Superconductivity in the Two-Band Hubbard Model in Infinite D: an Exact Diagonalization Study

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We apply an exact diagonalization method to the the infinite-D two-band Hubbard model. The method is essentially exact for the calculation of thermodynamic properties for all but the smallest frequencies and yields a resolution unavailable in Monte Carlo calculations. We establish the instability of the normal state with respect to singlet superconductivity at small frequencies at small doping, the regime of relevance for High-$T_c$ superconductors. We also present evidence for the existence of an instability towards triplet superconductivity in the large doping regime $n \sim 2$.

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The discovery of high-temperature superconductivity has enormously increased the interest in strongly correlated electron systems. Superconductivity in its various guises has been searched for in practically all available models. Of particular interest are models with several electronic bands, such as the three-band model of Emery [1] and of Varma, Schmitt-Rink and Abrahams [2]. These have been proposed as minimal models for the CuO planes in the new materials. In 2D, the three-band model has been been actively studied numerically, but even the most ambitious Quantum Monte Carlo calculations [3] have up to now given only inconclusive evidence.

Given the enormous complexity of the full problem in two or three dimensions it is natural to bring to bear the methods of the - now well established - infinite dimensional approach on this problem [4]. As for classical statistical mechanics systems, the limit of infinite dimensions constitutes a self-consistent mean field theory in which the spatial fluctuations are frozen and where the infinite-D many-body system is reduced to a self consistent single site problem. It is of considerable interest to clarify whether such models with several bands are able to show superconductivity even (or: at least) in large D, i.e. in the absence of spatial (e.g. antiferromagnetic) fluctuations. This is the aim of the present paper.

We investigate in detail the infinite-D two band Hubbard model, which was proposed in a recent paper [5] and studied with an extension of the Hirsch-Fye Quantum Monte Carlo (QMC) algorithm [6]. This method proved to be adequate for the investigation of the normal state, and several very interesting metal-to-insulator transitions were identified. However, the QMC algorithm did not allow a controlled investigation of the superconducting state or of the instability of the normal solution. The main result was that, at the temperatures accessible to the QMC method, the superconducting susceptibilities were large in two different regimes, the small doping regime (of relevance for high-$T_c$ superconductors) and a regime with density $n$ close to 2 for intermediate values of the Coulomb interaction.

In this paper we take up these two regimes ($n \sim 1$ and $n \sim 2$). We are interested in the normal state exclusively as a starting point for a linear stability analysis and investigate the regime close to the normal solution. Before presenting our results we will give a brief explanation of our exact diagonalization method ([7]) as applied to the problem of superconductivity. Just as for the Hubbard model [7], this method is far superior to the Quantum Monte Carlo method and allows us to decrease by at least an order of magnitude the limiting temperature (smallest accessible frequency).

The (CuO)$_d$-type which is the object of our study is defined by the Hamiltonian

$$
\mathcal{H} = - \sum_{i\in D,j\in P,\sigma} t_{ij} d_{i\sigma}^+ p_{j\sigma} + h.c. + \epsilon_p \sum_{j\in P,\sigma} p_{j\sigma}^+ p_{j\sigma} + \epsilon_d \sum_{i\in D,\sigma} d_{i\sigma}^+ d_{i\sigma} + U_d \sum_{i\in D} n_{i\uparrow} n_{i\downarrow} \tag{1}
$$

where the hopping is scaled as $t_{ij} \sim 1/\sqrt{2z}$ ($z$ is the connectivity of the lattice). In eq. (1) $(d_{\sigma}, p_{\sigma})$ represent two atomic orbitals on different sublattices $(D, P)$ of a bipartite lattice with $z \to \infty$ which, for the purposes of the present paper, is taken to be the infinitely connected Bethe Lattice. The repulsive Coulomb interaction acts only on the (’copper’) orbital $d_{\sigma}$, while the (’oxygen’) orbital $p_{\sigma}$ is uncorrelated. In the standard Nambu notation, $\Psi_d^+ \equiv (d_{\uparrow}^+, d_{\downarrow})$ (equivalently for $\Psi_p$) the d-orbital Green’s function can be written as a $2 \times 2$ matrix

$$
\mathbf{D}(\omega) \equiv -T < \Psi_d(\omega) \Psi_d^+(\omega) > = \begin{pmatrix}
G_d(\omega) & F_d(\omega) \\
F_d^*(\omega) & -G_d(-\omega)
\end{pmatrix} \tag{2}
$$
and the self-consistency equations for the Green’s functions are given by \[5\]

\[
\begin{align*}
D_0^{-1}(i\omega_n) &= i\omega_n + (\mu - \epsilon_d)\sigma_3 - t_{pd}^2\sigma_3 P(i\omega_n)\sigma_3 \\
\mathbf{P}^{-1}(i\omega_n) &= i\omega_n + (\mu - \epsilon_p)\sigma_3 - t_{pd}^2\sigma_3 D(i\omega_n)\sigma_3
\end{align*}
\]  

(note that \(D_0\) and \(D\) are \(2 \times 2\) matrices and that \(D_0^{-1}\) denotes the matrix inverse).

