How HF solutions for the TB interacting electrons in 2D predict SCES properties and suggest phenomenology for attaining RTS

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Former results for a Tight-Binding (TB) model of CuO planes in $La_2CuO_4$ are reinterpreted here to underline their wider implications. It is noted that physical systems being appropriately described by the TB model can exhibit the main strongly correlated electron system (SCES) properties, when they are solved in the HF approximation, by also allowing crystal symmetry breaking effects and non-collinear spin orientations of the HF orbitals. It is argued how a simple 2D square lattice system of Coulomb interacting electrons can exhibit insulator gaps and pseudogap states, and quantum phase transitions as illustrated by the mentioned former works. A discussion is also presented here indicating the possibility of attaining room temperature superconductivity, by means of a surface coating with water molecules of cleaved planes of graphite, being orthogonal to its c-axis. The possibility that 2D arrays of quantum dots can give rise to the same effect is also proposed to be considered. The analysis also furnishes theoretical insight to solve the Mott-Slater debate, at least for the $La_2CuO_4$ and TMO band structures. The idea is to apply a properly non-collinear GW scheme to the electronic structure calculation of these materials. The fact is that the GW approach can be viewed as a HF procedure in which the screening polarization is also determined. This directly indicates the possibility of predicting the assumed dielectric constant in the previous works. Thus, the results seem to identify that the main correlation properties in these materials are determined by screening. Finally, the conclusions also seem to be of help for the description of the experimental observations of metal-insulator transitions and Mott properties in atoms trapped in planar photonic lattices.

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I. INTRODUCTION

Band structure calculation is a central part of modern Solid State theory. The area has a long history in the literature along the continuous quest about the structure of matter [1-30]. A central open problem in this field is the connection between the so called first principles (or $ab – initio$) schemes with the Mott phenomenological methods [2, 3, 4, 13, 39]. Materials which had taken part in the center of the debate between the two conceptions were the transition metal oxides (TMO) and the HTSC materials [2, 14]. One particular substance in this set is the early superconducting material $La_2CuO_4$. Its first band structure calculations predicted a metal and paramagnetic characters, which were drastically different from its experimentally known insulating and antiferromagnetic nature [29]. These two qualities are strong correlation properties which can’t be derived from an $ab – initio$ HF independent particle description [10, 14, 34]. Seemingly paradoxical, in Refs. [38-40], a single band Hartree-Fock (HF) study was able to produce these strong correlation properties of $La_2CuO_4$, as independent particle ones, arising from a combination of crystal symmetry breaking with an entangled spin-spatial structure of the single particle states. However, the conclusion is not strange, after taking into account that the procedure employed was not an $ab – initio$ method. That is: the mean field approach was applied to a model in which the Coulomb interaction was screened by means of a phenomenological dielectric constant in order to match the band width of the spin polarized solution with the one associated to the single band crossing the Fermi energy in the Matheiss band structure evaluations for $La_2CuO_4$. Therefore the use of the HF scheme in these works has the same degree of applicability as the similar use of the mean field method for the evaluation of the AF order and the quasiparticles in the Hubbard models, which are considered to embody the SCES properties of the Mott substances, such as the $La_2CuO_4$ system. The direct inclusion of correlation effects in the considered model is clearly represented by the phenomenological way of including screening effects, which clearly add correlation to the model. An important difference with the Hubbard models is however, the fact that by not adopting the Hubbard strong approximations, the scheme was afterwards able to predict the existence of the pseudogap state ([38-40]), the nature of which is today still strongly debated [44]. We consider that a special merit of the present approach is that it identifies the relevant role of a particular form of correlations: namely...
screening, in determining the emergence of the insulating and AF character of the TMO and HTSC materials. The discussion in Ref. [38–40] considered a single band model of $La_2CuO_4$. Then, the derivation of the same results from an \textit{ab initio} band structure calculation could represent an appreciable contribution to clarify the links between the Mott and the \textit{ab initio} descriptions. This problem will be considered further elsewhere.

The present work is devoted to evidence general implications of the system investigated in Ref. [38–40]: the Tight-Binding model of 2D interacting electrons. The wide range of applicability of this model in 2D systems suggests that the appearance of SCES properties already in the HF approximation, in the context of the model as controlled by the overlapping and other parameters, can be of help in the search for physical systems of interest in nanotechnology. Then, after shortly reviewing Dirac’s fully unconstrained formulation of the HF problem, the mean field equations for the square 2D lattice model employed in [38–40] are written by allowing more freedom in the values of the parameters. Another main element is to allow a weaker translation symmetry. That is, the imposition of Bloch conditions on the HF self-energy terms, but in smaller sublattices being fractions of the total. We present the solutions obtained for the band structures of the TB model at half filling when the overlapping constant is varied by changing the width of the employed TB Gaussian orbitals. At small overlapping values the system developed an insulator gap which afterwards tends to close when the overlapping increases. This suggests the presence of an insulator to metal transition at even larger overlapping which however, lies outside the scope of the TB approximation. Apart from the parameter controlling overlapping, the others were chosen at the same values as in the model discussed in Ref. [38–40]. It can be noted that in addition with the connection with HTSC cuprates, from which the present analysis emerged, the received conclusions seem to furnish a clear understanding for the experimental observations of metal-insulator transitions and Mott properties in systems of atoms trapped in planar photon lattices [47,49].

