

## Electronic and Magnetic Properties of $\text{CuO}_2$ Plane<sup>†</sup>

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A mean field calculation of the two dimensional three band Hubbard models based on a Mori-projection operator formalism, which is called the projection operator mean field (POMF) approximation, is presented. The results are compared with those of the Quantum Monte Carlo (QMC) simulations. We find that the POMF results agree very well with those of the QMC. Then we use the parameters determined by the constrained density functional method to study the  $\text{CuO}_2$  plane by POMF. We find an antiferromagnetic insulating ground state with band gap and magnetic moment given by 1.97 eV and 0.65  $\mu_B$ , and a satellite peak around 13 eV below Fermi level. All these results agree with experiment. The effect of doping on the solutions is discussed.

Since the discovery of high  $T_c$  superconductivity in the copper oxides materials, theoretical study of strongly correlated electron systems has been once again a focal point in condensed matter physics. Many calculations in the past decade have demonstrated that the local spin density functional approximation (LSDA) gives a good description of ground state properties of many moderately correlated systems.<sup>1</sup> LSDA has become the de facto tool of first principles calculations in solid state physics, and has contributed significantly to the understanding of material properties at the microscopic level. For strongly correlated systems, the LSDA often fails. The failure of the LSDA is caused mainly by strong correlation effects. The valence electrons in the solid have a strong tendency to hop from atom to atom because this process will lower the kinetic energy due to the decreased spatial localization of the wave function. These kind of itinerant states are well described by the band picture. However, the Coulomb repulsion

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between electrons will oppose the hopping of the electrons between atoms. When the cost in potential energy arising from hopping outweighs the saving in kinetic energy, the electron becomes localized. Once the states are localized by strong intrasite Coulomb correlations, the magnetic interactions and tendency to integral occupation of such states strongly favors the antiferromagnetic ground state. Therefore antiferromagnetic materials are frequently strongly correlated systems. P. W. Anderson introduced a model<sup>2</sup> in order to understand why the majority of insulating magnetic materials were antiferromagnetic. Independently, John Hubbard studied the magnetism and metal-insulator transitions by introducing a separate model,<sup>3</sup> a generalized version of the Anderson model, which gives the approximate solutions to the many-body problem of a metal with strong intrasite Coulomb interactions. Since most of the parent structure of high  $T_c$  materials, such as  $\text{CaCuO}_2$ ,  $\text{La}_2\text{CuO}_4$ , and  $\text{YBa}_2\text{Cu}_3\text{O}_6$ , are antiferromagnetic insulators, the wavefunctions responsible for the magnetism are very likely to be localized. There are certain features in common for these High  $T_c$  materials, particularly the existence of the square  $\text{CuO}_2$  layers, which contribute to most of the unusual features of the normal, the magnetic, and the superconducting state. We believe that a detailed knowledge of the normal state electronic structure and excitationis will give important insight into the understanding of the nature of the superconductivity in these materials. Since the treatment of strong intra-atomic correlations in solids is difficult, it is appropriate at this stage to study model systems which hopefully reveal the correct qualitative physics. Quantum Monte Carlo methods have recently been used to study finite two dimensional Hubbard models, and have been extended to three band models to better study the  $\text{CuO}_2$  interactions.<sup>4,5</sup> The Quantum Monte Carlo methods are presently restricted to finite lattices, finite temperatures, and very large computers. We have developed a mean field calculation of the multi-band Hubbard model based on a projection operator scheme<sup>6</sup> which is able to treat the correlations for such models in a much faster but approximate fashion. The method also has the desirable feature that it can be generalized all the way to many atoms per unit cell with s, p, d orbitals included. We will apply the method to study the ground state in three band Hubbard models, and compare the results to those of the Quantum Monte Carlo method. Also, we will use parameters determined from LSDA, and from interpreting experimental data for the  $\text{CuO}_2$  plane, and compare the results to experimental measurement. Finally, we will study the effect on the solution of hole concentration.