The Green’s function \(D(i\omega_n)\) and the bath Green’s function \(D_0(i\omega_n)\) are connected by the single-site action

\[
S_{sup} = U_d \int_0^\beta d\tau n_{\uparrow\downarrow}(\tau)n_{\downarrow\uparrow}(\tau) - \int_0^\beta d\tau \int_0^\beta d\tau' \Psi_\downarrow^\dagger(\tau)D_0^{-1}(\tau - \tau')\Psi_\downarrow(\tau')
\]

This eq. \[4\] is at the base of the Quantum Monte Carlo approach to the solution of the \(d = \infty\) equations, which consists in a decoupling of the interaction term in \(U_d\) and a proper discretization of the integrals. Alternatively, the Green’s functions \(D(i\omega_n)\) and \(D_0(i\omega_n)\) may be viewed as impurity Green’s functions of an effective Anderson model \[8\] which, in the presence of a superconducting medium, is given by

\[
H_{AM} = \sum_{\sigma,l=1}^{n_s} \epsilon_l a_{l\sigma}^\dagger a_{l\sigma} + U n_{\uparrow\downarrow}n_{\downarrow\uparrow} + \sum_{\sigma,l=2}^{n_s} [V_l a_{l\sigma}^\dagger a_{1\sigma} + h.c.] + \sum_{l,k=1}^{n_s} \phi_{lk}[a_{l\uparrow}^\dagger a_{k\downarrow}^\dagger + h.c.]
\]

In eq. \[4\] we have used a compact notation with a site index \(l\), \(1 \leq l \leq n_s\), in which \(l = 1\) denotes the impurity. The matrix \(\phi\) provides explicit pairing terms between all the sites. The matrix is to be taken antisymmetric for the calculation of the triplet sector and symmetric in the singlet sector. Of course a strictly self-consistent solution based on the correspondence between eq. \[4\] and eq. \[3\] will only be possible in the limit of an infinite Anderson model \(n_s = \infty\).

The exact diagonalization method consists in approximating the function \(D_0(i\omega)\) in eq. \[3\] by the Green’s function of a (superconducting) impurity model eq. \[4\] with a finite, and even small number \(n_s\) of sites. Explicitly, \(D_0^{\text{And}}(i\omega)^{-1} = (i\omega - H)\) with \(H\) the single particle Hamiltonian (\(U=0\)) corresponding to eq. \[3\]. \(H\) is of course a strictly self-consistent solution based on the correspondence between eq. \[4\] and eq. \[3\]. The Green’s function is given by the standard formula \(G_0 d(i\omega) = i\omega - \epsilon_d - U_d/2 - \sum_{k=2}^{n_s} V_k^2/(i\omega - \epsilon_k)\).

In practice, we use a conjugate gradient method to determine the parameters \(V_k, \epsilon_k\), and \(\phi_{ij}\) minimizing the function

\[
E = \sum_{n=0}^{n_{\text{max}}} |D_0(i\omega_n) - D_0^{\text{And}}(i\omega_n)|/ (n_{\text{max}} + 1)
\]

Here the \(\omega_n\) denote the smallest Matsubara frequencies. Even at zero temperature we use \(\omega_n = (2n+1)\pi/\beta\) with \(\beta\) a fictitious temperature. This provides a lower frequency cutoff. All the results we present do not critically depend on the specific choice of the fitting function, and on \(n_{\text{max}}\).

For \(n_s \leq 6\) we are able to diagonalize exactly the Hamiltonian eq. \[4\], with a full calculation of the spectrum and of the eigenvectors. At temperatures accessible to QMC, the Green’s functions, susceptibilities, etc can then be compared with the extrapolated results of the Monte Carlo algorithm to very high precision. Since we are mainly interested...
in Green's functions in the zero-temperature limit, we may use the Lanczos method \[9\] and are then able to increase noticeably the size of the cluster. For the full superconducting Hamiltonian eq. \(5\) values up to \(n_s \sim 8\) may be handled without problems on a workstation \[14\].

The algorithm which we have just sketched is then iterated to convergence. Once this is reached we are able to estimate the quality of the calculation, which is entirely determined by the agreement of the two Green's functions \(D_0\) and \(D_0^{\text{And}}\). (Note that this is an intrinsic criterion). The agreement between the two functions has been found to be amazingly good. We insist that the fit of \(D_0\) by \(D_0^{\text{And}}\) is the only non-exact part of our procedure and seems to be a much less violent approximation than those introduced by the Trotter breakup (discretization of the integrals in eq. \(4\)) and by the stochastic noise of the Monte Carlo procedure.