The second issue examined consists in the application of the ideas in the model to develop an explanation of recent experimental results indicating the existence of granular room temperature superconductivity (RTS) as induced by chemisorption of water molecules on graphite powder [43]. These experiments detect the hysteresis loops shown by suspensions of the powder, which indicate the presence of magnetic properties in the grains. Due the presence of Oxygen in the water, one possibility could be to imagine the role of the presence of $O_2$ molecules in the system, due to the known ferromagnetic moment in this compound (See Ref. [57]). However, it is also possible that the powder becomes superconducting after doped with water [43]. We will explore here this last possibility, as motivated by observing some features with seem to link the system with the TB model of interacting electrons.

Recent \textit{ab initio} evaluations of the deposition of water on graphene had been performed in Refs. [43,46]. The authors of that work remark that the deposition of a single layer of water on the graphene leads to a 2D planar hexagonal crystal of water molecules sitting nearly $3.4 \text{ Å}$ above the graphene. The centers of the Oxygen atoms stay directly over the centers of the hexagons formed by the carbon atoms. They explain that the periodic potential created by the water molecules on graphene does not cause it to become metallic. However, they also argue that if a substrate of SiO$_2$ is added below the graphene, then the system might become conducting. This is a point that we consider as affording an opportunity for a TB model to be of relevance in describing the system. The idea is that graphite with a monolayer of water over the last graphene layer in it, can be considered as a graphene layer with a substrate of the same graphite. But as the simulations indicated, a substrate can help the last layer to become metallic. This view is also supported by the fact that the same graphite is a semi-metal. Therefore, assuming that the same predictions of SCES can be obtained from a TB model of 2D electrons with a lattice showing hexagonal structure, the last hexagonal graphene layer on the surface of the graphite (which is separated by a large distance from the other layers) could be eventually seen as TB metal upon which the deposited 2D crystal of water molecules exerts a strong dipolar periodic potential. As a consequence, it could be expected that this field may lead to create a TB binding band eventually producing an insulator and its corresponding pseudogap state along the lines discussed here. The elements of the discussion of the water doped graphite system also suggested the possibility that 2D arrays of quantum dots can give rise to the same effect, if no strong experimental limitations exist on the optimization of the ratio between the squared hopping parameter for the lattice of QDots and the width of the TB band determined by the potential generated by them.

The presentation proceeds as follows. The section 2 reviews the fully unrestricted HF procedure. Further, Section 3 presents the results of the insulator band structure with varying overlapping in the square two-dimensional TB model with interacting electrons. Next, section 4 discusses the possibility of obtaining room temperature superconductivity in water doped graphite surfaces and 2D lattice arrays of quantum dots. Finally, the results are summarized.

\section{II. THE FULLY UNRESTRICTED DIRAC'S HF SCHEME}

Let us briefly review here the fully unrestricted HF procedure employed in the following discussion. The state of a system of $N$ particles is described by the wavefunction depending on the particles spinor and spatial coordinates $f_n(x_1; s_1, ..., x_N; s_N)$, where $n$ represents the set of quantum numbers indexing the state $|28\rangle$. The HF approximation
is defined by assuming the above mentioned state as expressed by a linear combination of antisymmetric products of N orthonormalized orbitals \( \phi_k(x_i,s_i) \), with \( i = 1, \ldots, N \). Each one of the orbitals defines a single particle state. As usual, in what follows the word coordinate will mean the spatial as well as the spinor ones \([2, 27, 28]\).

