Composite operator candidates for a study of the \( p-d \) model

A Avella\(^{1,2,3}\), F Mancini\(^1,3\), F P Mancini\(^1\) and E Plekhanov\(^{1,2,3}\)

\(^1\) Dipartimento di Fisica “E.R. Caianiello”, Università degli Studi di Salerno, 84084 Fisciano (SA), Italy
\(^2\) CNR-SPIN, UoS di Salerno, 84084 Fisciano (SA), Italy
\(^3\) Unità CNISM di Salerno, Università degli Studi di Salerno, 84084 Fisciano (SA), Italy

E-mail: avella@physics.unisa.it

Abstract. We study the two-dimensional \( p-d \) model by means of a four-pole approximation within the Composite Operator Method framework. Many results of numerical simulations have been correctly reproduced by considering as basic composite field a four-component spinor field, including the \( p \) field, the two Hubbard operators for the \( d \) field, and a composite operator describing the \( p \) field dressed by the spin excitations of the \( d \) field. In this manuscript, we propose an alternative choice for the latter field, which takes into account charge and pair fluctuations too. The results of this study show that near half-filling one can safely neglect the contribution of charge and pair fluctuations and safely use the previously proposed field.

1. Introduction

It is believed that real oxide cuprate materials can be adequately described by the two-dimensional \( p-d \) model \([1]\). The model describes CuO\(_2\) layers, characterized by a strong intra-atomic Coulomb repulsion at Cu-sites and by a very highly correlation between the 3\( d \) electrons of Cu in the atomic orbital 3\( d_{x^2-y^2} \) and the \( 2p \) electrons of O in the atomic orbitals 2\( p_x \) and 2\( p_y \). Neglecting the Coulomb repulsion at O-sites and among the \( p- \) and \( d- \)electrons, as well as the O-O and Cu-Cu hopping terms, one can use a Bogoliubov transformation, to count out the antibonding degree of freedom of the \( p- \)electrons \([2]\). As a result, the Hamiltonian reads as

\[
H = \sum_i \left[ (\varepsilon_d - \mu) d^\dagger(i) d(i) + (\varepsilon_p - \mu) p^\dagger(i) p(i) + Un^d_\uparrow(i) n^d_\downarrow(i) \right] + 2t_{pd} \sum_i \left[ p^\dagger(i) d(i) + d^\dagger(i) p(i) \right].
\] (1)

We use the Heisenberg representation, \( i = (i, t) \) with \( i = R_i \) a Bravais vector in the CuO\(_2\) plane pointing at a Cu site. \( p(i) (p^\dagger(i)) \) and \( d(i) (d^\dagger(i)) \) are annihilation (creation) operators of \( p- \) and \( d- \)electrons in the spinor notation and satisfy canonical anticommutation relations. \( \mu \) is the chemical potential; \( \varepsilon_d \) and \( \varepsilon_p \) are the energy levels; \( n^d_\sigma(i) = d^\dagger_\sigma(i) d_\sigma(i) \) is the charge density operator of \( d- \)electrons with spin \( \sigma \). \( U \) describes the Coulomb repulsion at Cu sites. The short range hopping integral \( t_{pd} \) describes the hybridization between \( d \) and bonding \( p \) orbitals. For a
generic operator $\Phi(i)$ we define:

$$\Phi^{\gamma}(i) = \sum_j \gamma_{ij} \Phi(j),$$

(2)

where

$$\gamma_{ij} = \frac{a^2}{(2\pi)^2} \int_{\Omega_B} d^2 k e^{i k \cdot (\mathbf{R}_i - \mathbf{R}_j)} \gamma(k),$$

(3)

and

$$\gamma(k) = \sqrt{1 - \alpha(k)}, \quad \alpha(k) = \frac{1}{2} \left[ \cos(k_x a) + \cos(k_y a) \right].$$

(4)

In the above equations, $a$ is the lattice constant and $\Omega_B$ the volume of the unit cell in the reciprocal space. $\alpha$ corresponds to first neighbor projector, whereas $\gamma$ has a more complex structure as a result of the bonding - anti-bonding transformation.

As it has been illustrated in Refs. [3, 4], the study of highly interacting systems can be conveniently tackled by considering higher-order fields instead of the bare electronic operators $\{p, d\}$. These new operators, called composite operators, come out from the dynamics and include higher-order interactions among the original electronic fields. In the framework of the composite operator method [3, 4], one has first to identify the relevant composite fields. On the base of experimental and numerical results, we believe that one should use a four-component spinor field in order to capture sufficient physics to describe real oxide cuprate materials. The large covalence between oxygen and copper electrons leads to a large fluctuation of the energy of $p$-electrons at O sites, pointing out at the operator $p(i)$ - the bonding component for the $p_{\sigma}$ electrons on oxygen site - as the first field. The splitting of the $d$-band into the lower and the upper Hubbard sub-bands - due to the strong intra-atomic Coulomb interaction at Cu sites - naturally leads to the choice of the Hubbard projection operators $\xi(i) = [1 - n^d(i)]d(i)$ and $\eta(i) = n^d(i)d(i)$.