Figure 1 shows the projection operator mean field (POMF) and QMC results for the hole occupation on the Cu site,  $\langle n_{\text{Cu}} \rangle$ , and the O site,  $\langle n_{\text{O}} \rangle$ , for  $\beta = 8$ ,  $U_p = 0$ ,  $t_{dp} = 1$ ,  $t_{pp} = 0$ ,  $U_d = 6$ , and  $A = 2$ . Both the AF solution and the paramagnetic (PM) solution calculated by POMF are included in Fig. 1. We can see that the AF solution agrees better with the QMC results for  $n = 0.8, 0.9, 1.0$ , and  $1.1$ , where the total energy calculated using POMF for the AF solution is lower than that of the PM solution. For  $n = 1.2$  we find the total energy of the PM solution is lower than that of the AF solution and the PM solution agrees better with the QMC results. We can also see that when holes are added to the system away from half-filling,  $n = 1$ ,

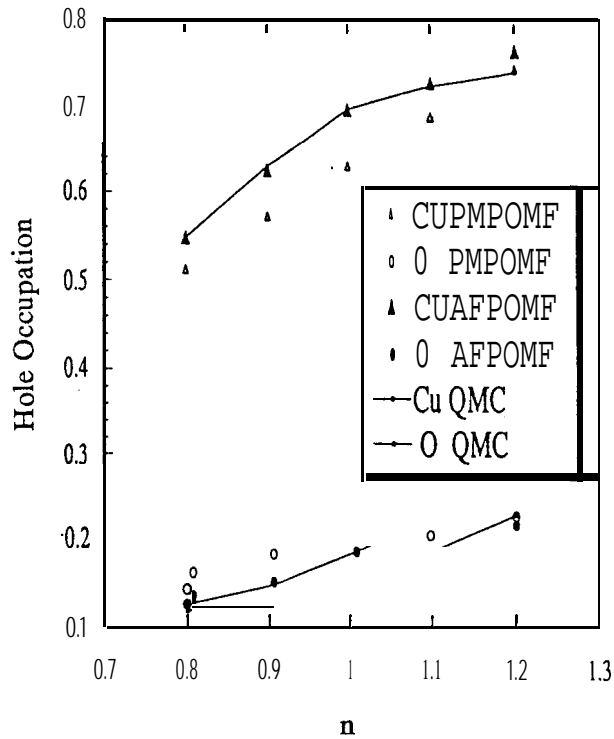


FIG. 1. The hole occupation numbers on the Cu site  $\langle n_{Cu} \rangle$  and the O site  $\langle n_O \rangle$  versus band filling  $n$  for  $U_d = 6$ ,  $A = 2$ ,  $t_{dp} = 1$ ,  $t_p = U_p = 0$ ,  $\beta = 8$  calculated using the POMF approximation and the QMC simulation (Ref. 4).

they go mainly to the oxygen site. On the other hand, if the electrons are added to the system, decreasing  $n$ , holes are mainly removed from the Cu sites. That is in agreement with experimental observation.<sup>7</sup> The squared magnetic moment  $\langle S_z^2 \rangle$  and the hole occupation on Cu sites  $\langle n_{Cu} \rangle$ , respectively, as a function of charge transfer energy  $A$  for  $U_d = 6$ ,  $t_{dp} = 1$ ,  $U_p = U_{dp} = t_{dp} = 0$ , and  $\beta = 10$  at half-filling calculated by POMF and QMC are shown in Figs. 2a and 2b. Again they agree quite well with each other. When the charge transfer energy increase, more holes go to the Cu sites and  $\langle S_z^2 \rangle$  increases as expected.

The agreement with the QMC results gives clear evidence for the utility of the present POMF method to study the three band Hubbard model. Thus we go to study the solution of the three band Hubbard model with parameters more suitable for the  $CuO_2$  plane using the POMF approximation. Recently, the parameters of the three band Hubbard model determined, both theoretically, from LSDA calculations,<sup>8,9,10</sup> and experimentally, by analyzing the photoemission experiments.<sup>11</sup> The values of the parameters determined by different groups are quite similar. The ranges for the values of the parameters are given by  $A$ , (1.5 eV - 4.0 eV);  $U_d$ , (8.8 eV - 10.5 eV);  $U_p$ , (4.0 eV - 6.0 eV);  $U_{dp}$ , (0.0 eV - 1.5 eV);  $t_{dp}$ , (1.07 eV - 1.6 eV) and  $t_{pp}$ ,