Let

\[
\hat{h}(x_1, \ldots, x_N) = \sum_i \hat{h}_0(x_i) + \frac{1}{2} \sum_{j \neq i} V(x_i, x_j),
\]

be the 2D electron system Hamiltonian, including the kinetic term, plus the interaction with the environment Hamiltonian \( \hat{h}_0 \) and the Coulomb interaction potential \( V \) among pairs of electrons. The HF equations of motion for the system follow after imposing the extremum condition on the mean energy functional, in the form

\[
\begin{align*}
\left[ \hat{h}_0(x) + \sum_{\eta_1} \sum_{s} \int d^2x' \phi^*_{\eta_1}(x', s') V(x, x') \phi_{\eta_1}(x', s') \right] \phi_\eta(x, s) \\
- \sum_{\eta_1} \int d^2x' \phi^*_{\eta_1}(x', s') V(x, x') \phi_{\eta_1}(x', s') \phi_\eta(x, s) = \varepsilon_\eta \phi_\eta(x, s),
\end{align*}
\]

where \( \eta = k_1, \ldots, k_N \) is the label in the basis of solutions. As usual the self-consistent Hamiltonian has two components: the direct and the exchange potentials \([31]\). The HF energy of the \( N \) electron system and the interaction energy of an electron in the \( \eta \) state with the remaining ones, are given by the expressions

\[
E_{HF} = \sum_\eta \langle \eta | \hat{h}_0 | \eta \rangle + \frac{1}{2} \sum_{\eta, \eta_1} \langle \eta, \eta_1 | V | \eta, \eta_1 \rangle - \frac{1}{2} \sum_{\eta, \eta_1} \langle \eta, \eta_1 | V | \eta, \eta_1 \rangle,
\]

\[
a_\eta = \frac{1}{2} \sum_{\eta_1} \langle \eta, \eta_1 | V | \eta, \eta_1 \rangle - \frac{1}{2} \sum_{\eta} \langle \eta, \eta_1 | V | \eta, \eta_1 \rangle.
\]

The bracket terms in \( [3] \) represent the following integrals:

\[
\begin{align*}
\langle m | \hat{h}_0 | p \rangle &\equiv \sum_s \int d^2x \ \phi^*_{m}(x, s) \ \hat{h}_0(x) \ \phi_{p}(x, s), \\
\langle m, n | V | o, p \rangle &\equiv \sum_{s, s'} \int d^2x d^2x' \ \phi^*_m(x, s) \phi_{n}(x', s') \ V(x, x') \ \phi_o(x', s') \ \phi_{p}(x, s),
\end{align*}
\]

where \( m, n, o \) and \( p \) denote any one of the possible quantum number indices.

It can be noted that the system of equations \([2] \) shows no constraint whatsoever on the spin and orbital structure of the single particle HF states, because it is written without imposing a spatially absolute direction for the spin quantization of the single electron orbitals. This fully unrestricted invariant formulation of the self-consistent HF procedure was first introduced by Dirac in Ref. \([31]\).

In general, finding the solution of \([2] \) is a complicated task. The iterative method is one of the most frequently employed for solving this kind of system and it is usually complemented by the imposition of symmetry restrictions that reduce the space of states to be sampled. However, such constraints can avoid obtaining special solutions not satisfying the fixed conditions. Although in some cases the constraints can be satisfied by the minimal energy state, the procedure can hide the existence of interesting excited states and inclusive could wrongly predict the excitation features in some cases, as had been seen in Ref. \([38, 40]\). A very common example of such restrictions, which are usually employed in band theory and quantum chemistry calculations, is to consider that single particle solutions of \([2] \) have the spin quantized in a fixed direction at every point of the space \([27, 28]\). That means, they satisfy

\[
\phi_k(x, s) = \begin{cases} 
\phi^{\alpha}_k(x) \ u_\uparrow(s) & \alpha \ \text{state}, \\
\phi^{\beta}_k(x) \ u_\downarrow(s) & \beta \ \text{state},
\end{cases}
\]

where \( u_\uparrow, u_\downarrow \) represent the Pauli spinors with spin up and down in a certain globally fixed direction, respectively. If the spacial functions \( \phi^{\alpha}_k \) and \( \phi^{\beta}_k \) are the same, the HF calculation is called a ”restricted” one, and if they are different, the procedure is called ”unrestricted” \([27]\). It was thus of interest to examine the consequence of considering the possible existence of non-separable single particle states being solutions of the HF problem in the context of a system showing antiferromagnetism. This was the main motivation in starting the investigation leading to the works in Refs. \([38, 40]\). Afterwards, the insulator gap appeared as a surprise.
Another important type of constraints posed on ab initio band theory evaluations is the a priori impositions of crystal symmetries. To beforehand impose a symmetry on the assumed to be searched solution, although it could be suggested in the studied system, has the risk of hiding a possible spontaneous breaking of that invariance. This could occur due to the reduction of the space of orbitals in which the search is done. In that case it can turn out that the obtained solutions will not be an absolute extremal of the energy functional, but a conditional one due to the fixed symmetry constraint.

