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Spontaneous symmetry breaking approach to La_2CuO_4 properties: Hints for matching the Mott and Slater pictures

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ABSTRACT

Special solutions of the Hartree–Fock (HF) problem for Coulomb interacting electrons described by a simple model of the Cu–O planes in La_2CuO_4 are presented. One of the mean field states obtained, is able to predict some of the most interesting properties of this material, such as its insulator character and the antiferromagnetic order. The natural appearance of pseudogaps in some states of this material is also indicated by another of the HF states obtained. These surprising results follow after eliminating spin and crystal symmetry restrictions usually imposed on the single particle HF orbitals, by employing the rotational invariant formulation of the HF scheme originally introduced by Dirac. Therefore, it is exemplified here, how up to know considered strong correlation effects, can be described by improving the HF solution of the considered system. In other words, it has been argued, that defining correlation effects as the ones shown by the system and not predicted by the HF best (lowest energy) solution, allows to explain important, up to know considered as strong correlation properties, as simple mean field ones. The discussion also helps to clarify the role of the antiferromagnetism and pseudogaps in the physical properties of the HTSC materials and indicates a promising way to start conciliating the Mott and Slater pictures in the physics of the transition metal oxides and other strongly correlated electron systems.

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The Hubbard-type models in the theory of strongly correlated electron systems are notably successful [1–10]. They remarkably reproduce the properties of Mott insulators, such as transition metals oxides and copper-oxygen layered HTc compounds [7]. However, the search for approaches having more basic foundations does not cease, hoping that they could open the way for obtaining more exact and specific results [11]. The so-called *first principle or Slater* procedures, are electronic structure calculations that begin by considering the interactions among electrons or atoms in vacuum. The study of the band structure they predict, in principle should offer a way for the precise determination of the physical properties of each material [11–13]. However, the above mentioned potentialities fail in describing many systems showing strong correlation effects [7].

The motivation of the present Letter emerged from a suspicion that the Hartree–Fock (HF) method, could had been underestimated in its possibilities for helping in clarifying the above mentioned difficulties [2,14]. As a net result of this work, we came to believe that a large deal of correlation effects, can be described in the framework of the HF scheme, after removing certain symmetry restrictions which obstacle the finding of the best HF solutions. By example, it has been early shown by Slater in Ref. [2], that sometimes the HF potential breaks the symmetry of the original crystalline lattice, creating magnetic structures and gaps. This symmetry breaking effect has been also more recently underlined and deepened in Ref. [15]. However, the removal of the lattice symmetry restrictions alone had not been able to describe the insulator properties of a large class of materials [1,7,11]. One of the central results of the present investigation, is the identification of another kind of symmetry restriction that seemingly had been overlooked for a long time. It corresponds to the usual assumption about the necessary α $(S_z = 1/2)$ or β $(S_z = -1/2)$ orientations of the

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spin of each solution for the HF orbitals [12,16]. For supporting this main statement, this work considered the HF problem as applied to a simple one band model of the superconducting material La_2CuO_4 [17], looking from the start for single particle orbitals being non-separable in their spacial and spinor dependences. That is, they will have the structure $\phi(x,s) \neq \phi(x)\psi(s)$, i.e. the orbitals have not an absolute common quantization direction for their electron spin. Note, that to proceed in this way means not other thing that to apply the Dirac's formulation of the HF procedure [14]. The results, as it will be seen, are able to describe the basic properties of the La_2CuO_4 [17]. We would like to stress that the obtained results do not look so radical if we consider the following circumstance: the correlation effects are associated with the difference shown by the system's properties with the ones predicted by the HF procedure applied to it. Therefore, what we have argued here, is simply that the there exist unexplored improvements of the mean field schemes which allow to predict properties which are currently considered as strong correlation ones. These modifications of the HF method are related with usual constraints which are imposed on the crystalline and spin properties of the single particle orbitals. The possibility of their employment for solving the long-standing debate between the Slater and Mott pictures in the theory of transition metal oxides and HTc superconducting materials will be considered elsewhere. In this Letter, we will firstly describe the physical basis of the model employed and after that, the results obtained for the various HF solutions will be presented. For the details of the concrete solutions we refer to the extended version of this Letter in Ref. [18].