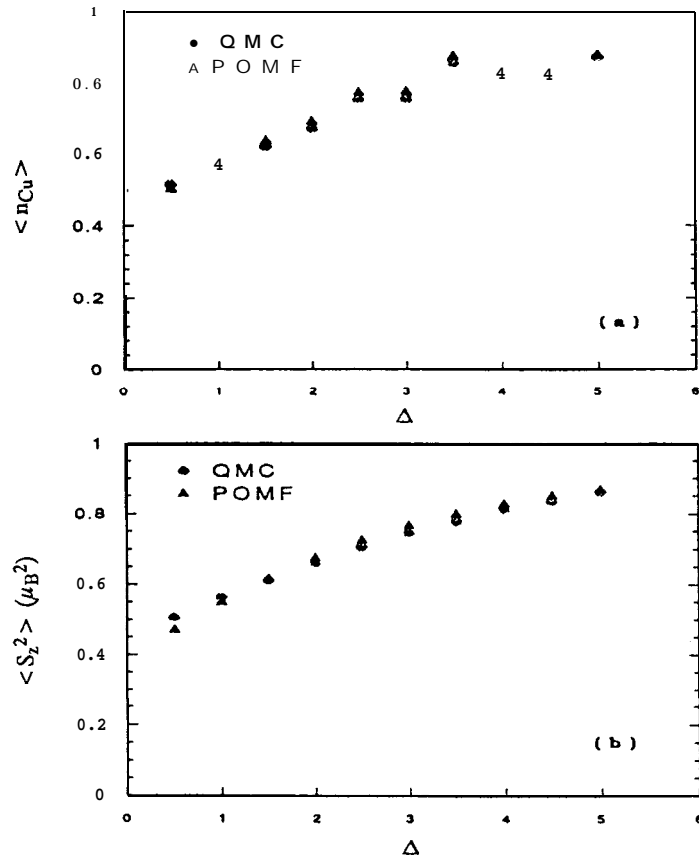


FIG. 2. (a) The squared magnetic moment  $\langle S_z^2 \rangle$  and (b) the hole occupation on Cu site  $\langle n_{\text{Cu}} \rangle$  versus charge transfer energy  $\Delta$  for  $U_d = 6$ ,  $t_{dp} = 1$ ,  $t_p = U_p = U_{dp} = 0$ , and  $\beta = 10$  at half-filling calculated using the POMF approximation and the QMC simulation (Ref. 4).

(0.33 eV - 0.65 eV). McMahan, Annett, and Martin<sup>10</sup> included two more orbitals, Cu  $d_{3z^2-r^2}$  and out of plane  $p_z$  in their calculation. In the calculations presented below, we will use the parameters determined by Hybertsen, Schluter, and Christensen (HSC)<sup>8</sup> as shown in Table I. HSC perform standard LMTO calculations with the use of the constrained local density functional approach to calculate the energy surface as a function of local orbital occupation in  $\text{La}_2\text{CuO}_4$ . Then they extract the parameters by matching the energy surface to the one obtained by a HF solution of the three band Hubbard model. Note that all the parameters listed in Table I are evaluated in the hole picture.

Since the intersite correlation is weak, we can include the  $U_{dp}$  terms in our calculation by the HF approximation, which replaces  $U_{dp} n_{d,\sigma} n_{p_j,\sigma'}$  by  $0.5 U_{dp} (n_{d,\sigma} \langle n_{p_j,\sigma'} \rangle + \langle n_{d,\sigma} \rangle n_{p_j,\sigma'})$ . Therefore the effect of the  $U_{dp}$  is just a constant shift of the on-site energies given by

TABLE I. Parameter values for the  $\text{CuO}_2$  plane used in the present calculation. All values are in eV

| $U_d$ | $U_p$ | $U_{dp}$ | D   | $t_{dp}$ | $t_p$ |
|-------|-------|----------|-----|----------|-------|
| 10.5  | 4.0   | 1.2      | 3.6 | 1.3      | 0.65  |

$$\varepsilon_d \rightarrow \varepsilon_d + 2U_{dp} \langle n_O \rangle$$

$$\varepsilon_p \rightarrow \varepsilon_p + U_{dp} \langle n_{Cu} \rangle$$

In order to study the antiferromagnetic ordering, we consider two  $\text{CuO}_2$  formula units per unit cell. Thus we now have six orbitals per unit cell. The half-filled upper band case, one hole per  $\text{CuO}_2$  unit, corresponds to 10 electrons (or 2 holes) per unit cell. The ground state of the system at half-filling,  $\mathbf{n} = 1$  per  $\text{CuO}_2$ , is found to be an antiferromagnetic insulator in our calculation. The band gap and the magnetic moment calculated by the POMF method is found to be 2.0 eV and  $0.65\mu_B$  assuming  $g = 2.0$ , and the corresponding results in experiment are given by 1.5 eV - 2.0 eV<sup>12</sup> and  $0.55\mu_B$ .<sup>13</sup> They agree quite well. The hole occupation on the Cu site and the root mean square magnetic moment  $\sqrt{\langle Sz^2 \rangle}$  are given by 0.708e and  $0.83\mu_B$ . Thus most of the hole is located on the Cu site, and the spin fluctuation is quite strong.