An example of the excellent quality of the solution is given by the normal state results \[11\] at zero temperature presented in fig. 1. Here, the functions \(G_{d0}(i\omega)\) and \(G_{d0}^{\text{And}}(i\omega)\) are displayed. The 'effective' temperature is \(\beta = 250\), \(U_d = 8\), and the density corresponds to the lightly doped regime of the two-band model. At \(n_s = 8\), the differences are below the resolution of the graph with a maximum difference on the order of \(10^{-2}\). At fixed value of \(n_{\text{max}}\) (here taken to be 64), we have noticed a systematic improvement of the quality of fit, expressed by a value of \(E\) in eq. \(6\) which decreases by a factor of \(\sim 4\) each time one more site is added \[12\]. As an illustration of this improvement we show in the insets of fig. 1 the self-consistent solutions at \(n_s = 4, 5, 6, 7,\) and \(8\). Above \(i\omega \sim 5\) the Green's functions are strictly identical.

We now consider the stability analysis of the normal state solution. A possible way of studying this stability is to calculate the pairing susceptibility. An alternative way used here is to establish the stability properties of the solution by introducing small terms \(\phi_{ij}\) in the Hamiltonian eq. \(5\), and following the evolution under subsequent iterations \[5\]. Under such conditions, the normal state solutions in fig. 1 very quickly acquire non-zero values of \(F(\omega)\), which indicate a superconducting instability. More rigorously, and in order to study quantitatively the effects of increasing \(n_s\), we may calculate the largest eigenvalue, and the corresponding eigenvector of the matrix \(\partial F(\omega)^{n+1}/\partial F(\omega)^n\) close to the normal state, where the superscripts on the \(F's\) indicate two subsequent iterations of the self-consistency loop. This involves a simple rescaling of the \(\phi\) at each iteration. We have done such calculations, which correspond to the well-known procedure of extracting the largest eigenvalues and eigenvectors of a matrix with the 'power method', starting from the parameters in fig. 1, for \(5 \leq n_s \leq 8\). We are able to identify a linear regime at small \(\phi\), with the largest eigenvalue always of the order \(\lambda_{\text{max}} \sim 2\). The corresponding (rescaled) eigenvectors for \(n_s = 6, 7, 8\) are plotted in fig. 2. Clearly, the agreement between these completely independent curves is excellent. We have checked this result in a variety of ways (by changing the effective temperature, the precise form of the function used in eq. \(3\), and the doping). This leads us to the conviction that the normal state solution of the \(d = \infty\) model at small doping is indeed unstable with respect to singlet superconductivity.

We have also studied the point investigated previously \[5\], i.e. values of the physical parameters corresponding to a total density of \(n \sim 2\), where the Hubbard interaction is just large enough to create a large overlap between the upper Hubbard band of the \(d\)-level and the \(p\)-level band. There our evidence for singlet superconductivity is very limited (at
least for frequencies larger than $\sim 1/200$). However, we have on that point found very clear evidence for superconductivity in the triplet sector. Following the procedure outlined above, we find consistently at small 'effective' temperature that any small terms in $\phi$, in addition to the normal state solution, blow up at a rate which corresponds to a largest eigenvalue of $\sim 1.8$ of the matrix $\partial F(i\omega)^{n+1}/\partial F(i\omega)^n$. In fig. 3 we show the zero-temperature normal state solution for $U_d = 4.5$, $\mu = \epsilon_p - \epsilon_d = 4$, calculated on a grid of points corresponding to an effective temperature of $\beta = 200$. The inset shows the most unstable eigenvector in the triplet sector. Its corresponding eigenvalue is $\lambda_{max} = 1.75$ [13]. Superconducting order of this kind has been first proposed by Berezinskii [14] in the context of $^3$He, and, very recently by Coleman, Miranda and Tsvelik [15] for heavy-fermion superconductors.

In conclusion, we have studied the infinite dimensional two-band Hubbard model with an exact diagonalization method, which has given very strong evidence for a superconducting instability at low temperature. Given the excellent fit of the Green's functions, and the smallness of the finite size effect (dependence on $n_s$), it seems to us to be difficult to escape the conclusion that the two-band model is indeed superconducting, with a strongly frequency-dependent order parameter. We have taken every effort to check the programs (exact diagonalization and Lanczòs) against each other and against the extrapolated Quantum Monte Carlo results at sufficiently high temperature. Close to the normal state solution we have also not been plagued by possible multiple solutions of the minimization in eq. (6). In fact, we have also been able to find perfectly converged solutions of the fully superconducting phase [16], but there the extrapolation with $n_s$, and the possible problem of multiple solutions are more critical. Therefore, the linear stability analysis presented here is the most convincing argument in favor of a superconducting instability of the two-band Hubbard model which we are able to give at the present time.