III. THE 2D SQUARE TB MODEL

The free hamiltonian of the model is considered in the form

$$\hat{h}_0(x) = \frac{\hat{p}^2}{2m} + W_\gamma(x) + F_b(x),$$

(5)

$$W_\gamma(x) = W_\gamma(x + R),$$

$$F_b(x) = \frac{e^2}{4\pi\varepsilon\varepsilon_0} \sum_R \int d^2y \frac{\rho_b(y - R)}{|x - y|}, \ b \ll p,$$

where $\hat{p}^2$ is the particle’s squared momentum operator; $m$ is the particle mass; $\varepsilon_0$ is the vacuum permittivity and the square lattice to which the free electrons bind is defined by

$$R = \begin{cases} n_x p \hat{e}_{x_1} + n_x p \hat{e}_{x_2}, \\ \text{with } n_x \in \mathbb{Z}, \end{cases}$$

with

$$Q = \begin{cases} 0, & \text{if } r=1, \\ p \hat{e}_{x_1}, & \text{if } r=2, \end{cases}$$

in which $\hat{e}_{x_1}$ and $\hat{e}_{x_2}$ point along the directions defined by the lattice’s nearest neighbors, see figure II. The lattice parameter $p$ is supposed now to be free, at variance with the case in Refs. [38–40], where it was fixed to the known distance between Cu nearest neighbors in CuO planes of La$_2$CuO$_4$: $p \approx 3.8 \ \text{Å}$.

The term $F_b$ represents the interaction between the particles and the ”jellium” neutralizing charges. The jellium is modeled as a gaussian distribution of positive charges

$$\rho_b(y) = \frac{1}{\pi b^2} \exp\left(-\frac{y^2}{b^2}\right),$$

sitting at each point of the square lattice and $b$ defines the degree of spreading around each of the lattice points. We also include the Coulomb interaction among pairs of particles in the form

$$V(x, y) = \frac{e^2}{4\pi\varepsilon\varepsilon_0} \frac{1}{|x - y|},$$

(6)

which, as remarked above, takes into account a dielectric constant $\varepsilon$ that is considered as generated by the effective environment.

The full square lattice will be divided in the two sublattices shown in figure II and the single particle eigenstates will be constrained to be eigenfunctions only of the reduced group of lattice translations transforming each of those sublattices on itself. This represent only a limited reduction of translation symmetry breaking in the final solution, since still the HF orbitals will be forced to be Bloch functions in the sublattices. However, the freedom allowed is sufficient to permit the appearance of antiferromagnetic solutions. We also will limit the discussion here to these important cases, in order to maintain the simplicity of the discussion in [38–40]. The points of the two sublattices will be indexed as $r = 1, 2$, and are defined as follows

$$R^{(r)} = \sqrt{2} n_1 p \hat{q}_1 + \sqrt{2} n_2 p \hat{q}_2 + Q^{(r)}$$

(7)

with $n_1$ and $n_2 \in \mathbb{Z},$ and

$$Q^{(r)} = \begin{cases} 0, & \text{if } r=1, \\ p \hat{e}_{x_1}, & \text{if } r=2, \end{cases}$$

in which $\hat{q}_1$ and $\hat{q}_2$ are the basis vectors on each one of them.

The condition of being a Bloch function in the sublattices is represented by the following eigenvalue equations of the operators $\hat{T}_{R^{(0)}}$ belonging to the reduced discrete translation group which transforms a given sublattice on itself:

$$\hat{T}_{R^{(0)}} \phi_{k,l} = \exp(i \cdot k \cdot R^{(0)}) \phi_{k,l}.$$
FIG. 1: The figure illustrates the decomposition of the full lattice in two sublattices in order to allow a lattice translation symmetry breaking.

For the Bravais lattice of the infinite crystal the Brillouin zone (B.Z.) associated to $\hat{T}_{R(0)}$ becomes the shadowed region in figure 2 a). The whole square in this figure represents the B.Z. associated to the group of translations leaving invariant the whole square lattice. However, in order to practically solve the equations it should be imposed periodic boundary conditions on the $\phi_{k,l}$ in the lattice boundaries $x_1 = -Lp, Lp$ and $x_2 = -Lp, Lp$ (see figure 2 b)). This condition determines the allowed set of momenta $k$

$$k = \begin{cases} \frac{2\pi}{Lp} \left( n_1 \hat{e}_{x_1} + n_2 \hat{e}_{x_2} \right), \\
\quad \text{with } n_1, n_2 \in \mathbb{Z} \\
\quad \text{and } -\frac{L}{2} \leq n_1 \pm n_2 < \frac{L}{2}.
\end{cases}$$

Therefore, we are demanding less crystal symmetry on the single particle HF states to be obtained, since a lower number of constraints are being imposed on the space of those states in which the solutions are sought.