When the system is doped away from half-filling, for example  $\mathbf{n} = 1.1$ , the system is found to be a paramagnetic metal by experiment. Therefore we present both the PM and AF solution for the case with doping,  $\mathbf{n} = 1.1$ . The hole occupation on the Cu site and  $\sqrt{\langle Sz^2 \rangle}$  are found to be 0.698e and  $0.78\mu_B$  for the PM solution and 0.741e and  $0.834\mu_B$  for AF solution respectively. Thus, consistent with experiment when holes are doped to the system away from half-filling they go mainly to oxygen sites,<sup>7</sup> 110% for the PM solution and 67% for the AF solution in our calculation. Also when the antiferromagnetism is destroyed by hole doping the  $\sqrt{\langle Sz^2 \rangle}$  show little dependence on doping.<sup>13</sup> Both these observations are consistent with our POMF results.

The electronic energy band structure in the electron picture along the (11) direction calculated using the POMF approximation for the AF solution at  $\mathbf{n} = 1.0$ , the AF solution at  $\mathbf{n} = 1.1$ , and the PM solution at  $\mathbf{n} = 1.1$  are shown in Fig. 3, and the corresponding density of states are shown in Fig. 4. One general feature of our results is that we obtain twelve bands instead of six bands for the system with six orbitals per unit cell. This is a consequence of the POMF method which keeps track of single and double occupancy. The number of electrons for the filled  $n$ th band with spin index  $a$  is determined by

$$N_{t\sigma}^{(n)} = \frac{1}{N} \sum_{k\nu} \langle C_{k\nu\sigma}^+(n) C_{k\nu\sigma}(n) \rangle$$

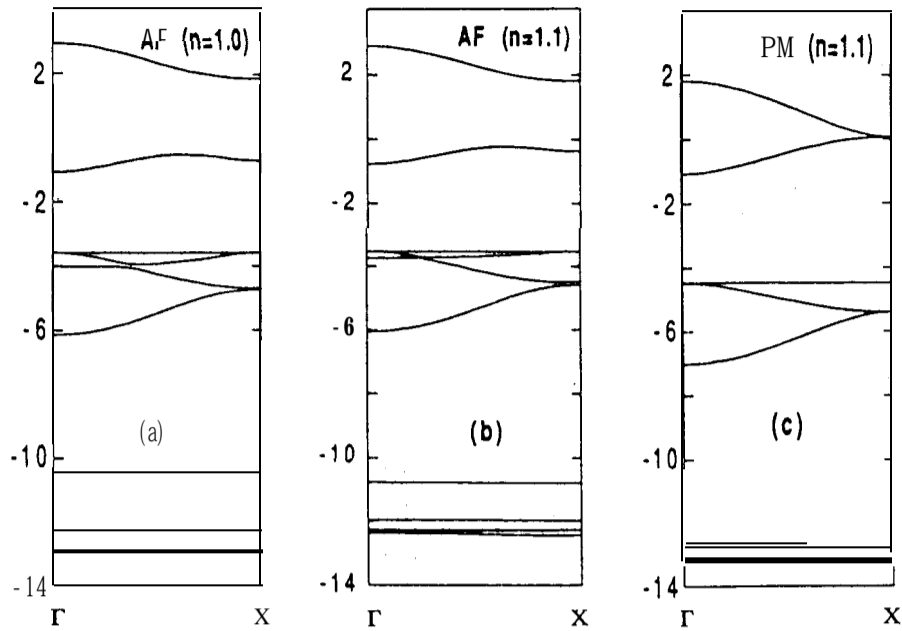


FIG. 3. The electronic structure along the (11) direction calculated using the POMF approximation for (a) antiferromagnetic solution at  $n = 1.0$ , (b) antiferromagnetic solution at  $n = 1.1$ , and (c) paramagnetic solution at  $n = 1.1$ . Parameters are the same as in Table I.

which is called the weight of that band. The weight for each band is usually less than one; however, the sum rule

$$\sum_{n=1}^{12} N_{t\sigma}^{(n)} = 6$$

is satisfied. There are many features of the density in Fig. 3 which agree with experimental measurement. There is a gap opening for the half-filling case. The structures around 5 eV below Fermi level with mainly O p character and around 13 eV with mainly Cu d character below Fermi level which are in reasonable agreement with experiment.<sup>14</sup> The structure around 13 eV below Fermi level, the satellite, is caused by the Coulomb repulsion  $U$  between two holes on the same Cu site, which has drawn much attention during the past decade.

