THE WAVEFUNCTION RENORMALIZATION CONSTANT FOR THE ONE- AND TWO-BAND HUBBARD HAMILTONIANS IN TWO DIMENSIONS

E. Louis,¹ G. Chiappe,¹ J. Galán,² F. Guinea,² and J. A. Vergés²

¹Departamento de Física Aplicada
Universidad de Alicante
Apartado 99, 03080 Alicante, Spain

²Instituto de Ciencia de Materiales
Consejo Superior de Investigaciones Científicas
Cantoblanco, 28049-Madrid, Spain

INTRODUCTION

The normal state of the recently discovered high-$T_c$ superconductors [1], exhibits many exotic properties that are not yet fully understood. A picture that is gaining acceptance assumes that the normal state is not a normal Fermi liquid [2-5] but rather it shows unconventional properties somewhat similar to those of the Hubbard model in 1D [6], namely: i) an unrenormalizable Fermi-surface phase shift, which implies a vanishing wavefunction renormalization constant ($Z$), ii) a one-particle spectral density that shows a strong peak at the Fermi energy, iii) a Fermi surface that obeys Luttinger’s theorem [7], and, iv) charge and spin separation.

Only in very few cases has a quantitative check of these properties been undertaken [8-15]. In particular, $Z$ has been calculated by exactly solving either the t-J [12] or the Hubbard Hamiltonian in $4 \times 4$ clusters. Charge and spin separation has also been recently investigated on finite clusters of the square lattice [13]. Unfortunately the behavior of these properties in the thermodynamic limit cannot be investigated at present by means of exact calculations.

In previous papers [16] we have presented an Unrestricted Hartree-Fock
(UHF) calculation of $Z$ for the one-band Hubbard model in the square lattice. UHF allows to consider clusters large enough to investigate the scaling of $Z$ with the system size. The results indicate that the system shows non-conventional behavior ($Z=0$) near half-filling. For a given value of $U$, $Z$ vanishes at low dopings, and becomes finite as doping is increased. For very large $U$ the value of $Z$ remains finite for all dopings, excluding half-filling. In this work we discuss these results outlining the reasons why we think that UHF may provide trustable information on $Z$. We also show that the results are not changed if the wavefunction is written as a linear combination of UHF solutions each one centered on a cluster site (this procedure significantly improves the UHF results for the total energy). Finally we present a calculation of $Z$ for the two-band Hubbard model; again, near half-filling, $Z$ scales to zero with the system size.

THE HUBBARD HAMILTONIAN AND THE UHF APPROXIMATION

The Hubbard Hamiltonian for one and two bands can be written in the general form \[ H = H_0 + H_1, \] (1)

\[ H_0 = \sum E_i n_{i\sigma} - \sum_{<ij>\sigma} t_{i,j} c_{i\sigma}^\dagger c_{j\sigma}, \] (2)

\[ H_1 = \sum_i U_i n_{i\uparrow} n_{i\downarrow} \] (3)

where the indexes $i,j$ run over the atoms of the CuO$_2$ planes in the two-band case, or over atoms at sites of the square lattice in the one-band case. The operator $c_{i\sigma}$ destroys an electron with a $z$-component of the spin $\sigma$ at orbital $i$, and $t_{i,j}$ is the hopping matrix element between orbitals located at atoms $i$ and $j$ (the symbol $<ij>$ denotes the sum over all pairs of nearest neighbors), $E_i$ are the orbital energies and $U_i$ is the intrasite Coulomb repulsion.