FIG. 2: Figure a) shows the continuous zone of momenta satisfying the periodic boundary conditions for the infinite lattice. Figure b) illustrates the discrete set of momenta which obey the imposed periodic boundary conditions in a finite square set of lattice points.

The Bloch basis which will be used for expanding the HF orbitals is written in the form

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

$$\hat{\sigma}_z u^{\sigma_z} = \sigma_z u^{\sigma_z},$$

$$\varphi_{R^{(r)}}(x) = \frac{1}{\sqrt{\pi a^2}} \exp\left(-\frac{(x - \mathbf{R^{(r)}})^2}{2 a^2}\right), \quad a \ll p,$$

where $N$ is the number of electrons in the system, $\hat{\sigma}_z$ is the spin $z$ projection operator, where $z$ is the orthogonal direction to the 2D lattice; $\sigma_z = -1, 1$, are the eigenvalue of the previously mentioned operator and $r = 1, 2$, is the label which indicates each of the sublattices. We are going to work on a half filling condition, then $N$ coincides with the number of cells in the square crystal with fixed periodic boundary conditions $N_c$. Note that due to the tiny overlapping among nearest neighbors approximation, the exact orthogonal character is only weakly lost between elements corresponding to different sublattices and having the same spin quantization. This fact is taken into account.
in the procedure for solving the HF equations. That happens because some nearest neighbors belong to different arrays. However, the orthogonality between different elements corresponding to the same sublattice, as well as unity norm for every elements, is rigorously maintained. This follows because they are constructed as Bloch states in their corresponding sublattices. Note that accordingly with the TB approximation, it will be considered that the effective potential created by the environment on each electron of the half filled band is a quadratic function having a minimum on the lattice points and strongly confining the electrons to it.

Now, let us consider the expansion of the HF orbitals in terms of the just defined Bloch basis. The mean field single particle states incorporating the before mentioned explicitly nonseparable form of the spin projections are given as

$$\chi_{l}(\mathbf{x}, s) = \sum_{r, \sigma} B_{r, \sigma} \chi^{(r, \sigma)}(\mathbf{x}, s),$$  \hspace{1cm} (9)

where \(l\) is the additional quantum number needed for indexing the stationary state in question, which we are going to define precisely below. After substituting (9), (5) and (6) in (2); followed by projecting the obtained result on the lattice points and strongly confining the electrons to it.

$$\mathbf{B}_{l} = \left| B_{l} \right|, \hspace{1cm} (10)$$

where each of the quantities

$$\mathbf{B}_{l} = \left| B_{l} \right|,$$

represents a vector having four components defined by the four possible pairs \((r, \sigma)\). The two appearing constants

$$\bar{\chi} \equiv \frac{mn^2}{4\pi \hbar^2 \epsilon_0 p},$$

$$\bar{\varepsilon}_{l}(\mathbf{k}) \equiv \frac{ma^2}{\hbar^2} \bar{\varepsilon}_{l}(\mathbf{k}),$$  \hspace{1cm} (11)

are dimensionless. In them, \(e\) represents the charge of the particles; \(\hbar\) is the reduced Planck constant; \(a\) is the characteristic radius of the Wannier orbitals \(\varphi_0\) while \(p\) is the nearest neighbors separation in the square lattice. It is clear now that we can define \(l = 1, 2, 3, 4\), as a label indicating each of the four solutions to be obtained for every value of quasi-momentum \(\mathbf{k}\). Also, all the implicit parameters in the 4×4 matrices defining the HF problem

$$\mathbf{B}^{0}_{\mathbf{k}} = \left| \mathbf{B}^{0}_{\mathbf{k}} \right|,$$

$$\mathbf{G}^{dir}_{\mathbf{k}} = \left| \mathbf{G}^{dir}_{\mathbf{k}} \right|,$$

$$\mathbf{F}^{ind}_{\mathbf{k}} = \left| \mathbf{F}^{ind}_{\mathbf{k}} \right|,$$

$$\mathbf{I}^{0}_{\mathbf{k}} = \left| \mathbf{I}^{0}_{\mathbf{k}} \right|,$$

$$\mathbf{B}^{1}_{\mathbf{k}} = \left| \mathbf{B}^{1}_{\mathbf{k}} \right|,$$

$$\mathbf{G}^{dir}_{\mathbf{k}} = \left| \mathbf{G}^{dir}_{\mathbf{k}} \right|,$$

$$\mathbf{F}^{ind}_{\mathbf{k}} = \left| \mathbf{F}^{ind}_{\mathbf{k}} \right|,$$