Finally, as has been discussed elsewhere [7], the method does for the time being not allow a precise calculation of the densities of states, and a renormalization group procedure is clearly called for. Such a method would allow the calculation of regular and superconducting densities of state. It would also allow calculations at finite temperature with much larger precision. The search for a numerical renormalization group procedure for $D = \infty$ is in our opinion an extremely exciting challenge to take up.

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[1] V. Emery Phys. Rev. Lett. 58, 2794 (1987).
[2] C. Varma, S. Schmitt-Rink and E. Abrahams Solid State Comm 62, 681 (1987).
[3] G. Dopf, A. Muramatsu and W. Hanke Phys. Rev. Lett. 68, 353 (1992)
[4] For a recent review and references, see e.g. D. Vollhardt, to appear in 'Correlated Electron Systems', proceedings of the Jerusalem Winter School of Theoretical Physics, V. J. Emery ed. (World Scientific). (preprint RWTH/ITP-C 6/92). 62 324 (1989).
[5] A. Georges, G. Kotliar, and W. Krauth, LPTENS preprint 93/10, to appear in Z. Phys. (1993)
[6] J. E. Hirsch and R. M. Fye, Phys. Rev. Lett. 56 2521 (1986)
[7] M. Caffarel and W. Krauth, LPQ preprint (1993)
[8] A. Georges and G. Kotliar Phys. Rev. B 45 6479 (1992)
[9] R. Haydock, V. Heine, and M. J. Kelly J. Phys. C 8, 2591 (1975)
[10] In practice, the Hamiltonian eq. (5) is rewritten in terms of Nambu spinors. The pairing terms are then transformed into spin-flip operators, and conserve the number of up-particles + down-holes. This symmetry has been implemented.
[11] This means that the anomalous Green’s function is forced to be 0 and that a self-consistent solution for $G_d(i\omega_n)$ is searched for. $F_d = 0$ is always a possible solution of the self-consistency equation eq. (4).
[12] This observation (which would indicate exponential convergence in $n_s$) is our main argument in favor of the algorithm. It seems rather unlikely that we would discover new physics at values of $n_s$ much larger than the ones treated in the presence of both an excellent fit and of extremely rapid convergence.
[13] In the triplet case we have very good convergence of the eigenvalues as a function of $n_s$, but the eigenvalues -although qualitatively the same - show some quantitative differences at small frequencies. Larger simulations are probably called for in order to settle this point.
[14] V. L. Berezinskii, JETP Lett. 20, 287 (1974)
[15] P. Coleman, E. Miranda, and A. Tsvelik Phys. Rev. Lett. 70 2960 (1993), and preprint
[16] W. Krauth and M. Caffarel, in preparation
Figure Captions

1. Zero temperature imaginary-time functions $G_{d0}(i\omega)$ and $G_{d0}^{and}(i\omega)$ (real parts: upper) (imaginary part: lower) vs $\omega$ $U_d = 8$, $\mu = \epsilon_p - \epsilon_d = 4$ as calculated with the Lanczos algorithm with $n_s = 8$ sites. Inset: Real part of the functions for $n_s = 4, 5, 6, 7$ and $= 8$. If $G_{d0}^{and}(i\omega)$ and $G_{d0}(i\omega)$ were exactly equal this would be the exact solution. Note the excellent fit of the two quantities for $n_s = 8$, and the systematic improvement with increasing number of sites. A quasi-exact solution is obtained at $n_s = 8$.

2. Largest eigenvector of the matrix $\partial F(i\omega)^{n+1}/\partial F(i\omega)^n$ close to the normal state solution of fig. 1. for $n_s = 6, 7$ and 8 (singlet sector). The corresponding eigenvalues are $\lambda_{max} \sim 2$ in all three cases.

3. Zero-temperature Green’s function $G(i\omega)$ in the normal state at $U_d = 4.5$, $\mu = \epsilon_p - \epsilon_d = 4$ at $n_s = 7$ (effective $\beta = 200$, $n_{max} = 64$). The misfit between $G_{d0}(i\omega)$ and $G_{d0}^{and}(i\omega)$ is given by $E = 1.5 \times 10^{-4}$ (!) (cf. eq. 6) and the maximum difference between the two functions is $7 \times 10^{-4}$. The inset shows the most unstable eigenvector in the triplet sector at $n_s = 7$. The corresponding eigenvalue is $\lambda_{max} = 1.75$. 