The most general effective Hamiltonian, within the UHF approximation, can be written as \[ H_1^{\text{eff}} = \sum_i \left( c_{i\uparrow}^\dagger c_{i\downarrow} \right) \left( \begin{array}{cc} <n_{i\uparrow}> & -<c_{i\uparrow}^\dagger c_{i\downarrow}>^* \\ -<c_{i\downarrow}^\dagger c_{i\uparrow}> & <n_{i\downarrow}> \end{array} \right) \left( \begin{array}{c} c_{i\uparrow} \\ c_{i\downarrow} \end{array} \right) - \sum_i U_i <n_{i\uparrow}><n_{i\downarrow}> - |<c_{i\downarrow}^\dagger c_{i\uparrow}>|^2 \] (4)

If spin flip terms characterized by a non-zero value of $<c_{i\uparrow}^\dagger c_{i\downarrow}>$ are ignored, the standard Hartree-Fock approximation of the Hubbard interaction is recovered. In this work we have only considered solutions with a single non-zero component of the local magnetization for the following reasons: i) near half-filling the vortex solutions described in \[ \text{[18, 19]} \] lie at much higher energies than the Ising solutions (magnetic polaron or extended), and, ii) at moderate dopings vortices become more competitive but only for an even number of particles. In general, solutions with transverse magnetization are more extended and lead to lower values of $Z$. 
THE WAVEFUNCTION RENORMALIZATION CONSTANT

The wave-function renormalization constant is given by

$$\sqrt{Z} = \frac{< \Psi(N)|c_{\alpha}\Psi_{\alpha}(N + 1)>}{< \Psi(N + 1)|c_{\alpha}^\dagger c_{\alpha}^\dagger|\Psi(N + 1)>}$$  \hspace{1cm} (5)$$

where $\alpha$ stands for the appropriate quantum numbers and the $\Psi$'s are the ground state wave-functions. In calculating $Z$ we proceed as follows. We start from the Slater determinant for $N$ electrons and empty the one-electron state of highest energy. This is equivalent to identify the operator $c_{\alpha}^\dagger$ in Eq. (2) with

$$c_{E_n,\sigma} = \sum_k \gamma_{k\sigma}(E_n)c_{k\sigma},$$  \hspace{1cm} (6)$$

where $E_n$ and $\sigma$ are the energy and spin of the empty UHF level of lowest energy, and $\gamma_{k\sigma}(E_n)$ are coefficients obtained in the UHF calculation. For this choice of the operators in Eq. (5) the normalization constant in this equation is equal to one. Simultaneously, we introduce a small random distortion (maximum modulus of $10^{-6}$) on the starting mean field, both on local charges and magnetizations. The addition of this distortion has two objectives: a) to break the degeneracy of the filled state of highest energy as occurs in cases such as half-filling, and, b) to draw the iteration process towards the state of lowest energy. Then we initiate the iteration process \cite{18, 19} until selfconsistency is achieved.

The square root of the wave-function renormalization constant $Z$ is given by the overlap between the resulting Slater determinant and the initial one, which can be calculated through the following expression,

$$< \Psi(N)|\Phi(N)> = \begin{vmatrix} <\psi_1|\phi_1> & \cdots & <\psi_1|\phi_N> \\ . & \cdots & . \\ <\psi_N|\phi_1> & \cdots & <\psi_N|\phi_N> \end{vmatrix}$$  \hspace{1cm} (7)$$

where $\Psi(N)$ and $\Phi(N)$ are two Slater determinants for $N$ particles, and $\psi_i$ and $\phi_i$ the corresponding mono-electronic wavefunctions.

One-band Hamiltonian

The one-band Hubbard Hamiltonian has been solved on finite clusters of size $L \times L$ (with $L$ up to 16). For the parameters in Eqs. (1-3) we took, $t_{i,j} = 1$, $E_i = 0$ and $U_i = U$. The ground state for intermediate values of $U$ is, in the case of a single hole, the magnetic polaron, whereas for many holes it corresponds to magnetic polarons disorderly distributed through the whole cluster. At $U = \infty$ the UHF ground state is ferromagnetic for all fillings \cite{16}.
Figure 1: UHF results for the wave-function renormalization constant $Z$ vs the cluster size ($L \times L$) for the one-band Hamiltonian and 6.25% doping.