Let $\hat{\mathcal{H}}(x_1,\ldots,x_N) = \sum_i \hat{\mathcal{H}}_0(x_i) + \frac{1}{2}\sum_{j\neq i} V(x_i,x_j)$, be the N-electrons system Hamiltonian, including kinetic plus interaction with the environment Hamiltonian $\hat{\mathcal{H}}_0$, besides Coulomb interaction among pairs of electrons V. The HF equations of motion were solved by allowing for non-separable solutions for the orbitals $\phi_\eta(x,s)$, where $\eta = k_1,\ldots,k_N$ are the labels of the HF basis they form. The system of HF equations is rotational invariant when formulated in the general HF procedure firstly introduced by Dirac in Ref. [14]. Its explicit expression for the here considered problem can be found in Ref. [14,18].

Let us first present the effective band model used to describe the dynamic of the less bounded electrons in La_2CuO_4. It is known that at low temperature La_2CuO_4 is an antiferromagnetic-insulator [17]. However, in evident contradiction with the experiments the Linear Augmented Plane Waves (LAPW) band calculations predicts for it metal and paramagnetic zero temperature properties [12]. Nevertheless, such band studies results at least show that the conduction electrons are strongly coupled to the Bravais lattice centers of the copper oxygen planes. Clearly this tight-binding behavior is determined by the interaction of the electrons with its surrounding effective environment. The less bounded electron in the La_2CuO_4 molecule is the Cu^{2+}'s not paired one. At difference from O^{2-} ions, Cu ones do not have their last shell (3d) closed. Those copper 3d electrons partially fill the last band of La_2CuO_4 solid and in what follows they shall be referred as: the electron gas. It seems appropriate to consider those electrons as strongly linked to CuO_2 cells and with special preference for the Cu centers [5]. Thus, our Bravais lattice is going to be the squared net coincident with the array of copper sites (see Fig. 1). Further, the presence of electrons pertaining to the various fully filled bands in the material plus the nuclear charges, will play a double role in the model. Firstly, they will act as an effective polarizable environment screening the field of the charges in the electron gas. It will be reflected by a dielectric constant ϵ reducing the Coulomb interaction. Secondly, the mean field created by the environment will act as a periodic potential W_γ, tight-binding the electrons to the Cu centers. The interaction F_b among the electron gas and a "jellium" neutralizing its charges is also considered. It was modeled as a Gaussian distribution of positive charges $\rho_b(\mathbf{y}) = \frac{1}{\pi b^2}\exp(-\frac{\mathbf{y}^2}{b^2})$, surrounding each lattice point and having a characteristic radius b. Summarizing, the free Hamiltonian of the model takes the form

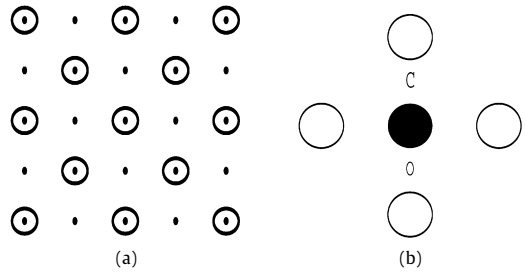

Fig. 1. The figures show: (a) The point lattice associated to the Cu–O planes. For removing the symmetry restrictions, it was helpful to separate the lattice in the two represented sublattices; and (b) shows the corresponding base of the Cu–O planes.

$$\hat{\mathcal{H}}_0(\mathbf{x}) = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m} + W_\gamma(\mathbf{x}) + F_b(\mathbf{x}),$$
$$W_\gamma(\mathbf{x}) = W_\gamma(\mathbf{x}+\mathbf{R}),$$
$$F_b(\mathbf{x}) = \frac{e^2}{4\pi\epsilon\epsilon_0}\sum_{\mathbf{R}}\int d^2y \frac{\rho_b(\mathbf{y}-\mathbf{R})}{|\mathbf{x}-\mathbf{y}|}, \quad b \ll p, \tag{1}$$