We also calculated the magnetic moment as a function of doping. Antiferromagnetic, ferromagnetic (FM), and paramagnetic solutions were investigated. The magnetic moment on the Cu site for AF solution and the magnetic moment on the Cu site for FM solution calculated using POMF approximation are shown in Fig. 5a. Here the magnetic moment on the Cu site for the AF solution calculated using the HF approximation is also included in Fig. 5a for comparison.

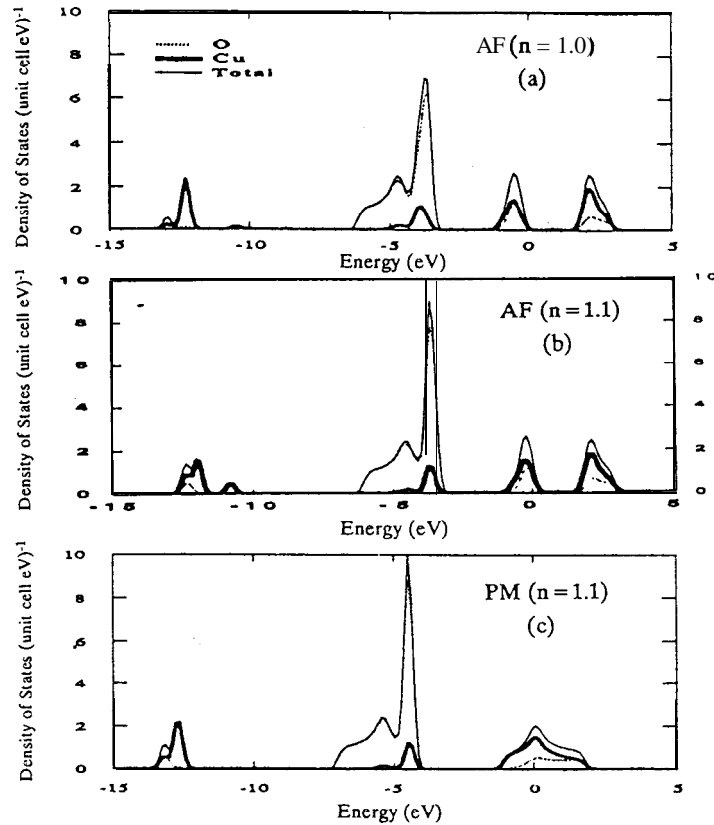
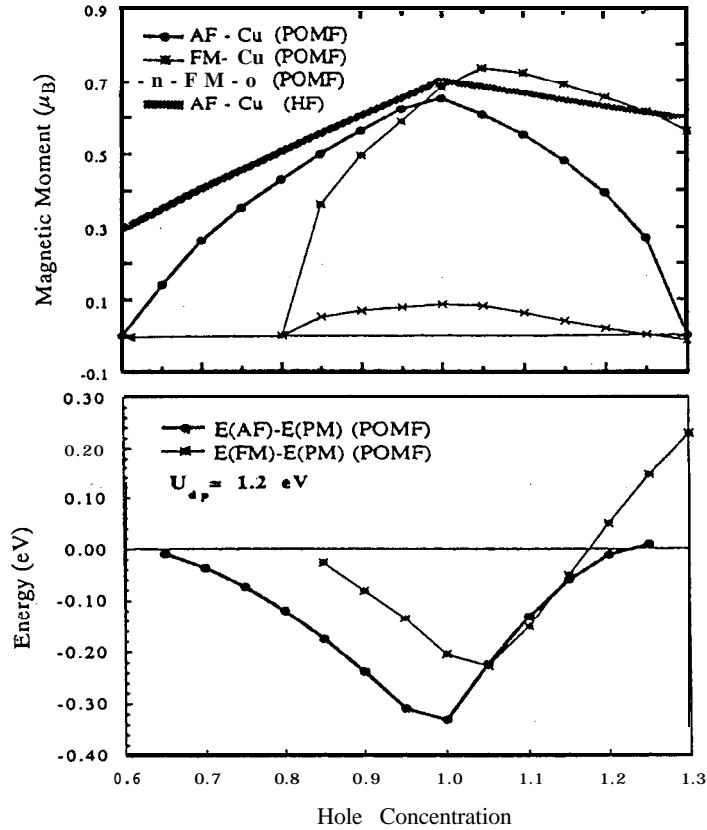


FIG. 4. The density of states calculated using the POMF approximation for (a) antiferromagnetic solution at  $n = 1.0$ , (b) antiferromagnetic solution at  $n = 1.1$ , and (c) paramagnetic solution at  $n = 1.1$ . Parameters are the same as in Table I.