Our results for $Z$ at half-filling clearly indicate that it slowly decreases with $L$ for all $U$. The UHF results for the $4 \times 4$ cluster are in good agreement with the exact results reported in Refs. [10, 12]. The scaling of $Z$ to zero with the system size, can be understood as follows. The changes in the charge and spin configurations that result from emptying one of the degenerate levels at the top of the lower Hubbard band are non-uniformly localised along lines. Thus, as the one-hole selfconsistent solutions are localized, it can be expected that the overlap between the two should decrease with the size of the cluster. It should be noted that as at half-filling the system is an antiferromagnetic insulator, strictly speaking it does not make sense to talk about its Fermi or non-Fermi like character. We note, however, that homogeneous HF solutions would have led to a finite $Z$ even at half-filling. Thus, the present results clearly indicates that for a small, still finite, density of holes the system should show non-conventional behavior.

Figure 2: Schematic phase diagram for the one-band Hubbard model according to the results for $Z$. The parameters are the fraction of holes referred to half-filling ($x$) and $U$. $Z$ vanishes in a region close to half-filling. As regards finite doping, we have analyzed the case of 6.25% holes. The results of Figure 1 indicate that, for 6.25% of holes, $Z$ scales to zero for $U = 20$ whereas it remains finite for $U = 10$. This defines a transition from Fermi to Luttinger-like behavior at an intermediate $U$. Thus, we may expect that at large enough $U$ the constant $Z$ will again be finite. At $U = \infty$ the UHF results show that $Z$ remains finite at all dopings, except at half filling (this is a consequence of the ferromagnetic character of the UHF ground state away from half-filling). On the other hand, in the dilute limit the results of Ref. [20] indicate that $Z$ is finite for all $U$.

The numerical data for $Z$, in the cases for which it decreases with $L$, can be fitted by means of the expression [16]
\[ \sqrt{Z} = a \exp(-b \ln L) \quad (8) \]

This equation coincides with that suggested years ago by Anderson [2, 21], and indicates that there exists an unrenormalizable phase shift at the Fermi energy. Actual results for \( b \) show appreciable errors due to the difficulty of the calculations. In all cases analysed here, \( b \approx 0.5 \). The resulting phase shift \( \delta \), obtained by comparing Eq. (8) with that in refs. [2, 21], is \( \delta \approx \pi/\sqrt{2} \), or by introducing the Fermi wave number, \( \delta \approx 0.9k_Fa \), in excellent agreement with the result of [2].

The previous results suggest the phase diagram for the one-band Hubbard model depicted in Figure 2. The region where the system is expected to show non-conventional behavior is close to half filling and finite \( U \). For a given finite \( U \), the system will first (low doping) be a Luttinger liquid and become a Fermi liquid as doping is increased.

**Two-band Hamiltonian**

We have chosen the following set of parameters, \( E_p - E_d = 4.0, U_d = 6.0, t_{pd} = 1.0 \), and the remaining parameters equal to zero. This choice gives, for instance, a reasonable fit of the experimental data for the magnetization. Clusters containing up to \( 12 \times 12 \) unit cells, have been considered. Both electron and hole dopings have been investigated. For a single hole the ground state is, in both cases, the magnetic polaron [19]. The results for \( Z \) at half-filling are shown in Figure 3. As in the case of the one-band Hamiltonian, \( Z \) decreases with \( L \) as in Eq. (8). The scaling of \( Z \) to zero is very similar for both types of doping.

Figure 3: UHF results for the wave-function renormalization constant \( Z \) vs the cluster size \((L \times L)\) for the two-band Hamiltonian at half-filling. Results for both hole and electron doping are shown.
BEYOND UHF

The magnetic polarons, although show the appealing features of all mean field solutions \[18, 19\], have many drawbacks. The two most outstanding are the non-uniform distribution of the excess charge [13-15], in contrast with the exact solutions [5-9], and an energy, significantly higher than the exact one \[15\]. In particular the former could be the origin of the behavior of $Z$ discussed above. The usual way followed in quantum chemical calculations to go beyond HF is the so-called Configurations Interaction (CI). In the case of the magnetic polarons a particular CI seems rather clear, namely, the one that allows the localised polarons to move through the whole cluster. We have explored this CI for a single hole, by writing its wavefunction as a linear combination of Slater determinants for the single polarons (SP) localised on all cluster sites. The exact Hamiltonian has been solved in this basis set. We call this solution a multipolaron (MP).