$$\mathbf{I}^{0}_{\mathbf{k}} = \left| \mathbf{I}^{0}_{\mathbf{k}} \right|,$$

$$\mathbf{B}^{1}_{\mathbf{k}} = \left| \mathbf{B}^{1}_{\mathbf{k}} \right|,$$

$$\mathbf{G}^{dir}_{\mathbf{k}} = \left| \mathbf{G}^{dir}_{\mathbf{k}} \right|,$$

$$\mathbf{F}^{ind}_{\mathbf{k}} = \left| \mathbf{F}^{ind}_{\mathbf{k}} \right|,$$

$$\mathbf{I}^{0}_{\mathbf{k}} = \left| \mathbf{I}^{0}_{\mathbf{k}} \right|,$$

$$\mathbf{B}^{1}_{\mathbf{k}} = \left| \mathbf{B}^{1}_{\mathbf{k}} \right|,$$

$$\mathbf{G}^{dir}_{\mathbf{k}} = \left| \mathbf{G}^{dir}_{\mathbf{k}} \right|,$$

$$\mathbf{F}^{ind}_{\mathbf{k}} = \left| \mathbf{F}^{ind}_{\mathbf{k}} \right|,$$

$$\mathbf{I}^{0}_{\mathbf{k}} = \left| \mathbf{I}^{0}_{\mathbf{k}} \right|,$$

are dimensionless. The set of quantities (12) constitute the matrix representations of the periodic potential created by the mean field \(W_{\gamma}\), the direct and exchange terms in (2), the interaction potential with the neutralizing "jellium" of charges \(F_{\gamma}\) defined in (5) and the overlapping matrix among the wavefunctions of the basis, respectively. Each one of the four pairs, \((t, \alpha)\) and \((r, \sigma)\) defines a row and a column respectively, of the matrix in question for each momenta value. The explicit forms of the matrix elements are given in Ref. [30] after assuming no restriction in the parameters. The normalization condition for the HF single particle states and the HF energy of the system take the forms

$$1 = B^{l}_{\mathbf{k}} \cdot I_{\mathbf{k}} B^{l}_{\mathbf{k}}, \hspace{1cm} (13)$$

$$E^{\text{HF}} = \sum_{\mathbf{k}, l} \Theta(\bar{\varepsilon}_{l}(\mathbf{k})) \bar{\varepsilon}_{l}(\mathbf{k}) \frac{1}{2} B^{l}_{\mathbf{k}} \cdot (G^{dir}_{\mathbf{k}} - G^{ind}_{\mathbf{k}}) B^{l}_{\mathbf{k}}, \hspace{1cm} (14)$$

where \(\Theta\) is the Heaviside function. The system (10) is non linear in the variables \(B^{l}_{\mathbf{k}}\), which are the four components of each vector \(B^{l}_{\mathbf{k}}\). Thinking in terms of numerically solving the equations by the method of iterations, it is convenient to pre-multiply them by \(I_{\mathbf{k}}\) for each \(\mathbf{k}\). Note that for each \(\mathbf{k}\) four eigenvalues \((l = 1, 2, 3, 4)\) will be obtained, or
equivalently, four bands on the B.Z. From Eq. (10), it can be observed that in the representation (8), the HF potentials and in general the total hamiltonian of the system, resulted as being block diagonal with respect to the sets of states indexed by the same \( k \). This fact is a direct consequence of the translation symmetries leaving invariant the sublattices.

In next section we will consider a half filling condition, that is, the HF solution will have one electron per cell. In addition a periodic lattice of \( N = 20 \times 20 \) electrons will be also assumed. The occupied states inside the B.Z. are indicated in figure 2(a) by the points inside the shadowed region.

IV. SCES PROPERTIES AND OVERLAPPING CONTROLLED GAP IN THE 2D TB MODELS OF INTERACTING PARTICLES

In this section we present the results for the energy bands of the considered TB model as determined by the solution of the system of equations Eq. (10) for the same system investigated in [38–40] but assuming that the overlapping in the TB model is changing. The change is implemented by modifying the parameter \( \tilde{a} \). As in [39], the solutions were found by using the method of successive iterations. The parameter defining the width of the jellium charge \( \tilde{b} = 0.05 \) is fixed. On the other hand, the parameter \( \tilde{a} = a_p \) is modified in order to correspondingly vary the overlapping. The expression for \( \tilde{\gamma} \) (the quantity which defines the width of the free TB band associated with the model as \( 4\tilde{\gamma} \)) is defined by the model in terms of \( \tilde{a} \) as (See [38–40])

\[
\tilde{\gamma} = \exp\left( -\frac{1}{4\tilde{a}} \right) - 0.05,
\]

FIG. 3: The set of plots shows the band structure of the HF self-energy modes for six values of the parameter \( \tilde{a} \) in the range 0.25 – 0.30 in steps of 0.01. The value of \( \tilde{a} \) defines the width (in units of \( p \)) of the Gaussian orbitals in the neighborhood of each lattice points. Note that increasing overlapping by taking \( \tilde{a} \) larger, with the lattice fixed, reduces the energy gap.