Fig. 5b shows the energy difference between the AM solution and the PM solution,  $E(\text{AF}) - E(\text{PM})$ , and the energy difference between the FM solution and the PM solution,  $E(\text{FM}) - E(\text{PM})$ , calculated using the POMF approximation. We can see that there is a small region around  $n = 1.1$  where the FM solution is the ground state. However, this does not agree with experiment. The  $U_{dp}$  term strongly favors the FM solution. No FM ground state was found if we reduced the value of  $U_{dp}$  down to 0.8 eV. The magnetic moment and the energy differences as a function of hole concentration for  $U_{dp} = 0.8$  eV are shown in Figs. 6a and 6b. Therefore the value of  $U_{dp}$  determined by Hybertsen's group,  $U_d = 1.2$  eV, may be too large. By replacing the value of  $U_{dp}$  by 0.8 eV, we found the AF magnetic moment and band gap are given by 1.8 eV and  $0.635\mu_B$  for half-filling. The  $\sqrt{\langle Sz^2 \rangle}$  is given by  $0.823\mu_B$  which indicates that the spin fluctuation is quite strong. When the system is doped away from half-filling, we found that the holes introduced by doping go mainly to oxygen sites, 66% for AF solution and 106% for PM solution; and the  $\sqrt{\langle Sz^2 \rangle}$  are almost not changed,  $0.826\mu_B$  for AF solution and  $0.778\mu_B$  for PM



**FIG. 5.** (a) The magnetic moment on the Cu site for AF solution and the magnetic moment on the Cu site and the oxygen site for FM solution as a function of hole concentration calculated using the POMF approximation. The magnetic moment on the Cu site for AF solution calculated using the HF approximation is also included for comparison. (b) The magnetic energy,  $E(\text{AF})-E(\text{PM})$  and  $E(\text{FM})-E(\text{PM})$ , as a function of hole concentration calculated using the POMF approximation. Parameters are the same as in Table I.

solution. All these results are also in reasonable agreement with experiment.

The magnetic moment calculated using POMF approximation is depressed by doping and disappears for doping of about 0.25 holes or 0.4 electron per  $\text{CuO}_2$  unit. The disappearance of long range ordering is faster for hole doping than that for electron doping. The HF approximation gives a larger moment at half-filling, and the long range ordering is less rapidly destroyed than that in the POMF approximation. Experimentally, the magnetic order of  $\text{La}_{2-x}(\text{Sr/Ba})_x\text{CuO}_4$  disappears at the concentration of  $x = 0.03$ ,<sup>15</sup> which is about a factor of 10 faster than what we have in the POMF approximation. Although we obtain an AF ground state at  $n = 1.1$ , we believe the PM solution will give a better description of the real system for that hole concentration. Thus, we will focus on the AF solution for  $n = 1$  and the PM solution for  $n =$