Thus, we write the wavefunction of a single hole ($N_s - 1$ electrons) as a linear combination of single polaron Slater determinants centered on all cluster sites

$$\Psi_{MP}(N_s - 1) = \sum_i a_i \Phi_i(N_s - 1)$$

where MP stands for multipolaron, and $\Phi_i(N_s - 1)$ is the wavefunction for the magnetic polaron centered on site $i$. The coefficients $a_i$ are obtained through diagonalization of the exact Hamiltonian.

The ground state wavefunction for a single hole includes all the SP wavefunctions with the same weight, and, therefore, gives an excess charge uniformly distributed throughout the whole cluster, as in the exact case. Note, however, that the $S_z$ component of the single polaron ($S_z = 1/2$) is preserved by the multipolaron approximation. The results for the energy necessary to create one hole (the difference between the energies of the system with one and zero holes) in the SP and MP approximations, are reported in Table I. As expected, the MP approximation lowers the energy of the single polaron. The most important changes are found for intermediate values of $U$. The correction rapidly decreases with $U$, and tends to zero for infinite $U$. On the other hand we note that the correction does only slightly depend on the size of the cluster. This can be easily understood by noting that the interaction between polarons rapidly decreases with the distance.

We note that although the MP solution restores the translational symmetry of the Hubbard hamiltonian, features associated with the initial, localized solutions, remain; in particular the behavior of $Z$ is not changed. This is so because, in our CI scheme, each of the solutions which enter in the final wavefunction contains a "continuum" of levels which is substantially modified by the addition of an extra electron. The orthogonality catastrophe which is responsible for the absence of coherent quasiparticles within the Hartree-Fock approximation is unchanged in the final wavefunction.

CONCLUDING REMARKS

We have presented the first investigation of the magnetic polarons...
Table 1: Energy (in units of $t$) required to create a hole in the single polaron (SP) and multipolaron (MP) approximations, for three cluster sizes ($L$) and several values of the intrasite Coulomb repulsion ($U$). Exact results are taken from Refs. [7,8]. The HF solution for the $4 \times 4$ cluster and $U = 4$ is not the single polaron (see text).

| $L \times L$ | exact $U=4$ | SP $U=4$ | MP $U=4$ | SP $U=6$ | MP $U=6$ | SP $U=8$ | MP $U=8$ | SP $U=10$ | MP $U=10$ | SP $U=12$ | MP $U=12$ |
|-------------|-------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 4           | -1.0434     | -0.7352  | -0.7270  | -0.7942  | -0.9219  | -0.9366  |
| 6           | -1.4148     | -0.8956  | -0.9033  | -1.2143  | -1.2413  | -1.2419  |
| 8           | -1.6784     | -1.0719  | -1.0793  | -1.3731  | -1.3940  | -1.3941  |
| 10          | -1.8640     | -1.2092  | -1.2190  | -1.4662  | -1.4868  | -1.4868  |
| 12          | -2.0015     | -1.3146  | -1.3267  | -1.5326  | -1.5527  | -1.5527  |
| 16          | -2.1954     | -1.4627  | -1.4767  | -1.6249  | -1.6432  | -1.6432  |
| 20          | -2.3281     | -1.5601  | -1.5741  | -1.6871  | -1.7034  | -1.7034  |

function renormalization constant for the one-band Hubbard Hamiltonian in the square lattice. Our results suggest that it may show non-conventional behavior in the thermodynamic limit, as discussed by previous authors [2-5]. The region of the parameter space ($U$ and filling) where $Z$ vanishes is narrow and close to half-filling. The way in which $Z$ scales with the size of the system makes this problem very difficult to investigate by means of exact calculations.