While the choice of the first three fields is quite intuitive, it has proved a difficult task the right choice of the last field. Indeed, one would like to take into account quantum fluctuations associated with the Cu-O bonds. By taking higher-order time derivatives of the Hubbard fields, one may generate a hierarchy of composite operators. In particular the field $\pi$, defined as

$$\pi(i) = \frac{1}{2} \sigma^\mu n^d_k(i)p^\gamma(i) + \xi(i)p^{\gamma^\dagger}\eta(i),$$

(5)

appears as a good candidate, since it describes p-electronic excitations accompanied by the nearest neighbor d-electron spin, charge and pair fluctuations. However, in a series of papers [5, 9, 10], we chose the fourth field as

$$p_s(i) = \sigma_k n^d_k(i)p^\gamma(i).$$

(6)

This field describes p-electronic excitations accompanied by the nearest neighbor d-electron spin fluctuations only. In the above equation, $\sigma_k$ are the Pauli matrices, $n_d$ is the particle number per site of d electrons, and $n^d_k(i) = d^\dagger(i)\sigma_k d(i)$ is the spin density operator of d-electrons. The reason for this choice is based on the experimental evidence that spin fluctuations are predominant over all other fluctuations in the region of physical interest (i.e., near half filling).

Thus, by considering as basic composite field the four-component spinor field:

$$\psi(i) = \begin{pmatrix} p(i) \\ \xi(i) \\ \eta(i) \\ p_s(i) \end{pmatrix}$$

(7)
Figure 1. The double occupancy $D$ as a function of $n_T$, for $U = 6$, $\Delta = 4$, and $T = 0.1$. The solid line is obtained by considering the field $\psi(i)$ as defined in eq. (7). The dotted line obtained by taking $\pi(i)$ instead of $p_s$.

the Hamiltonian (1) can be solved in the pole approximation [3, 4]. In this approximation, the field (7) is indeed an eigenoperator of the Hamiltonian (1) with eigenenergy $\varepsilon(k)$. As a consequence, a solution of the Hamiltonian can be obtained.

Within this framework, the retarded Green’s function and the pertinent correlation functions turn out to be functions of a finite set of parameters, in terms of which one finds a solution of the model. The unknown parameters, which depend on the choice of the basis, can be determined by means of the Pauli principle and/or a decoupling procedure [3, 4]. We refer the interested reader to Ref. [5] for computational details. As it is shown in Ref. [5], this choice of the composite field $\psi(i)$ correctly reproduces many results of numerical simulations [6, 7, 8] and also qualitatively reproduces the band structure exhibited by the undoped single-layer La$_2$CuO$_4$ [9].

2. The field $\pi$: results and discussion
In this short manuscript, we would like to take a step back and estimate the error done by neglecting the charge and pair fluctuations in the choice of the fourth field. In particular, as fourth field we consider the field $\pi(i)$, as defined in Eq. (5). We recall that $\pi(i)$ is the higher-order non-local field generated by the dynamics of the Hubbard operators $\xi(i)$ and $\eta(i)$. We shall focus our attention on the comparison between the results obtained by the two different choices of the fourth basic field. The differences between the two solutions greatly depend on the value of the total filling $n_T$. In particular, we will show that near half filling ($n_T = 3$) the spin fluctuations prevail over the charge and pair fluctuations, reducing, thus, the difference between the two solutions. In the following, we take $t_{pd} = 1$ as the unit of energy.

In order to test the adequacy of our original choice of the field $p_s$, we shall consider the double occupancy per site of d electrons $D$ and the chemical potential $\mu$. In Fig. 1, we report, as a function of the total number of electrons $n_T$, the double occupancy for $\Delta = 4$, $U = 6$, $T = 0.1$. As one can clearly see, the agreement between the two solution is good in the underdoped region, drifting apart in the overdoped region.

In Fig. 2, we show the dependence of $n_T$ on the chemical potential for $U = 6$, $\Delta = 4$, and $T = 0.1$. The best agreement between COM predictions and QMC results [6], is clearly given by considering the field $p_s$. The comparison between the two choices leads to the conclusion
that considering also the charge and pair fluctuations in the definition of the fourth field does not dramatically improve the results obtained by considering only the field \( p_s \), at least near half filling and in the underdoped region.

3. Conclusions
In summary, by means of a four-pole approximation, within the Composite Operator Method, we have studied the \( p-d \) model and, in particular, we focused our attention on the comparison between alternative choices of the basic composite field. We came to the conclusion that taking into account a wider set of fluctuations in an overall approximate framework does not naturally leads to more accurate results.

Acknowledgements
We acknowledge the CINECA award under the ISCRA initiative (project MP34dTMO), for the availability of high performance computing resources and support. A. A. thanks the Max-Planck-Institut FKF Stuttgart for hospitality and financial support.

References
[1] Emery V and Reiter G 1988 Phys. Rev. B 38 4547.
[2] Matsumoto H and Tachiki M 1990 Suppl. Prog. Theor. Phys. 101 353.
[3] Mancini F and Avella A 2004 Adv. Phys. 53 537.
[4] Avella A and Mancini F 2011 Strongly Correlated Systems: Theoretical Methods (Springer Series in Solid-State Sciences) vol 171 (Berlin Heidelberg: Springer-Verlag) chap The Composite Operator Method (COM) p 103.
[5] Fiorentino V, Mancini F, Žaškinas E and Barabanov A F 2001 Phys. Rev. B 64 214515.
[6] Dopf G, Muramatsu A and Hanke W 1990 Phys. Rev. B 41 9264.
[7] Scalettar R T, Scalapino D J, Sugar R L and White S R 1991 Phys. Rev. B 44 770.
[8] Dopf G et al. 1992 Phys. Rev. Lett. 68 2082.
[9] Avella A, Mancini F, Mancini F P and Plekhanov E 2011 J. Phys. Chem. Sol. 72 384.
[10] Avella A, Mancini F, Mancini F P and Plekhanov E 2011 J. Phys.: Conf. Series 273 012091.