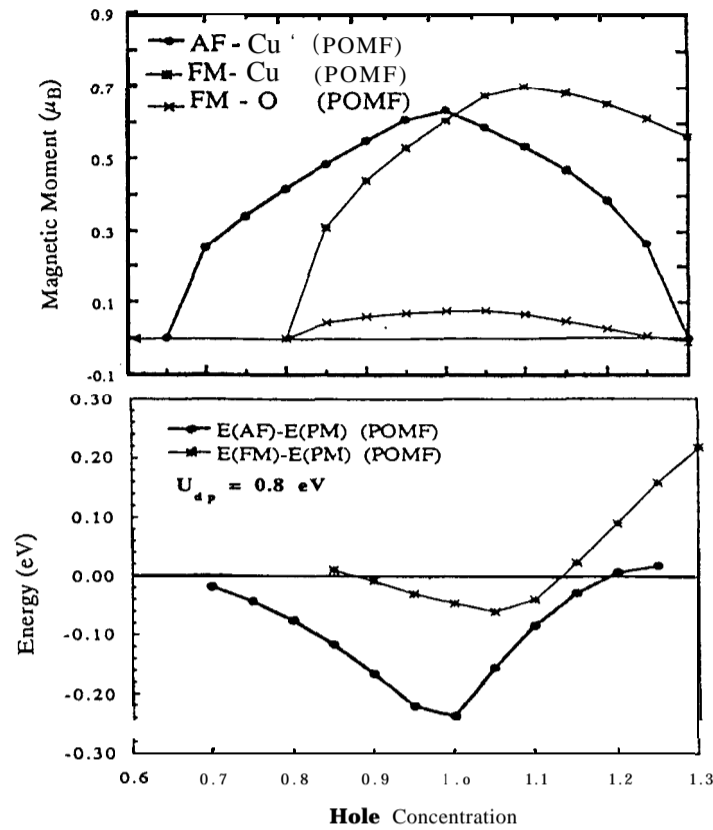


FIG. 6. (a) The magnetic moment on the Cu site for AF solution and the magnetic moment on the Cu site and the oxygen site for FM solution as a function of hole concentration calculated using the POMF approximation. The magnetic moment on the Cu site for **AF** solution calculated using the HF approximation is also included for comparison. (b) The magnetic energy,  $E(\text{AF})-E(\text{PM})$  and  $E(\text{FM})-E(\text{PM})$ , as a function of hole concentration calculated using the POMF approximation for  $U_{dp} = 0.8$  eV. The other parameters are as given in Table I.

1.1 in the rest of this paper.

Before we study the ferromagnetic response with an applied field, let us examine the PM solution for the half-filled case. We find there is a single band crossing the Fermi level, which is the anti-bonding band of Cu  $d_{x^2-y^2} - 0 p_{x,y}$ , and the amount of oxygen  $p_{x,y}$  admixed into Cu  $d_{x^2-y^2}$  conduction bands near the Fermi level is less than 25%. This is considerably less than the 60% obtained in the LSDA<sup>16</sup> but consistent with experimental observation.<sup>17</sup> To calculate the moment on each site induced by the applied field, we need to reduce the charge transfer energy  $A$  from 3.6 eV to 2.0 eV in order to prevent a spontaneous ferromagnetic solution. For  $A = 2.0$  eV, the induced moment on the Cu site and the oxygen site are given by  $0.0167\mu_B$  and  $0.0037\mu_B$  when we shift the spin up (down) bands by  $-0.005$  ( $+0.005$ ) eV corresponding to a mag-

netic field of  $8.64 \times 16$  G. If we reduce the value of  $A$  further,  $A = 1.5$  eV, we find the induced moment on the Cu site and the oxygen site are now given by  $0.0069\mu_B$  and  $0.00212\mu_B$  when the same amount of energy shift is applied. The contribution of the total induced moment per unit cell by oxygen sites is given by 38% for  $A = 1.5$  eV and 30% for  $A = 2.0$  eV. Therefore, we conclude that there is only small amount of oxygen 2p admixture into the Cu 3d conduction bands and the contribution of the oxygen sites to the induced ferromagnetic form factor is small, all these are consistent with the experimental observation.”

At last, we examine the effect on the satellite by the hole concentration which is shown in Fig. 7. Only paramagnetic solutions are considered. We can see that the binding energy of the satellite decreases and its intensity increases as the hole concentration increases. This is agree with experimental observation. Fig. 8 shows the extended valence band spectra for  $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$  and  $\text{YBa}_2\text{Cu}_3\text{O}_{6.25}$  crystal measured by Arko et al.<sup>14</sup> The binding energy of the satellite of  $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$ , which has more holes in the  $\text{CuO}_2$  plane, is lower than that of  $\text{YBa}_2\text{Cu}_3\text{O}_{6.25}$ . We note that much of the experimental spectra which is evident between 6 eV and  $E_F$  comes from the Cu and oxygen bands which were not considered in our model.

We have used a projection operator method to study the three band Hubbard model, and compared the results to those calculated using Quantum Monte Carlo simulation. The excellent