It is worth mentioning that our route towards the results which show highly unconventional behavior is itself very conventional. We apply the most standard technique in the study of many-body systems: the Hartree-Fock approximation. While the method, and the results, seem to be a contradiction of terms, we think that the opposite is true. Precisely because the method is so standard, it is biased in favor of normal (Fermi liquid) behavior. In fact, we recover such behavior in the low density limit, as we should. Also, the AF insulator at half filling is well described within our approximation. The main deviation of our results from conventional behavior is the proliferation of solutions which break translational symmetry, near half-filling. It is also in that region where we find $Z=0$. Restoring the translational symmetry by means of a CI scheme, while improving the results for the total energy, does not change the results for $Z$.

Some results for the two-band Hamiltonian, indicate that this model may also show non-conventional behavior, no matter the type of doping.

**ACKNOWLEDGEMENTS**

The financial support from the spanish CICYT (grant MAT91-0905-C02) is gratefully acknowledged. One of us (G. Chiappe) wishes to thank the "Ministerio de Educación y Ciencia" for a postdoctoral fellowship and the "Fundación Gil-Albert for a partial grant."
References

[1] J. G. Bednorz and K.A. Muller, Z. Phys. B 64, 88 (1986).
[2] P.W. Anderson, Science 235, 1196 (1987); ibid, Phys. Rev. Lett. 65, 2306 (1990); ibid, 64, 1839 (1990).
[3] N. Nagaosa and P.A. Lee, Phys. Rev. Lett. 64, 2450 (1990).
[4] L.B. Yoffe and P.B. Wiegmann, Phys. Rev. Lett. 65, 653 (1990).
[5] C.M. Varma, P.B. Littlewood, S. Schmitt-Rink, E. Abrahams and A.E. Ruckenstein, Phys. Rev. Lett. 63, 1996 (1989).
[6] F.D.M. Haldane, J. Phys. C 14, 2585 (1981).
[7] J.M. Luttinger, Phys. Rev. 121, 942 (1961).
[8] X.G. Wen, Phys. Rev. B 42, 6623 (1990).
[9]
[10] G. Fano, F. Ortolani and A. Parola, Phys. Rev. B 46, 1048 (1992).
[11] H.E. Castillo and C.A. Balseiro, Phys. Rev. Lett. 68, 121 (1992).
[12] E. Dagotto and J.R. Schrieffer, Phys. Rev. B 43, 8705 (1991).
[13] E.A. Jagla, K. Hallberg and C.A. Balseiro, Phys. Rev. B 47, 5849 (1993).
[14] S. Sorella, this volume.
[15] W. Metzner, this volume.
[16] G. Galán, G.Chiappe, E.Louis, F.Guinea y J.A.Vergés, Phys.Rev.B 46, 3163 (1992); E. Louis, G. Chiappe, J. Galán, F. Guinea and J.A. Vergés, Phys. Rev. B, 48, 426 (1993).
[17] J. Hubbard, Proc. Roy. Soc. (London) Ser. A 276, 238 (1963)
[18] A.R.Bishop, F.Guinea, P.S.Lomdahl, E.Louis y J.A.Vergés, Europhys. Lett. 14, 157 (1991); J.A.Vergés, E.Louis, P.S.Lomdahl, F.Guinea y A.R.Bishop, Phys.Rev.B 43, 6099 (1991).
[19] J.A. Vergés, F. Guinea and E. Louis, Phys. Rev. B 46, 3562 (1992).
[20] J.R. Engelbrecht and M. Randeria, Phys. Rev. Lett. 65, 1032 (1990); ibid, Phys. Rev. Lett. 66, 3225 (1991).
[21] P.W. Anderson, Phys. Rev. 164, 352 (1967).