvalue of \( \lambda = \lambda \alpha \) and we do that by the power method using the full algorithm. To do this, we run the algorithm described in the previous section a large number of times, starting with a small value of the off-diagonal term \( F (\tau, \tau') \) of the Green’s function. In the normal state, \( F (\tau, \tau') \) will converge to zero and two subsequent runs will yield two functions \( F (\tau, \tau') \) and \( F' (\tau, \tau') \) obeying

\[
F' (\tau, \tau') = \int d \tau'' \lambda (\tau, \tau'') F (\tau'', \tau') \sim \lambda_{\text{max}} F (\tau, \tau').
\]

\( \lambda_{\text{max}} \) is the largest eigenvalue of the matrix \( \lambda \) (cf. (26)) and \( F' (\tau - \tau') \) converges to the corresponding right eigenvector, which is also the eigenvector corresponding to the most unstable eigenvalue of the susceptibility matrix.

In Fig. 11, we show \( \lambda_{\text{max}} \) vs \( n \) at a relatively high temperature \( \beta = 15 \) in the singlet sector, i.e., after explicitly
Fig. 11. $\lambda$ vs $n$ at $\beta = 15$ and $L = 16$ (upper curve), 32, and 64 (lower curve) at the special point $\Delta_0 = 4$, $U_0 = 4.5$, $\mu - e = 4$

Fig. 13. The real part of $F_3(\beta \omega)$ vs $\omega$ on the special point at $L = 128$ and inverse temperatures $\beta = 64$ (full line), $\beta = 70$ (dotted line), and $\beta = 80$ (dashed line)

Fig. 12. Green's functions $G_3(\tau)$ and $F_3(\tau)$ at the special point $\Delta_0 = 4$, $\mu - e = 4$, at $U_0 = 4.5$, $\beta = 64$ and $L = 128$. The inset shows $F_3(\tau)$ and $F_3(\tau)$

Fig. 14. Imaginary part of $G_3(i\omega)$ on the special point at $L = 128$ and inverse temperatures $\beta = 64$ (full line), $\beta = 70$ (dotted line), and $\beta = 80$ (dashed line)

anti-symmetrizing the functions $F(\tau)$ and $F_0(\tau)$ with respect to $\beta/2$. In order to assess the importance of finite $\Delta \tau$ effects, we have plotted $\lambda_{\text{max}}$ for $L = 16$, 32, 64. Let us stress that this extrapolation is the only error in our calculation, since the statistical uncertainty and the uncertainty stemming from the self-consistency condition are extremely small. All of our data is consistent with quadratic convergence in $\Delta \tau^2$ for small values of $\Delta \tau$ which we have clearly established for the Green's function itself.

The susceptibility seems to have a local maximum close to the density $n = 1$, and is again large at around $n = 2$. We notice that the tendency towards superconductivity
is largest near half filling and near $n \sim 2$, i.e. in the mixed valence regime.

We have been able to produce perfectly converged superconducting solutions of the mean-field equations in the singlet case for temperatures within our reach. The solution for $F(\tau)$, at temperatures just below $T_c(\Delta \tau)$ is very similar to the largest eigenvector of the susceptibility matrix above $T_c$. The finite value of $\Delta \tau$ produces large finite size effects in the value of $T_c(\Delta \tau)$. At this point we have established that $\beta_\tau(L=64)=37$, $\beta_c(L=128)=59$ and $\beta_\tau(L=192)=75$: A reliable finite size scaling of this quantity to determine the value of the critical temperature requires larger simulations and will be described elsewhere. Here we use the fact that the largest eigenvector of the susceptibility matrix converges very well to discuss the nature of the possible superconductivity in this system. Of particular importance is the different and strong frequency dependence on the copper and the oxygen sites.

Examples of such numerical solutions are given in Fig. 12 for 128 time slices, at the value which seems to be most favorable for the appearance of superconductivity $\Delta \tau = 4$. The Fourier transform of the order parameter on the copper site near $T_c$ are displayed in Fig. 13. Notice (inset of Fig. 12) that the pairing amplitude is much larger on oxygen sites than on copper sites, as expected, and that the equal-time pairing $F(0)$ is nearly zero on copper sites.

7. Conclusion

In this paper we introduced a controlled approach to the study of the occurrence of superconductivity in strongly correlated systems. We extended the mean field approach to the strong correlation problem of [4] to derive a self consistent picture of a correlated superconductor which becomes exact in infinite dimensions. As in the corresponding treatment of the normal state [4] an impurity model plays the role of the mean field hamiltonian. The impurity model corresponding to a correlated superconductor is an Anderson impurity model embedded in a superconducting medium. The quantities that correspond most closely to the Weiss field is now a set of two functions that describe the diagonal and the off-diagonal response of the effective medium. A numerical solution of the self consistent equations for the Green's functions revealed a strong frequency dependence of the superconducting order parameter.

Using this method we investigated the most promising regions for high temperature superconductivity in the present version of the extended Hubbard model in large dimensions. The lowest tendencies towards superconductivity were found when the normal phase is in a mixed valence regime.

There are several natural extensions of this work. One can study the effect of adding extra interactions in the hamiltonian on the superconducting transition temperature of the system. While the critical temperatures we found are relatively high, a better understanding of the behaviour of the solution of our equations may lead to higher transition temperatures. Finally, as emphasized throughout the text, larger simulations are called for. They should allow the finite size scaling analysis which can fully elucidate the existence of the superconducting state proposed here. A completely open problem is the study of the physical properties of this superconducting state. We stress that because of the strong correlations a non perturbative treatment like the one outlined in our paper is necessary for tackling this problem.

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References

14. Note that, in the atomic limit $\tau_0=0$, the total hole density vs. chemical potential is given by: $n_{\text{atomic}} = \Theta (\mu - \epsilon_d) + \Theta (\mu - (\epsilon_0 + U_d)) + 2 \Theta (\mu - \epsilon_0)$
16. In this section we follow the Hirsch and Fye notation and define the Green's functions with an extra minus sign relative to the other sections