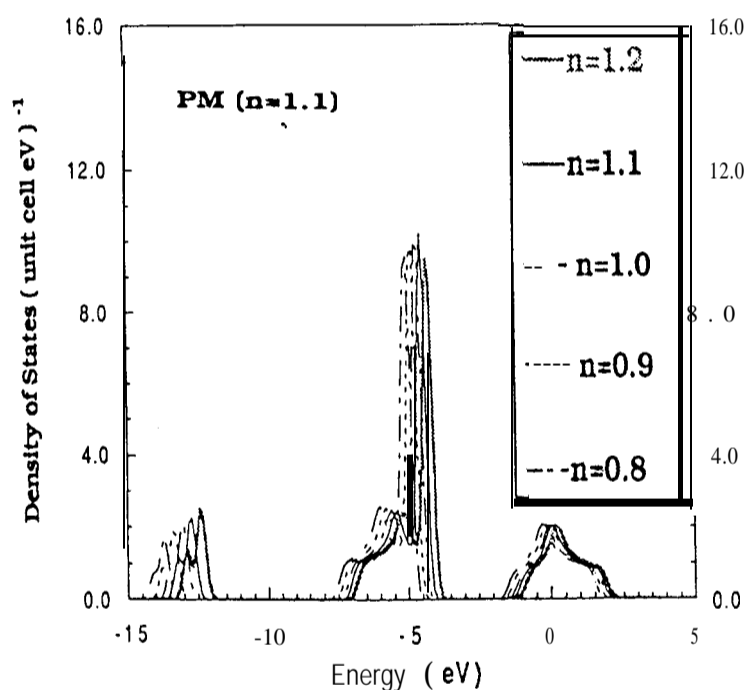


FIG. 7. The comparison of the total density of states of paramagnetic solution for  $n = 0.8, 0.9, 1.0, 1.1,$  and  $1.2$ . Parameters are the same as in Table I.

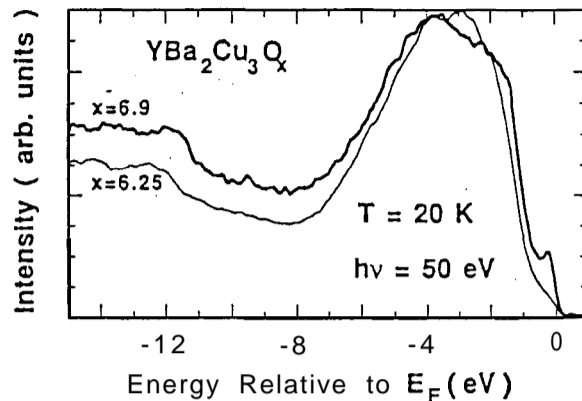


FIG. 8. The extended valence band spectra for  $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$  and  $\text{YBa}_2\text{Cu}_3\text{O}_{6.25}$  crystal measured by Arko et al. (Ref. 14).

agreement with QMC results encouraged us to further examine the parameters for the  $\text{CuO}_2$  plane. Therefore, we used the parameters determined by the constrained local density functional method to study the  $\text{CuO}_2$  plane with the POMF method. We obtained an antiferromagnetic insulator ground state with magnetic moment and band gap given by  $0.65\mu_B$  and  $2.0\text{ eV}$  which is in good agreement with experiment.<sup>12,13</sup> The value of  $\sqrt{\langle S_z^2 \rangle}$  is given by  $0.83\mu_B$ . Thus spin fluctuations are quite strong,  $\sqrt{\langle S_z^2 \rangle} - \langle S_z \rangle \approx 0.51\mu_B$ . We also showed the suppression of the antiferromagnetism by hole doping is faster than that by electron doping. The long range magnetic ordering disappears at  $x$  equal to 0.3 for hole doping and 0.4 for electron doping. This is too large compared with experiment measurements, which suggest  $x = 0.003$  for  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ .<sup>15</sup> By study of the paramagnetic solution of the  $\text{CuO}_2$  plane at  $n = 1.1$ , we obtain a reasonable description of the normal state properties of the High  $T_c$  superconducting materials. There are two key features in the total density of states, around  $5\text{ eV}$  and  $13\text{ eV}$  below the Fermi level, which is a consequence of strong electron correlations. The  $\sqrt{\langle S_z^2 \rangle}$  with small doping,  $n = 1.1$ , in the paramagnetic solution is given by  $0.78\mu_B$ , which indicates that the local moments are preserved when the long range magnetic ordering is destroyed by a small amount of doping. This is again in agreement with experimental observation.<sup>12</sup> When holes are doped to the system away from half-filling they go mainly to oxygen sites, 110% for the PM solution and 67% for the AF solution in our calculation. This also agrees with experimental observation.<sup>7</sup> We also show that the  $U_{dp}$  strongly favors the FM solution, and the value of  $U_{dp}$  should be small in order to prevent the FM ground state. The amount of oxygen 2p admixture into the Cu 3d conduction bands is reduced by strong correlation effect as caused by larger  $U$ . The contribution of the oxygen sites to the induced ferromagnetic form factor is smaller than 30% which is consistent with experiment.<sup>17</sup> Finally, we studied the effect on the satellite of hole concentration. We found the binding energy of the satellite decreases and its intensity increases as the hole con-

centration increases, which is again in agreement with experimental observation.<sup>14</sup>

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