The lattice unit cell was also fixed to the distance between the nearest neighbor Cu atoms: \( p = 3.8 \ A^0 \). The iteration process for solving the equations started from a state selected to show antiferromagnetic order. This allowed to achieve the convergence toward the solution presented in this subsection, because there could exist a kind of barrier for the convergence from an initial paramagnetic state. Figure 3 shows a set of band structures corresponding to varying values of the width of the gaussian Wannier orbital. They correspond to lattices of 20x20 cells. The bands are depicted on the scale of energies \( \frac{m^2}{2\hbar^2} \). The plots show how the insulator energy gap decreases as the overlapping increases when the orbital size \( \tilde{a} \) becomes larger. The results for the bands are almost in the thermodynamical limit for the 20 × 20 lattice size employed, since the bands are practically unchanged when a lattice of 30 × 30 unit cells is considered. The presented calculation exemplifies how a highly unconstrained HF solution of a 2D model of TB interacting electrons is able to predict SCES properties as Mott types of insulator gaps.
V. RTS IN WATER DOPED GRAPHITE AND 2D QDots LATTICES?

In this section a possibility will be discussed for attaining room temperature superconductivity (RTS) when graphite is doped with water on its surface. At the end of the section, and suggested by the analysis of water doped graphite system, some remarks indicating the possibility of RTS in 2D lattices of Quantum Dots will be also advanced. The possibility of RTS in graphite doped with water had been suggested by recent experiments reporting the detection of granular room temperature superconductivity in graphite powder, which was previously subject to temperature treatment when suspended in water [43]. The measured hysteresis loops in samples made with the powder, signaled the presence of superconductivity and allowed to estimate a critical temperature higher than room one. On the other hand, recent ab-initio calculations of clusters of water molecules over graphene in [45, 46], had indicated that water molecules tend to form an hexagonal monoatomic layer on top of the graphene, which can act as an imposed periodic external potential on it. The authors remark that the deposition of a single layer on the graphene leads to 2D planar hexagonal crystal of water molecules, staying slightly above the graphite’s last graphene plane.

![Image of water molecule over graphene](image.jpg)

**FIG. 4:** The figure illustrates the possible action of the hexagonal array of water molecules which ab-initio calculations predict to be formed when water is sufficiently doped with water molecules [45, 46]. Only one molecule of water is illustrated for simplicity. The hexagon of Carbon atoms shown at the left, and not having the influence of the molecule of water, is for comparatively illustrate the effect of the molecules on the electrons clouds. The distances between the atoms are roughly proportion with the ones defined by the simulations, and a last graphene layer in graphite was considered, as indicated by its bounds with the next layer below. Note that the electronegativity of Oxygen should tend to repel the electron density along the C-C bonds. This effect can be also reinforced by the image of the water dipole moment in graphite, which is a semi-metal. Thus, the possibility exists that the action of the periodic potential created by a water monolayer on graphite could generate a TB band of the kind which the cuprates show. [38–40].

The centers of the Oxygen atoms rest directly over the centers of the hexagons formed by the carbon atoms. They explain that the periodic potential created by the water molecules on graphene does not affect it up to a point in which it becomes metallic. However, it was also argued that, if a substrate of SiO₂ is added below the graphene monolayer, then the system becomes metallic. This is a property that we interpret as opening an opportunity for obtaining RT superconductivity. The idea is described in what follows. Firstly, graphite with a monolayer of water molecules over the last graphene plane in it, can be considered as a graphene layer with a substrate of the same graphite. But, as the simulations indicated, a substrate can help the last layer to become metallic. The validity of this property is directly supported by the fact that the same graphite is a semi-metal. Therefore, assuming that the same predictions of SCES can be obtained from a TB model of 2D electrons with a lattice showing hexagonal structure, the last hexagonal graphene layer on the surface of graphite (which is separated by a large distance from the other layers) could eventually act as a TB metal, upon which the deposited 2D crystal of water molecules exerts a strong dipolar periodic electric potential. To illustrate this possibility consider figure 4 in which one of the water molecules doping the surface of graphite is pictured according to the ab-initio structure of a single layer of water interacting with the surface of graphene.