where $\hat{\mathbf{p}}_i^2$ is the ith electron's squared momentum operator; m is the electron mass; ϵ_0 is the vacuum permitivity and lattice vectors $\mathbf{R} = n_{x_1} p\hat{\mathbf{e}}_{x_1} + n_{x_2} p\hat{\mathbf{e}}_{x_2}$ with n_{x_1} and n_{x_2} being integers, move on Bravais lattice. This last will be referred hereafter as the *the absolute* lattice. The versors $\hat{\mathbf{e}}_{x_1}$ and $\hat{\mathbf{e}}_{x_2}$ are resting on the direction defined by the lattice's nearest neighbors (see Fig. 1(a)). The distance between Cu nearest neighbors is $p \approx 3.8$ Å [17]. The interaction among pairs of electrons is taken in the form $V(\mathbf{x},\mathbf{y}) = \frac{e^2}{4\pi\epsilon\epsilon_0}\frac{1}{|\mathbf{x}-\mathbf{y}|}$, which includes the dielectric constant associated to the presence of the effective environment.

As already mentioned, we are seeking here for HF solutions with orbitals having a non-separable spin and orbit structures. Thus, it was considered that the spin can show a different projection for the different Wannier orbitals to be superposed for defining those orbitals. The spin for each of them will be either or α or β type, according they are linked either to one or the other of the two sublattices shown in Fig. 1(a). The points of these sublattices were defined as follows: $\mathbf{R}^{(r)} = \sqrt{2}n_1 p\hat{\mathbf{q}}_1 + \sqrt{2}n_2 p\hat{\mathbf{q}}_2 + \mathbf{q}^{(r)}$, $r = 1,2$; with n_1 and $n_2 \in \mathbb{Z}$, and in which the vector $\mathbf{q}^{(r)} = 0$ if $r = 1$ and $\mathbf{q}^{(r)} = p\hat{\mathbf{e}}_{x_1}$ when $r = 2$; and where $\hat{\mathbf{q}}_1$ and $\hat{\mathbf{q}}_2$ form the basis versors on each one of them. The searched solutions were constructed as eigenfunctions of the operators $\hat{T}_{\mathbf{R}^{(r)}}$ belonging to the translation group transforming each sublattice on itself: $\hat{T}_{\mathbf{R}^{(r)}}\phi_{\mathbf{k},l} = \exp(i\mathbf{k}\cdot\mathbf{R}^{(r)})\phi_{\mathbf{k},l}$. Therefore we imposed periodic boundary conditions on the $\phi_{\mathbf{k},l}$ in the absolute lattice's boundaries $x_1 = -pL$ and pL, L, $x_2 = -pL$ and pL (see Fig. 1(a)). This condition determines the allowed set of quasimomenta $\mathbf{k} = \frac{2\pi}{Lp}(n_1\hat{\mathbf{e}}_{x_1} + n_2\hat{\mathbf{e}}_{x_2})$, with $n_1, n_2 \in \mathbb{Z}$ and $-\frac{L}{2} \leqslant n_1 \pm n_2 < \frac{L}{2}$. Note that we are demanding less than the full crystal symmetry on the single particle states which we are looking for. Let the single particle states represented in the explicitly non-separable form

$$\phi_{\mathbf{k},l}(\mathbf{x},s) = \sum_{r,\sigma_z} B^{\mathbf{k},l}_{r,\sigma_z}\varphi^{(r,\sigma_z)}_{\mathbf{k}}(\mathbf{x},s),$$

where l is the additional label needed for indexing the stationary states. The tight binding Bloch basis $\varphi^{(r,\sigma_z)}_{\mathbf{k}}$ appearing is defined as

$$\varphi^{(r,\sigma_z)}_{\mathbf{k}}(\mathbf{x},s) = \sqrt{\frac{2}{N}}u^{\sigma_z}(s)\sum_{\mathbf{R}^{(r)}}\exp\big(i\mathbf{k}\cdot\mathbf{R}^{(r)}\big)\varphi_{\mathbf{R}^{(r)}}(\mathbf{x}),$$
$$\hat{\sigma}_z u^{\sigma_z} = \sigma_z u^{\sigma_z},$$

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