Further, figure 5 shows the band structures of $La_2CuO_4$ ([29]), $YBa_2Cu_3O_7$ ([50]) and graphite ([51]). Note from
FIG. 5: The plot shows the band structures of three materials: a) $La_2CuO_4$ (50), b) $YBa_2Cu_3O_7$ (50) and c) Graphite (51). Note that the bands crossing the Fermi level in $La_2CuO_4$ have nearly 4 eV in energy width. On the other hand the same kind of bands ranges only approximately 2 eV in energy in YBCO. Graphite bands being closer from above and below to the Fermi level are very close in energy.

The plots that the bands crossing the Fermi level in $La_2CuO_4$ have nearly 4 eV in energy width. On the other hand, the same type of bands range only approximately 2 eV in energy in the YBCO material. Then, let us consider that as the model of $La_2CuO_4$ the width of the resulting TB like band given by the HF solution, becomes roughly proportional to the resulting insulator gap, after the constraints on the HF scheme had been deleted. This assumption in turns indicates that in the case of $YBCuO$, since the width of the TB like bands are nearly half the ones of the $La_2CuO_4$, the insulator gap resulting of applying the model to this material (let us call it $U$ in what follows) might be also nearly a half of the one obtained for $La_2CuO_4$. But, note that the model considered here can be seen as kind of improvement of the single-band Hubbard (or t-j) one. But, these models indicate a critical temperature $T_c$ for superconductivity obeying $T_c \sim \frac{U}{t}$. Therefore, assuming that the hopping parameter $t$ is similar for both cuprate materials, it follows that the prediction is in agreement with the t-j model result, about that the $T_c$ of $YBCuO$ should nearly double the one of the $La_2CuO_4$. Therefore, after examining the band structure of graphite, the following observation seems to support the possibility of realizing higher critical temperatures in the graphite water systems. Note from figure 5 that the pure graphite bands which are closer from above and below to the Fermi level, are very near in energy one to another. This property suggests that the action of the hexagonal dipolar potential created by the water molecules, might be able to generate a TB binding band, showing an energy width few times smaller than the one in YBCuO materials. Henceforth, under the generation of the insulator HF solution discussed here, this band might be able to determine a value of $U$ also few times smaller than the corresponding value in YBCuO. In addition, the hopping parameter $t$ could be also possible to become higher in the "graphite-water" system. Thus, the analyzed situation suggests the possibility for the appearance of RTS in graphite doped with water as reported in [43]. Finally, it can be noted that the above discussion correctly identify that a small insulator gap of the considered TB model could contribute to enhance $T_c$. This property opens the possibility of developing 2D nanotechnology systems being described by a periodic TB models of interacting electrons, which could enhance the nowadays attained critical temperatures. In particular, a directly coming to the mind possibility is the growing of a 2D periodic array of Quantum Dots being driven by an external potential. Then, by varying the potential, the electron density can be to controlled, and a hole doped 2D system being similar to the CuO planes in $La_2CuO_4$ could be developed. Therefore, assumed that not a strong experimental limitations arises for increasing the values of the parameter $\frac{U}{t}$ in the considered 2D
system, the possibility is suggested of rising the critical temperatures with respect to the ones attained in the cuprates. The study of the nowadays experimentally realizable values for $t^2/U$ will be considered elsewhere.

Conclusions

We consider former results for a Tight-Binding model of CuO planes in $La_2CuO_4$ with the objective of underlining their wider implications. It is illustrated how interacting electrons systems described by the TB model can show strongly correlated electron properties appearing in the mean field approximation. For this outcome it becomes relevant to complement the HF scheme by incorporating crystal symmetry breaking effects and non-collinear spin orientations of the final HF orbitals. The results also furnish a general theoretical insight for solving the old standing Mott-Slater debate, at least for the $La_2CuO_4$ and TMO band structures. The idea suggested is to apply a properly non-collinear GW scheme to the electronic structure calculation of those materials. This view is strongly supported by the fact that the GW method can be conceived as a generalized HF procedure, in which the screening polarization is also determined. Thus, the possibility arises for predicting the just phenomenologically fixed value for the dielectric constant in $La_2CuO_4$, which is central in deriving the SCES properties of $La_2CuO_4$ from the TB model in that references. Henceforth, the whole discussion points to identify the main correlation properties in these materials as mainly determined by screening. Preliminary arguments are also presented indicating the possibility of attaining room temperature superconductivity by means of a doping with water molecules surfaces of graphite, being orthogonal to its c-axis. The discussion opens an opportunity to understand the recent reports of granular superconductivity at room temperatures in graphite powder [43]. It should be mentioned that whole discussion seem to be of help in the description of the observations of metal-insulator transitions and Mott properties in systems of atoms trapped in planar photon lattices [47-49]. Finally, the analysis also furnishes insights about how to approach the old, but yet conflicting results about the appearance of a magnetic order in the jellium model and the metallic systems at variable electron densities [36, 37].

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